Research and Innovation actions

Chemistry, Molecular & Materials Sciences and Technologies Virtual Research Environment (CMMST-VRE)

Call EINFRA-9-2015

Executive summary

Objective of the document: The present proposal aims at building added value onto the Chemistry, Molecular & Materials Sciences and Technologies (CMMST) communities by grafting them onto a Virtual Research Environment (VRE). The proposed VRE will empower with e-infrastructure technologies the tools and applications for research, education and innovation of the CMMST communities. These communities, in spite of being loosely coupled aggregates of independent academic research laboratories most likely not sharing a common distributed ICT platform or a common operating or experimental frame, can benefit from the highly collaborative environment of a VRE. The key objective of the proposal is to build, based on a dedicated e-infrastructure, a European CMMST VRE engineered according to a synergistic model paving the way to competitive collaboration and market oriented sustainable activities.

Partners of the project: The proposal is driven by the intention of INSTM to concert the efforts of COMPCHEM and other EGI (European Grid Infrastructure) VOs to the end of establishing a VRE in the CMMST area by leveraging on networked resources with the support of three important players of the field: EGI, MTA-SZTAKI and INFN. This endeavour is meant to address the needs of some EU initiatives and public institutions (e.g. COST CMST Actions, MoSGrid, Scalalife, ENEA, EM and ITN TCCM consortia) plus those of some large popular European associations (EUCHEMS and ECTN) and ESFRI projects (like ELIXIR). In addition, a cluster of SMEs utilizing their own resources, EGI.eu and some of its NGIs (as well as some large scale facilities consortia like PRACE and XSEDE) are the key technology partners of the project.

Goals of the VRE: the specific goals of the project are:
a) *orchestrate the activities of the e-infrastructure experts and of the members of the involved communities so as to enable an effective intra- and trans-community networked implementation and coordination of a collaborative/competitive (synergistic) research environment by:*
- allowing a selection of the compute resources based on quality parameters and a composition of higher level of complexity chained applications through the coordinated usage of distributed hardware and software,
- fostering the use of specialized web portals and workflows facilitating the production of data and know how in science and innovation, the direct re-use of the produced data and knowledge in education, training and further research
- rewarding the work done by its proactive members on behalf of the community.
b) *enable the production and the provision of computational services useful to molecular and materials disciplines when carrying out multi-scale treatments necessary to reproduce the observables of realistic systems in the area of energy, environment, materials, pharmacology, chemistry, biology, biotechnologies, medicine, etc. by means of:*
- state-of-the-art first principles electronic structure and nuclei dynamics computations,
- high level of accuracy multiscale design of complex molecular systems,
- knowledge management for training and education in sciences and technologies.
c) *turn (in collaboration with the partner SMEs) the versatility of the adopted e-infrastructure tools, the richness of the developed CMMST knowledge and the credit mechanism supporting the synergistic operating into a business model enabling an efficient transfer of the activities to the market ensuring business sustainability*

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Tasks: Both technical and non-technical tasks concerned with the building of the CMMST VRE will be performed.

The ICT tasks of the VRE will consist of collecting the requirements, validating the developed procedures, disseminating them, carrying out related integration, user support and knowledge transfer, adopting existing scientific gateways, workflows, data management and commons and associating them with the synergistic model and a credit based economy.
The CMMST tasks of the VRE will consist of porting state-of-the-art first principles electronic structure and nuclei dynamics codes, implementing accurate multiscale simulators of smart energy carriers in combustion, energy storage, space missions, bioinorganic chemistry, using both ab initio and empirically parametrized kinetic data, designing materials and modelling supramolecular phenomenologies, handling extended information systems for the investigation of the structure and processes of complex molecular systems relevant to pharmacology, medicinal and biological systems, and managing distributed knowledge processes.

Perspective developments: Establishing the VRE will allow the CMMST communities to significantly enhance their e-infrastructure based activities aimed at developing higher level of complexity applications and fully exploiting the features of a synergistic distributed environment. This will enable the mentioned communities to play a significant role in the innovation market, reduce the distance between public research & education and innovative startups and SMEs, get ready to operate on the market.

I. TERMINOLOGY

A complete project glossary is provided at the following page: http://www.egi.eu/about/glossary/.

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1. Excellence

In this section we describe the concept and objectives of the proposed Chemistry, Molecular & Materials Science and Technology (CMMST) Virtual Research Environment (VRE) designed to provide the members of the various CMMST communities with an efficient operational ground based on e-infrastructures and related innovative features and tools aimed at offering higher quality services in science, education and innovation.
The project is coordinated by INSTM (http://www.instm.it/) the largest Italian (Florence based) CMMST

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consortium of Universities and Research Institutes. The project leverages both on the support of EGI (http://www.egi.eu/), INFN (http://www.infn.it/index.php?lang=en), MTA-SZTAKI (https://www.sztaki.hu/) key players in e-infrastructure technologies and on the participation of the members of the CMMST Virtual Research Community (VRC) recently established by the COMPCHEM Virtual Organization (VO) and other EGI VOs (see https://wiki.egi.eu/wiki/Towards_a_CMMST_VRC). Resources and technologies of EGI (and of some of its NGIs (National Grid Infrastructures)) as well as those of PRACE, EUDAT, and Helix-Nebula will be considered for that purpose. The project aims at involving in the participation to such activities the members of popular CMMST large associations (like EUCHEMS and ECTN), initiatives (like MoSGrid(https://mosgrid.de/portal), Scalalife (http://www.scalalife.eu/), ENEA (http://www.enea.it/en), ESFRI ELIXIR (http://www.elixir-europe.org/), COST CMST (http://www.cost.eu/), the joint Master and Doctorate TCCM Erasmus+ (http://emtccm.qui.uam.es/) networks and clusters of SMEs (like DRAG).

Additional elements of excellence are:

among the EGI VOs COMPCHEM (https://www3.compchem.unipg.it/compchem/) is the largest international CMMST VO born out of the EGI projects for classical and quantum molecular dynamics computations;

among the other CMMST communities MoSGrid (https://mosgrid.de/portal) is the largest project devoted to ab initio based molecular and molecular mechanics simulations operating on PRACE and XSEDE while COST CMST (http://www.cost.eu/COST_Actions/cmst) is the largest European collaborative network in chemical science and technology research consisting of more than 200 research laboratories belonging to the most recently approved actions;

among the joint Master and Doctorate Erasmus+ networks the TCCM (Theoretical Chemistry and Computational Modelling) is the largest CMMST consortium of European Universities (see http://emtccm.qui.uam.es/) devoted to computing technologies;

among the large EU wide associations ECTN (http://ectn-assoc.cpe.fr/) is a leader in the field of Virtual education with more than 100 collaborating chemistry departments while EUCHEMS (http://www.euchems.eu/) is the general European academic, professional and industry chemistry organization counting over 150.000 members.

among the CMMST spinoffs and SMEs DRAG is the cluster coordinated by ECTN.

To the just pinpointed excellence of the CMMST activities, however, does not rely on a common distributed ICT platform (or a common experimental or operational frame) because related communities are unstructured aggregates of several independent academic research laboratories having common scientific goals. Yet, they are well suited to benefit from the highly collaborative environment of a VRE. Therefore, even if it is unthinkable to create at present a unitary CMMST scientific organization, the above mentioned partners and stakeholders will add strength to their excellence by grafting their communities into a **synergistic** VRE in which users and resource providers are encouraged to compete through collaboration. In particular, the project aims at:

- 1) **orchestrating** and **supporting** the activities of the involved communities in using the existing e-infrastructure resources and tools (including supercomputers and cloud technologies) in order to boost mutual interactions and enhance competitive collaboration;
- 2) **applying** and **adapting** e-infrastructure technologies to the CMMST disciplines in order to develop more advanced approaches, produce further innovation and enhance related knowledge management;
- 3) **structuring** and **evolving** the present quality based credit mechanisms into a systematic sustainable (even beyond the lifespan of the H2020 project) market oriented business model.

Key excellence feature of the proposed synergistic approach is its quality based credit mechanism supporting (as will be discussed in more detail later):

- the "selective use" of the heterogeneous computing elements of a Distributed Compute Infrastructure (DCI) as well as of related tools and applications based on Quality of Service (QoS) parameters allowing an intra- and trans-community "a la carte" composition of higher level of complexity usecases,
- the "collaborative competition" (based on both Quality of User (QoU) and QoS parameters) promoting a continuous enhancement of the services developed by the community members,
- the "credit award & redemption system" introducing an intra- and trans-community service based economy
- the SMEs (academic spinoffs and startups, etc.) driven "business model proof of concept" aimed at supporting a high level of sustainability and market compatibility.

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1.1 Objectives

Here a description of the specific objectives of the CMMST-VRE project which are expected to be achieved during its duration is given in more detail.

OBJECTIVE 01: ***The orchestration of the activities of the involved communities and support in managing and using the existing e-infrastructure resources and tools.***

The basic objective of the proposed CMMST VRE is the *orchestration of the activities of the e-infrastructure experts and of the members of the involved communities so as to enable accurate multi-scale multi-disciplinary applications interlacing different areas of molecular and materials science and technology expertise and treatments*.

To this end the CMMST-VRE will leverage on both the built in ICT expertise of EGI (and associated partners like CESNET, IBERGRID, etc.), INFN, SZTAKI, ENEA, University of Westminster, University of Perugia and the external support of other technology providers like EUDAT, CINECA in order to exploit the innovative features of the presently available e-infrastructures and related tools (which have already shown to be highly beneficial for research and innovation progress also in other scientific and technological domains). Moreover, the Molecular and materials know how and technologies of INSTM (as well as those of the members of the recently established CMMST VRC and other related large communities as well) provide also the ground necessary to carry-on the related collaborative multi-scale interdisciplinary applications (like the use of some embryo tools bearing QoS functionalities suited for identifying compute resources suitable for supporting higher level of complexity applications through the coordinated usage of High Performance (HPC) and High Throughput (HTC) Computing distributed hardware and software already experimented with CINECA on PRACE machines).

To properly orchestrate the CMMST activities and make them sustainable, however, the VRE needs to aim at much more than that. It will aim, in fact, at enabling *an effective intra- and trans-community networked implementation and coordination of a collaborative/competitive (synergistic) environment. This will allow the selection of the compute resources based on the already mentioned quality parameters, the composition of higher level of complexity chained applications through the coordinated usage of distributed hardware and software, the exploitation of specialized web portals and workflows facilitating the production of data and know how in science and innovation, the direct re-use of the produced data and knowledge in education, training and further research and the reward as well of the work done by its proactive members on behalf of the community.*

Accordingly, OBJECTIVE 01 has been articulated into the following sub-objectives:

a: ***Management and coordination***

In general management and coordination is not a sub-objective and their usual features are described later in section 3.2. Yet, being the management and coordination of the CMMST VRE a test ground for the orchestration of the activities and the e-infrastructure of the present VRE, the design of a dynamic governance structure (in our case the synergistic one) is indeed a sub-objective of the project. For this reason, the governance model and the resource usage are chosen to be enough simple and robust to be easily varied during the lifetime of the project according both to the quality parameters and to the feedbacks from the stakeholders (EUCHEMS, ECTN, ITN TCCM Joint doctorate).

b: ***Requirements collection, validation and dissemination***

This sub-objective aims at collecting the requirements and validating the capabilities of the high-level activities of the VRE in supporting the computing tasks of data processing, like user-driven workflows and data-driven pipelines. It will be concerned, therefore, with the assessment of the proposed evolution and actual implementation of gateways and simulation workflows for providing user communities with efficient access, selection and utilization of high throughput and high performance computing resources for the various scientific use cases related to the considered accurate multi-scale interdisciplinary applications of the involved scientific communities. This implies the definition and implementation of a set of validation procedures for high-level computing tasks and workflows established with the help of the SME members of the project. The validation will be also concerned with knowledge exchange, feedbacks and requirement sharing for environments in which community-specific high-level solutions are proposed either for

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dissemination, production or pre-production components. For this purpose online and offline events and contributions to various types of activities to be held within and outside the project will be organised.

c: ***Integration, user support and knowledge transfer***

This sub-objective aims at fostering the aggregation of the different CMMST communities inside the VRE ICT activities by enhancing the awareness of their members about the possibility of both making available distributed computing resources and adopting standard, reusable tools of existing e-infrastructures to the end creating a common VRE computing and storage environment. Moreover, this sub-objective aims at familiarizing the CMMST members with the distributed know how necessary to exploit e-infrastructures resources and tools by means of specific training events and tutorials. This implies the adding of further value to the activities of the members of the communities and the stimulating of active participation to the development of improvements and new activities. This comprises the offering of support and training in utilizing the proper tools and methodologies aimed both at facilitating the porting of the codes of inexperienced users and the singling out the factors that can determine his/her success (or setbacks). Specific care will be put in creating support and training activities in which ICT and selected field-experts closely work with the users in order to address their specific requirements, code building, multi-platform porting and storage.

d: ***Gateways and workflows for the synergistic model implementation***

This sub-objective aims at finding solutions for high-level computing tasks of data processing (e.g. like user-driven workflows and data-driven pipelines), for simulation workflows, and any other stand-alone computing activities and related components, tools and interfaces built on top of the existing technological solutions (frameworks and gateways), for devising the best solution for enabling the concerted use of both the existing users' data and applications of the involved communities on the ground of the adoption of the already mentioned QoS and QoU mechanisms. This implies the development of the gateway layer enabling users to get proper access to the needed resources of the underlying e-infrastructures, the implementing of a first prototype multiplatform workflow for the underlying usecases facilitating interoperability among different workflow systems and the user communities by incorporating the functionalities of GriF (an embryo tool ranking resources and users in terms of QoS and QoU (C. Manuali, A. Lagana', GRIF: A New Collaborative Framework for a Web Service Approach to Grid Empowered Calculations Future Generation of Computer Systems, 27(3), 315-318 (2011)) and enabling the ranking and selection of the computing resources to be used. This implies the identification of technologies and services suitable to support the project and to operate on different architectures and platforms. The synergistic model, therefore, aims also at pivoting the use of the e-Infrastructure using cloud technologies under the requirements of the user communities and the agreed community policies. This prompts the evolution towards PaaS and SaaS (Software as a service) solutions for each usecase and proper virtual images for the e-infrastructure SaaS services, the transformation of the developed prototype applications into a pre-production or production workflow interacting with the already mentioned validated tools and procedures.

e: ***Data management and commons for a credit based economy***

This sub-objective aims at developing the required high-level data-management functionalities as required by the need for validating existing tools and promoting the credit based economy of the synergistic model aimed at encouraging proactive users to carry out activities (either as work performed within the VRE commitments or even as new procurements) useful to the communities to the end of enhancing research and innovation. QoU and QoS quality parameters and their accurate determination through extended statistical analyses will be utilized for the evaluation of the Terms Of EXchange (TOEX) between the activities carried out and the credits to be awarded as well as between the credits to be redeemed and the services or the financial resources to be provided in return (C. Manuali, A. Lagana', A Grid Credit System Empowering Virtual Research Communities Sustainability, Lecture Notes Computer Science, 6784, 397-411 (2011)). The award and redemption of credits motivates proactive users to carry out activities (either as work performed within the VRE commitments or even as new procurements) useful to the communities to enhance research and innovation knowledge.

This implies the identification of the technologies and services to be developed for Data Management suited to support the project and operate with different platforms in a synergistic way, the singling out of easy-to-use Interfaces able to provide convenient access to logically consistent data operations. This will include also a framework that supports interaction, composition and visualization, the working out of (de facto) format standards in order to facilitate data search and data sharing among different scientific areas.

To summarize Objective 01 aims, therefore, at assembling the ingredients necessary to implement, support and further promote for sustainability a synergistic model of computing that reduces the extended

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fragmentation of the computational methods adopted by CMMST researchers by leveraging on consolidated and to be validated e-infrastructure technologies of well established partners. This objective aims at enhancing also full interoperability among codes, data, tools and laboratories by encouraging the sharing of packages and results derived from the community endeavours and outcomes thereby exalting the scientific impact of distributed computing.

OBJECTIVE 02: ***The application, adaptation and dissemination of the e-infrastructure technologies to the CMMST disciplines***

The CMMST VRE will enable the production and provision of computational services for molecular and materials disciplines necessary when carrying out the multi-scale treatments on which various disciplines rely in order to reproduce the observable properties of realistic systems for a large variety of applications in the field of energy, environment, materials, pharmacology, chemistry, biology, biotechnologies, medicine, etc. This type of services is usually provided at three different levels.

The first level of service is the one concerned with state-of-the-art from first principle electronic structure (sublevel a1) and nuclei dynamics (sublevel a2 that most often, though not always, makes use of sublevel a1) calculations. This level of service (the CMMST flagship service) provides ab initio information on molecular geometries and energies as well as on related spectroscopic and single (or half) collision scattering properties (such scheme is a generalization of the simulator GEMS (Grid Empowered Molecular Simulator) already described in the literature that serves both the electronic structure and the nuclei dynamics communities). Both sublevels 1a and 1b prompt the concerted usage of highly accurate electronic structure and nuclei dynamics calculations based on the synergistic use of different computing resources and technologies and the definition of (at least de facto) data format standards. They represent the most advanced research ground for both methodological ab initio developments (including the design and testing of new concurrent algorithms) and the rationalization of molecular structures and processes;

The second level (b) of trans-community services is the one concerned with Complex molecular systems. In this case the use of (either on- or off-line (eg the distributed remote theoretically and experimentally generated databases of structural and dynamical (or kinetics) properties) molecular systems for higher scale calculations of chemical properties. Service applications considered here are concerned with:

- b1 Accurate multiscale modelling of smart energy carriers in combustion, energy storage, space missions, bioinorganic chemistry, using ab initio and empirically parametrized kinetic data;
- b2 Computational design of materials and supramolecular phenomenologies (like clathrate hydrates capture of gases and the properties of ionic liquids), automatic parameterization of molecular dynamics force fields;
- b3 Handling of extended data bases for the investigation of the structure and processes of complex molecular systems relevant to pharmacology, medicinal and biological systems.

The above level (b) services can either exploit the use of level (a) services or replace them with their own (simplified) ones.

The third level (c) of trans-community services is the one concerned with the management of distributed Knowledge to the end of supporting rationalization, dissemination and education related to CMMST sciences and technologies. At this level we consider here self-learning (c1) and self-assessing (c2) services for both the specific CMMST VRE training and the more general educational endeavours for molecular science and technologies based disciplines able to trigger virtuous learning cycles (in particular those associated with the assemblage, use, and trial-and-error mutual improvement of Learning Objects (LO)s).

Accordingly OBJECTIVE 02 has been articulated into the following sub-objectives:

a: ***Ab initio molecular structure and dynamics simulations***

This sub-objective is the most theoretically and computationally challenging molecular science goal of the proposed VRE. It aims in fact at grafting on the e-infrastructure the highest level theoretical researches and computations allowing to offer as a service the most accurate and advanced molecular structure and dynamics computational investigations and to assemble the already mentioned General Ab-initio Simulator, (GENIUS, General Electronic and Nuclear Intra-and-inter-molecular Universal Simulator). GENIUS leverages on the porting on the e-infrastructure of both high level ab initio electronic structure packages (requiring usually computing platforms having large memory sizes and relying on tightly coupled parallel computational tasks) and ab initio based quantum, semiclassical and quasiclassical codes dealing with nuclei motion. This is indeed the case of the codes used by the COMPCHEM, MosGrid and COST MOLIM Action (http://www.cost.eu/COST_Actions/cmst/Actions/CM1405) communities dealing mainly with spectroscopic

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investigations and molecular motions. These applications often require also fitting (using ad hoc designed global functional forms or force fields) potential energy hypersurfaces and classical molecular dynamics computations based on loosely coupled (or even totally uncoupled) computing tasks and reduced memory sizes. This makes the combined usage of different computing platforms and the exploitation of workflowed QoU and QoS functionalities an asset for such computations.

b: ***Complex molecular systems and processes simulations***

This set of sub-objectives are the most innovation and technology oriented ones and target massive multiscale simulations often requiring also the combined usage of different computing platforms and workflows dealing with classical mechanics treatments (sometimes even non atomistic) of large systems and higher scale statistical and/or dynamical treatments.

b1: ***Modeling energy transfer processes***

This sub-objective aims at porting on distributed computing environments a set of computational procedures integrating scattering and kinetic systems of equations (together with data and phenomenological formulations of related parameters) dealing with the most advanced molecular and materials collisional processes simulations exploiting the computational determination of the efficiency of detailed energy transfers. Related highly innovative simulation packages deal with the accurate microscopic determination of the action of the smart energy carriers intervening, for example, in clean combustion (like in the SMARTCATS COST Action http://www.cost.eu/COST_Actions/cmst/Actions/CM1404), in the modeling of spacecraft reentry (like in the Phys4entry project http://users.ba.cnr.it/imip/cscpal38/phys4entry/index.html), in the evaluation of Carbon dioxyde reduction (like in the production of carbon neutral fuels));

b2: ***Materials by design***

This sub-objective aims at the porting on distributed computing environments of condensed matter codes dealing with the simulation of the formation of new materials. This implies for the chosen use cases the porting on the available e-infrastructures of the set of codes of the CMAST virtual laboratory of ENEA (http://www.afs.enea.it/project/cmast/index.php). The CMMST VRE will also port the codes dealing with the ionic liquid modeling codes of CHRO, the quasi-automatic parameterization of the force fields in molecular dynamics simulations of CHSA, with the rationalization of the action of some additives on methane storage as clathrate hydrates (https://www.youtube.com/watch?v=xJeg7paZCeY);

b3: ***Data for biomed***

This sub-objective aims at porting on distributed computing environments procedures for Cross-type data integration, visualisation and exploitation of data linking in chemistry and biology. To this end a huge amount of information available in public databases will be used and new ones will be produced by means of multiscale simulations. Among the programs of interest for this purpose a family of efficient Quantum Mechanics/Molecular Mechanics (QM/MM) simulation codes will be considered for porting on the available e-infrastructures and for being grafted within workflows in order to be made available as services at the CMMST VRE. Such procedure will be adopted for the porting of the main public databases for GPCR (G protein-coupled receptors) and for the implementation of the use of high throughput in silico virtual screening aimed at identifying interesting leads and at characterizing the interaction with known ligands (http://www.gpcr.org/7tm/webservices). Similar multiscale computational procedures devoted to the evaluation of kinetic and thermodynamics parameters will be adopted also for enzymes (http://www.researchgate.net/topic/enzyme_kinetics) in order to elucidate the mechanisms of related catalytic effects and for other Bio-molecular modeling of the computational Life Science communities (http://www.scalalife.eu/). Extended data bases will be handled (in tight connection with the ESFRI project ELIXIR) in order to investigate structure and processes of complex molecular systems relevant to pharmacology, medicinal and biological systems; code workflow and user service will be implemented and validated for use in computational enzymology to the end of improving our understanding of enzyme-catalyzed reactions by using multiscale simulation tools;

c: ***Knowledge management and e-learning for molecular sciences***

Distributed knowledge developed and stored for the purpose of providing the above mentioned innovation services will be utilized for the purpose of providing e-learning services both under the form of Learning Objects (c1, being progressively improved thanks to their shared usage and to its association with the credit system) and under the form as well of materials to be used for self assessment procedures (c2). In both cases use will be made of Moodle as Learning Management System. This service will be designed not only for the training of the project but also, thanks to the collaboration with the cluster of spinoffs led by the Academic Spinoff Master-up, for the more general use of enhancing molecular sciences knowledge by the ECTN (Higher Education), EurChem (Professional), CEFIC (industrial) and EUCHEMS (general) associations but

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also for the measuring of acquired competences in General chemistry on a European scale in a sustainable way.
To summarize Objective 02 targets significant advances in a wide spectrum of the CMMST area ranging from research and methodology (in subobjective (a)) to promising innovation services (by relying (either directly or indirectly) both on services of type (a), though most often largely simplified, and on a massive use of databases generated from sources of different types (including monitoring and empirical procedures)) in subobjective (b) and knowledge management in education and training ones in subobjective (c). In the first case the achievement of new research primes for which the proper chaining of computing platforms is important is the key target, in the second case fully realistic simulations of innovative technologies are the key target while in the world latter case the existence of dynamic evolution procedures for data collection and improvements is the ultimate target.

OBJECTIVE 03: ***Structuring and transforming the credit mechanism into a systematic sustainable market oriented business model.***
The goal of this third objective, that deeply involves the technology providers and the cluster of SMEs participating to the project, is to establish and maintain a set of exploitation activities (in a structured and systematic way during the project) which are aimed at accelerating the post-project uptake of the results achieved. Key elements of such exploitation activities will include assessment of the optimal business model to adopt in order to transfer related technologies to the market in a way that ensures the widest uptake and profitability as well as business sustainability. Such transfer will leverage both on the gathering of a proper cluster of solid technology providers and on the establishing of a credit mechanism to support the synergistic model adopted by the CMMST VRE based on an objective evaluation of the already mentioned TOEX (terms of exchange between credits and revenues generated). Such TOEX are agreed between the Communities and the Stakeholders in order to ensure that the results of the project (software and services) are provided at a professional level with alignment to the established standards. The SMEs members of the project will take care of validating related procedures and of producing a guide to sustainability and exploitation of the intellectual property.
To summarize Objective 03 is the most long range strategic one. It targets, in fact, the self-sustainability of the involved communities that is pursued through the design and implementation of a credit system and its evolution into a suitable business model thanks to the engagement of the partner SMEs and a proper set of technology providers in such process.

1.2 Relation to the work programme

The present proposal aims at developing a Virtual Research Environment tailored to suit the needs of the Chemistry, Molecular & Material Science and Technology communities. In particular, the proposal is addressed to equip the CMMST researchers of the already mentioned COMPCHEM and MOSGRID Virtual organizations, ENEA, INFN, SCALALIFE and COST CMST Actions communities plus two Erasmus^{+} Consortia gathering several tenths of EU Higher Education Institutions (TCCM ((http://emtccm.qui.uam.es/) for Theoretical Chemistry and Computational Modelling Master and Joint PhD and EURASIACAT (https://sites.google.com/site/emeurasiacat/home) for Advanced Education European-Asiatic Exchange Programme in Materials Science and Catalysis including 6 Asia Pacific countries) and several other individual European laboratories with a Virtual Research Environment in which domain-driven services are made available to their members. Stakeholders of the initiative are some more general associations like EUCHEMS (over 150.000 members) and ECTN (over 100 University Chemistry and Chemical Engineering Departments) and a cluster of SMEs.

Challenges:
- supporting **capacity building** in interdisciplinary research communities to empower researchers through development and deployment of service-driven digital research environments, services and tools tailored to their specific needs

  The proposal aims at increasing capacity building in CMMST areas and at empowering, through the development and the deployment of service-driven digital environments, the offering of services and tools thanks to the synergy implemented between some major e-infrastructure technology providers (like

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EGI.eu, INFN, MTA-SZTAKI, ENEA and the University of Westminster) and some members of the CMMST communities. In contrast to many previous research projects CMMST will focus on domain scientists representing the Chemistry, Molecular & Material Science and Technology communities. Domain scientists may combine in-silico simulation and in-vitro experiments to advance this discipline. Running simulations requires expertise in computing infrastructure to access compute and data resources and skills in use of simulation software packages that domain scientist may not have. To support them CMMST will further extend the WS-PGRADE/gUSE science gateway framework and elaborate the CMMST VRE platform around this framework. This VRE platform will manage scientific experiments as workflows and provide seamless access to compute and data resources. In this VRE platform three types of actors will cooperate: technology developers, workflow developers and domain scientists. Technology developers will create the CMMST VRE platform extending existing services and tools considering the community requirements. They will customise this platform according to a particular CMMST community's requirements and deploy community specific VREs. Workflow developers in collaboration with domain scientists will elaborate workflows implementing use cases identified by the CMMST communities and upload them in public repositories. The CMMST VRE platform will provide customised graphical user interfaces for domain scientists to support searching, downloading, parametrising, submitting and monitoring scientific experiments as workflows. As a result, even domain scientists with basic IT skills can find, download and run scientific experiments on the customised CMMST VRE. This approach will signicantly increase of the munber prospective users from a few hundreds workflow developers to a few thousand domain scientists.

- Virtual Research Environments (VRE) should **integrate resources across all layers** of the e-infrastructure (networking, computing, data, software, user interfaces), should foster cross-disciplinary data interoperability and should provide functions allowing data citation and promoting **data sharing** and trust.

  The CMMST VREs will be built on the WS-PGRADE/gUSE science gateway framework. This framework provides access to major compute and data resources through the DCI Bridge and Data Avenue Service. The DCI Bridge manages access to all major computing infrastructures such as clouds (EGI Federated Cloud), clusters, desktop and service grids (EGI Grid). and supercomputers. The Data Avenue service supports all major data formats and data transfer protocols to manage input, intermediate and output data used and/or produced by scientific experiments. The CMMST VRE platform will allow sharing both data resources (input, intermediate and output data) and methodology (workflows) via a new workflow management strategy. Many of the existing workflows are too complex and monolithic, i.e. they support only one specific scientific experiment. Even the slightest change in the scientific experiment may require a complete re-design of the workflow. To address this issue WP4 (Scientific Gateways and Workflows) will develop a new strategy to be based on the concept of atomic workflow - workflow library – compound workflow. Atomic workflow is a workflow that provides a specific and well-defined function that can be used in complex workflows (called as compound workflows) as a building block similarly to Lego bricks. Workflow developers elaborate the atomic workflows and publish them in workflow libraries. These libraries contain atomic workflows of one specific domain for example docking library molecular dynamics library, etc. Workflow developers in cooperation with domain scientists combine atomic workflows into compound workflows to implement specific scientific experiments. They publish these workflows in public repositories. This strategy will enable both data and methodology sharing at domain scientist level in a more efficient way than previously.

Scope:

- Each VRE should **abstract from the underlying e-infrastructures** using standardised building blocks and workflows, well-documented interfaces, in particular regarding APIs, and interoperable components

  The WS-PGRADE/gUSE framework has a built-in workflow system - the WS-PGRADE workflow system - that enables creating, submitting and monitoring workflows representing scientific experiments. This workflow system enables workflow developers to elaborate scientific experiments as workflows and domain scientists to run them offering user interfaces customised for them, i.e. there is a separate developer and user view. The workflow system manages compute and data resources through the DCI Bridge and the Data Avenue Service and works as abstraction layer between the infrastructure and the

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users. This abstraction hides the underlying e-infrasturcture.

- VREs will be composed of **generic services** delivered by e-infrastructures and **domain specific services** co-developed and co-operated by researchers, technology and e-infrastructure providers, and possibly commercial vendors.

  CMMST will develop both generic and domain specific services. WP4 (Scientific Gateways and Workflows), and WP5 (Data Management and Commons) will mainly be responsible for further development of generic services, while domain specific services will be developed by WP6, WP7 and WP8. Regarding generic services, WP4 will further develop and extend WS-PGRADE/gUSe based services that are already widely available in existing e-infrastructures, such as EGI. New and improved services will be created addressing for example Quality of Service and Quality of User requirements, federated authentication support, advanced workflow services, improved data and compute infrastructure support, and logging services. WP5 will create common high-level data management services by integrating and extending existing technologies, such as EUDAT and Data Avenue, WP5 will also develop generic services to support the Rewards/Credits system proposed by the project, front-end services to support the integration of data back-end services into user facing interfaces, and a metadata repository and its related services to support cataloguing and publishing data from large scale heterogeneous data services. Domain specific services will mainly be addressed by WP6 (related to ab initio electronic structure nuclei dynamics simulations), WP7 (related to complex molecular systems and processes simulations) and WP8 (related to knowledge management and e-learning for molecular sciences). The development of all services will be in cooperation between domain specific scientists (chemists) and distributed computing specialist computer scientists, and will also be validated by CMMST partner SMEs.

- VRE proposals should clearly identify and build on **requirements from real use cases**, e.g. for integration of heterogeneous data from multiple sources and value-added services for computing, modelling, simulation, and data exploration, mining and visualisation, taking due account of privacy aspects.

  CMMST will be driven by its targeted user communities. The requirements for generic and domain specific services will be formulated by the CMMST communities based on their real use-cases, and will be synthetised by WP2. Once the generic requirements are collected, WP4 and WP5 will translate these to compute and data related requirements before implementing generic services. Finally, domain specific services (e. g. workflows and portlets) will be created on top of these generic services by developers and researchers associated with the user communities. CMMST specifically will address data integration from multiple sources (WP5), value-added services for computing, modelling, simulation, and data exploration, mining and visualisation in the form of computational workflows (WP4), and enhanced authentication services for addressing privacy (also WP4).

- VREs should **re-use tools and services** from existing infrastructures and projects at national and/or European level as appropriate

  CMMST general services will be based on the results of several previous European projects. CMMST will develop new services based on these existing and widely used technologies. The current gUSE framework was created by the SCI-BUS project and used by over 50 user communities wordwide, including several EGI and PRACE user communities. Workflow interoperability framework and workflow repository that is fully interoperable with WS-PGADE/gUSE was developed inside the SHIWA and ER-FLOW projects. Services operated by exsiting European e-infrastructures, such as EGI and EUDAT will be utilised and will serve as the bases for the CMMST reference architecture. New services will always be tested and harmosed to these existing e-infrastructures.

- VRE will define the **ontologies and semantics**, the 'what' metadata, as well as the best computing models and levels of abstraction (e.g. by means of open web services) to process the rich semantics at machine level (the so called 'how' metadata), as to ensure interoperability

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A significant aspect of CMMST VRE platform is that it envisages engaging and strengthening the collaboration across diverse scientific communities. These communities often make use of large volumes of data which is potentially useful across different communities and therefore becomes a pivotal factor in bringing together and fostering effective relationships among such communities. This proposal will facilitate establishing and further enhancing these data-oriented collaborations by developing a set of tools to achieve a synergistic data management framework. Furthermore, the CMMST will manage the heterogeneity among the data semantics and standards adopted by different participating communities and addresses this diversity by developing specific backend plugins to support multiple contemporary data formats and standards. These plugins not only address the non-trivial challenge of diversity in data semantics but also serve to support a level of abstraction in making the access to these data sources convenient.

- VREs may also support **proof of concept, prototyping and deployment of advanced data services and environments**, and access to top-of-the-range connectivity and computing

  The CMMST-VRE will allow diverse scientific communities to improve the quality of their research by enabling synergistic access to diverse data sources via a common scientific gateway. CMMST-VRE will achieve this via
  - Development and deployment of generic data services to manage data from potentially heterogeneous data sources, formats and semantics.
  - Developing bespoke tools to facilitate existing data analytics frameworks adopted by participating scientific communities.
  - Development and deployment of a reference framework to facilitate integration of data visualization tools adopted by specific communities.
  - Development, deployment and evaluation of a proof of concept metadata repository to support data cataloguing and publication from large scale heterogeneous data services.

- VREs may **target any area of science and technology**, especially **interdisciplinary** ones, including ICT, mathematics, web science and social sciences and humanities. Focusing on the ICT infrastructures needed for addressing the Societal Challenges is especially encouraged. Proposals should indicate the number of researchers they target as potential users

  The CMMST-VRE is focused at addressing the specific needs of Chemistry, Molecular & Material Science and Technology communities. In particular, the proposal is addressed to equip the CMMST researchers of the already mentioned COMPCHEM and MOSGRID Virtual organizations, ENEA, INFN, SCALALIFE and COST CMST Actions communities plus two Erasmus^{+} Consortia gathering several tenths of EU Higher Education Institutions (TCCM ((http://emtccm.qui.uam.es/) for Theoretical Chemistry and Computational Modelling Master and Joint PhD and EURASIACAT (https://sites.google.com/site/emeurasiacat/home) for Advanced Education European-Asiatic Exchange Programme in Materials Science and Catalysis including 6 Asia Pacific countries) and several other individual European laboratories with a Virtual Research Environment in which domain-driven services are made available to their members. Stakeholders of the initiative are some more general associations like EUCHEMS (over 150.000 members) and ECTN (over 100 University Chemistry and Chemical Engineering Departments) and a cluster of SMEs.

1.3 Concept and approach

This section describes how the Service Activities (SA) will offer access to state-of-the-art infrastructures, high quality services, and will enable users to conduct excellent research.

SA - Service Activities

E-infrastructure technologies often have a learning curve which requires scientists to develop expertise foreign to their domains thereby limiting the extensive adoption of such technologies. CMMST-VRE services strive to lower these barriers and to the end of carrying out the related *targeted applications porting*

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and training the already mentioned sets of CMMST popular usecases have been taken as working ground. Accordingly, the Applications Porting (SA) work packages identify such flagship applications as well as related common frameworks and common libraries in use within the involved communities and are targeted to port them to distributed environment. The following are the SA activities distributed over the already mentioned WPs.

SA0 – BASIC SERVICE ACTIVITIES:

WP03: Integration, user support, and knowledge transfer

The basic goal of service activities is to establish an environment to foster the collaboration among the project members belonging to the CMMST communities which are currently working in different environments and to apprise them about:

- the opportunity to engage with distributed resources to improve their research quality,
- the availability of reusable tools on the existing e-infrastructures to be used to create a common VRE computing and storage environment,
- the existence of distributed know-how supporting the users in learning and exploiting such resources.

This is envisaged to be achieved as part of WP03 (as specified in detail in the related Table) by creating a strong link between the generic services available in the existing e-infrastructures and the applications developed within the project. To this end the technical features of existing e-infrastructures will be analyzed along with the definition of specific pilot scenarios to facilitate testing and validation of the proposed usecases and related services. Furthermore, knowledge dissemination activities will be conducted focused at available distributed resources, standard and reusable tools available via existing e-infrastructures, and creation of common computing and storage environment. This is aimed at enabling users across different participating communities of CMMST to benefit from these resources to improve the quality of their research.

To this end a strong link between the generic services available in the existing e-infrastructures and the applications developed within the project will be created. Furthemore, the expertise and the provisioning of guidelines and best practices will be shared with the developers so as to enable their activities more generic and beneficial to other researchers within and outside the VRE. This WP will also devise a support structure for the members of the project and provide appropriate tools in order to effectively address the problems users may face during their activities. This will leverage on the existing support structures of the different e-infrastructures as well as on the developer teams of the services being developed within the project.

SA1 - USE CASES SET 1:

WP06: Ab initio combined electronic structure and nuclei dynamics simulations

This activity is fundamental to the project. It assures, in fact, both the service of continuous advancement in CMMST basic methods and algorithms development for new approaches and the service of supplying basic electronic structure and nuclei dynamics detailed data (potential energy hypersurfaces, coupling matrices, reaction probabilities and cross sections, etc.) as a ground for higher scale treatments. Part of the activity of this WP will consist of porting a set of CMMST codes to the available distributed computing environemnts making use of different features of existing e-infrastructures. This is envisaged to enable addressing non-trivial structural and dynamical challenges to fulfill the specific requirements of cutting edge computational probelms. The richness of the related GENIUS simulator allows the assembling of a large variety of codes and workflows of which:

i. The first family of codes (subset 6.1) consists of selected first-principles electronic structure and few-body quantum nuclei dynamics packages running on platforms having a large memory size able to perform tightly coupled HPC parallel calculations. These codes start from a limited input describing the nature of the system considered and produce a large amount of intermediate (orbitals, wavefunction integrals, spatial distributions, etc.) and final (see the previously mentioned quantities) data. In this case use of the PRACE platform will also be made by the MoSGrid community operating in collaboration with the US counterparts (via the MoSGrid-XSEDE cooperation). The focus on the mentioned packages will be both on Born-Oppenheimer (BO) and non-BO techniques and different levels of theory for the evaluation of the spectroscopic and scattering properties of molecular systems. A strong link with the recent development of theoretical and computational approaches coupling electronic and nuclei motions in spectroscopic studies will also be established.

ii. The second family of codes (subset 6.2) to be ported on both HPC and HTC distributed platforms

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will be concerned with uncoupled (or loosely coupled) few and many-body classical and semiclassical molecular dynamics (for which on-the-fly approximate ab initio and force field electronic structure treatments of the interaction are often preferred). Also in this case interoperability with XSEDE machines will be seeked.

iii. To complement the above mentioned tasks is the one (subset 6.3) aimed at implementing GENIUS (General Electrons Nuclei Intra-inter-molecular Universal Simulator) as a platform for the other WPs and combine the ported applications in selected workflows.

Concrete examples of coordination between both families of codes (accurate electronic structure and nuclei dynamics) will be established in order to enable full ab initio simulations in an a-la-carte fashion by choosing at run time the most suitable machines and the preferred packages. Other families of codes worth to be implemented and inserted in the mentioned workflows are those related to fitting of potential energy hypersurfaces and/or other higher scale properties obtainable by performing additional statistical and/or dynamical treatments.

SA2 - USE CASES SET 2:

WP07: Complex molecular systems and processes simulation

This activity is devoted to innovation targeted multi-scale calculations building on the atomistic accurate determination of the electronic structure and nuclei dynamics detailed data provided as a service WP6.

The codes of these use cases start usually from extended (quite often etherogenous in terms of grid resolution, data accuracy, metadata, and sets of data detail (of the same level like the orbitals, wavefunctions integrals, spatial distributions, etc. or different level like thermodynamics, fluodynamics, geographical data, etc.) information taken from different databases to produce at completion even larger amounts of data using different specialized procedures.

We consider in the project three important families of applications:

a) Modelling smart energy carriers (subset 7.1)

This activity consists of porting a set of codes related to the detailed simulation of gas phase energy transfer processes to the available distributed computing environments. Other codes are those related to the simulation of clean combustion object of the recently approved COST CMST Action SMARTCATS. Distributed calculations parameterizing the evaluation of rate coefficients of the processes taking place during the combustion of alternative fuels will be finalized to the formulation of the temperature dependence of the rate coefficients of the intervening elementary processes also via the comparison with experimental data. A second set of codes to be ported deal with the simulation of an innovative experimental prototype based on the catalyzed reduction of CH_4 through massive computations performed by varying initial conditions in order to reproduce the measurements of a prototype industrial apparatus using excess electric power.

A third set of codes to be ported will be those enabling the simulation of the processes taking place at the gas-surface interface of spacecrafts entering planetary atmospheres in order to produce data of interest for the European Space Agency (ESA).

b) Supramolecular effects and condensed phase (subset 7.2)

This activity consists of porting a set of codes related to the simulation of the formation of new condensed phase materials to the available e-infrastructure. The major part of this activity is achieved in part by enabling accessibility of community members to the applications available at the ENEA virtual laboratory i.e. CMAST for materials design. This is accomplished by adapting related interfaces and workflows already operating on the CRESCO high performance computing (HPC) platform. The choice of the CRESCO HPC platform is motivated by the availability of several popular packages of particular relevance to the CMMST VRE including the paralleized plane wave/pseudopotential version of a code based on the Density Functional Theory (DFT).The DFT is an integrated suite of computer codes performing electronic-structure calculations and materials modeling at the nanoscale, a code carrying out atomistic and molecular simulations of solid state, liquid, molecular and biological systems. Further applications considered for porting will be a user friendly tool focused at generation of classical force fields for crystalline and microporous materials from scratch (requiring only crystallographic data and, when available, vibrational spectra), a software made of a multi-scale knowledge base that organizes the existing computational techniques used in the simulation of room temperature ionic liquids.

c) Pharmacology and Medicinal chemistry (subset 7.3)

This activity consists of porting on the e-infrastructure a set of codes exploiting the features of distributed environments for pharmacological and medicinal chemistry applications. The first use case is made by the procedure for feeding the GPCR database and producing information on new safer drugs production,

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crystallographic breakthroughs enabling receptor function and drug design studies with easy to use data visualisation tools and extension of the current residue diagrams and phylogenetic trees.
The second set of codes enable accurate multiscale calculations of kinetic parameters and elucidating plausible catalytic mechanism(s) of enzyme processes of interest. The procedure will facilitate the evaluation of related effects, including inhibition, point mutations, protonation states, external stimulus and tunnelling and support an improved understanding of enzyme action. The procedure will offer also valuable feedbacks on the structural aspects.
The third usecase will be concerned with adapting the functionalities of Scalalife to the distributed computing environment by implementing support tools for both users and developers. This will enable an efficient usage of the applications, analysis and profiling of codes, deployment and benchmarking on HPC systems. The procedure will also provide support to resource providers (such as HPC centers) with best practices for application setup and tuning.

SA3 - USE CASES SET 3:
WP08: Knowledge management and e-learning for molecular processes
This activity consists of developing a description of the General Chemistry syllabus based on a Europe-wide analysis of the curricula for Higher Education and ECTN Eurolabel standards. Furthermore, it will carry out an analysis of the situation of ECTN EChemTest self evaluation sessions with special concern for the General chemistry level (subset 8.1). On this ground porting on distributed computing environments of a set of tools and procedures developed for the handling of Molecular and materials science knowledge both under the form of Learning objects and under the form of self evaluation sessions will be made. This implies the development of specific methodologies and taxonomies to handle General chemistry contents as well as the dissemination of the related best practices on a European scale.
To this purpose (subset 8.3) an e-learning environment (Moodle based) will be used to access a repository of SCORM Learning Objects (LO) maintained by federated institutions on a set of servers (G-LOREP). Furthermore a Cloud based service for enabling the e-assessment of competencies and skills (EOL, Exams On Line), will be made available to the VRE (subset 8.2) mainly for certificating acquired knowledge and skills in the General Chemistry discipline (EChemTest). The e-learning environment will also help in user training tasks by establishing a series of tutorials and support pages based on the following established best practice: identify the steps of the procedure (job generation, submission, etc.), illustrate each step by a screen shot, write understandable short text for each screen shot, implement the step by step description eg several html pages), enclose a running example file and the related output, modify according to the feedback of a revision by an α-user.

JRA – Research Activities

Here we describe how the Joint Research Activities will contribute to quantitative and qualitative improvements of the services provided by the infrastructures.

JRA1
WP04: Gateways and workflows for the synergistic model implementation
The Scientific Gateways work package will determine common requirements for high-level computing tasks of data processing (e.g. user-driven workflows and data-driven pipelines), for simulation workflows, and any other stand-alone computing activities and related components, tools and interfaces built on top of the existing technological solutions (frameworks and gateways). It will also take care of activating the transition to a common implementation as it becomes available. The analysis of the past experiences of the CMMST VRC have singled out the tendency of the related communities to make a concerted use of both the existing users' data and applications on the ground of the adoption of agreed quality mechanisms. Out of the same analysis it has been concluded that the porting of a common set of tools and applications using shared techniques have a large, immediate impact to the community and that robust candidates to doing this are P-GRADE and SHIWA whose performances for CMMST applications will be evaluated. The gateway layer will enable the users to get proper access to the required resources of the underlying e-infrastructures, the implementation of a first prototype multiplatform workflow for the usecases of the CMMST communities, the facilitation of the interoperability among different workflow systems and the evolution towards PaaS (Platform as a Service) and SaaS (Software as a service) solutions for each usecase along with apporpriate virtual machine images for the e-infrastructure SaaS services, and the transformation of the developed prototype applications into a pre-production or production workflow interacting with the already mentioned

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validated tools and procedures. In this respect, specific attention will be paid to quality evaluation by testing and further implementing the advanced features of GRIF that provides quantitative and qualitative parameters allowing the optimization of the use of the resources and the involvement of the users in the production of services. In this way, we shall be able to rank the available software tools and protocols to be included in the offer of service and joint research activities. In addition, the assessment efforts will help to keep the CMMST-VRE platform continuously updated in terms of state-of-the-art procedures. Such developments will be readily made available to users.
The number and periodicity of events together with the quality ranking of the resource sites and of the proactive users will be adopted as an indicator of the state of advancement of this objective.

JRA2
WP05: Data management and commons for a credit based economy
The CMMST applications often make use of and create large datasets that, at the same time, are indispensable for several scientific and engineering communities activities and represent a valuable outcome of their knowledge production. An important component of the CMMST-VRE activities, in this respect, is the handling of the outcomes of European initiatives in producing digital data and metadata aimed at preserving heritage, fostering related research and consolidating the ground on which further CMMST activities will leverage.
For this reason CMMST-VRE will address significant efforts to strengthen the collaboration and mediation among the internal and external domains. In particular the work will focus on developing the mandatory high-level data-management functionalities as required by the need for promoting the credit based economy of the synergistic model aimed at encouraging prospective users to carry out either work within the VRE commitments or as new procurements in the interest of the communities to the end of enhancing research and innovation. In particular, the tools carrying out continuous quality evaluation will be utilized for determining the TOEX between the activities carried out and the credits to be awarded (and between the credits to be redeemed and the services or the financial resources to be provided in return as well). This requires the identification of the technologies to be developed for data representation and management suited to facilitating data search and data sharing among different domains by articulating areas of common interest and identifying common approaches to the manage complex data-driven applications. This is important for the design of quality activities in which both experimental acquisitions and theoretical simulations produce a large and continuous stream of information to make the appropriate representation, storing, accessing, retrieving and handling of data a challenging problem and a key step to model the dynamics of the e-infrastructures using techniques of Complex Network Analysis, Machine Learning and Data Mining.

Sharing and use of the existing basic operations services

Here we describe how the project will share and use existing basic operations services (e.g. authorisation and accounting systems, service registry, etc.) with other e-infrastructure providers giving on-line references.
Here we list and summarize the platforms, the services and the support to be provided to the CMMST VRE by the NGIs of EGI. The section starts with the description of two EGI platforms: the EGI HTC platform and the Federated Cloud Computing (FCC) platform followed by a description of the basic operational and other general services including support activities (such as dissemination). Related software tools and human services will be used by the CMMST VRE to coordinate the communities of the project, to facilitate among them communication, to assure continuous exchange of relevant information between the VRE and the rest of EGI, and to reach new members as well.
Platforms, tools and services described in this section are all operated by either VRE members or the NGIs. The software tools have a web interface that is accessible through some graphical portal (URLs are indicated in the text). The two platforms provide rather low level access mechanisms. These can be extended and made more user friendly by adopting science gateways and portals often built out of flexible frameworks. Some of these tools, such as portals and application gateways, have additional interfaces in the form of web gadgets and/or programming APIs which facilitate their strong integration with the domain specific services of the community.

EGI high-throughput platform

EGI high-throughput platform is a global high-throughput data analysis infrastructure, linking hundreds of independent research institutes, universities and organisations delivering top quality computing resources. As

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of January 2015, EGI offers more than 370,000 CPU cores of installed computing capacity interoperating through the Unified Middleware Distribution and supporting about 1.8 million computing jobs per day. Within this platform resources are allocated to 'Virtual Organisations' (VOs). Each VO represents a scientific community and the resources these communities have access to among those of the production infrastructure. The computational chemistry community operates in EGI through 6 VOs and several regional VOs (like the VO of Central Europe).

EGI Federated Cloud platform

EGI Federated Cloud[1] is a single, standards-based, open system to federate academic clouds from multiple providers, offering scalable computing resources with increased flexibility. It provides advanced compute capabilities for research, virtualised resources to run any chosen environment, cloud storage for easier sharing of data, and a number of support services to ensure applications run as efficiently as possible. EGI Federated Cloud can be used for running cloud-based applications and services needed by CMMST researchers. The EGI Federated Cloud platform currently operates in testbed mode, and is open for early adopter scientific use cases.

Operation services

EGI Operation services[2] are technologies, processes and people required to federate computing and data resources from resource providers into EGI. They provide a cost-efficient framework to manage operations within a federated environment, while retaining responsibility for local infrastructure. EGI Operations services can be used by the CMMST communities to federate clusters, storage and desktop systems into EGI, and share these capacities in a secure manner with VRC members.

Applications database

The EGI Application Database (AppDB)[3] is a centralised service that stores and provides information about the rich variety of software that has been integrated with the EGI production infrastructure. AppDB gives visibility to and facilitates the re-use of scientific software and associated tools by providing a platform for developers to publish their software in the repository part and/or to provide user-friendly description of their software and related access conditions. AppDB can be used to publish information about scientific applications, tools, science gateways, workflow systems and middleware components. The CMMST members can use existing entries from AppDB, and can publish their own software in the database, making these available not only to the other members, but also to research communities around the world. AppDB has a 'web gadget'[4] that enables the integration of lists of its relevant software into any website. The list presented in such a gadget is clickable, so those who wish to get further information about items in the list are redirected to the particular entry. AppDB can be used, therefore, as a central 'shop window' by the CMMST VRE to search for and browse applications, tools, science gateways, workflows and middleware software from EGI.

Training Marketplace

The EGI Training Marketplace[5] is an online registry of training events, training materials, training resources (e.g. computing sites for training), webinar events and university courses that are relevant to EGI user communities. The service allows users to browse and search for tailored content, and institutions, projects and communities to advertise their training offering. The Training Marketplace provides rating and commenting facilities for the registered items, and web gadgets for integration with third party websites. It can be used to publish events, training material, online courses that the communities develop for their members and share the information through the training Marketplace web portal.

[1] http://www.egi.eu/solutions/fed-cloud/index.html
[2] http://www.egi.eu/solutions/fed-ops/index.html
[3] http://appdb.egi.eu
[4] http://go.egi.eu/gadgets
[5] http://training.egi.eu

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Document Database

EGI Document Database[6] (DocDB) is a powerful and flexible collaborative document server. It was originally developed for use by the BTeV collaboration at Fermilab and is now used by twenty or more other experiments, Fermilab divisions, organizations, national laboratories, and companies (a partial list). DocDB is well suited for managing and sharing documents (not just official publications) among groups of up to several hundred people. It can be used to publish and manage (version control, updates) internal and public documents that the VRE produces with the read and write permissions for documents to be controlled separately.

Requirement Tracker

EGI Requirements Tracker[7] (RT) is used by European Grid Infrastructure collaboration to collect, store, monitor and provide solutions to requirements and recommendations communicated by scientific communities. It is a powerful and flexible tool with a web frontend and the ability to accept requests submitted by email. RT can be used to submit requirements and recommendations allowing to keep track of their status, and to receive alerts about progress and solutions. Submitted requirements can be also tracked either via custom RT dashboards or custom RT web gadgets.

Webex tele and video conference system

Webex[8] is a high level communication platform which provides on-demand collaboration, online meeting facilities, web conferencing and video conferencing services. EGI.eu, the coordinator of the EGI collaboration has a subscription to Webex. The CMMST VRE can use this EGI Webex account to organise teleconferences for coordination calls, and for interaction calls with EGI. The Virtual Team project that authored this document was also using this system for its teleconferences.

EGI SSO and GrIDP Identity Federation

EGI Single Sign On (SSO) system provides the federated authentication and authorization mechanisms within EGI services. With an EGI SSO account one can access the protected features of EGI services, for example to register applications in the Applications Database, to add new documents to the Documents Database, to register new training events or materials into the Training Marketplace and so on. Anyone can obtain an EGI SSO account at http://www.egi.eu/sso. EGI does not provide identity vetting for the SSO, i.e. the real identity of the requester is not checked, the accounts are issued based on the data the requester provides.

The EGI SSO system participates as an Identity Provider in the Grid Identity Pool (GrIDP) identity federation[9]. GrIDP is jointly managed and operated by GARR and INFN Catania from Italy, supporting cross-institutional e-Infrastructure services and providing federated authentication to its members. EGI SSO account holders through GrIDP can access high-level services, such as web portals and science gateways, in an easy yet secure and confidential way, using the credentials provided by the EGI SSO system.
The CMMST VRE can use the EGI SSO system to get controlled access to the protected services of the EGI Tools, and can use the GrIDP federation to access services with EGI SSO accounts. In addition it can offer services that are accessible with accounts issued by the Identity Providers of GrIDP[10].

Sex gender analysis

Here we describe how sex and/or gender analysis is taken into account in the project's content.

The proposal has been assembled by issuing a generalized call for expressions of interest to the members of the stakeholders of the project and WP leaders have been selected within the groups expressing the wish to participate to its activities in the tasks of their competence by applying positive discrimination for women whenever possible. Moreover, Sonja Herres Pawlis (RWTH) will take care of all aspects of such issue occurring during the life time of the project and other two women will act as advisors of the project (Otilia

[6] http://documents.egi.eu
[7] http://go.egi.eu/requirements
[8] http://www.webex.com
[9] http://gridp.garr.it/
[10] http://gridp.garr.it/identity-providers.html

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Mo, Director of the Department of Chemistry of the Autonoma University of Madrid, Spain and Elda Rossi, Head Technologist, CINECA, Casalecchio di Reno, Italy).

Towards a synergistic interdisciplinary VRE, the opportunistic versus the grant model resources management

Here we describe and explain the overall concept underpinning the project, the main ideas, models and trans-disciplinary considerations;

The evolution of computing technologies has led, in general, to two models of resources allocation:

- the first (the centralized grant model) assigns specific amounts of shared resources to users' proposals selected after an ex ante evaluation (based on criteria set by the facility management) at scheduled calls;
- the second (the local opportunistic model) assigns the available resources so as to match the requests of the registered users as they come without strict selection with case by case adaptations (often in the form of queuing policies).

The grant model is resource provider oriented and is in general adopted by large scale supercomputing facilities (as well as by medium-large size computer centres) in which specialized staff is devoted to the maintenance of HW and SW. The local opportunistic model, instead, is user oriented and is in general adopted either by research groups or departments running their machines for internal use (with the help of some permanent or temporary technical staff).
Although widely adopted, both the centralized and the local opportunistic model have recently shown to be insufficient to meet alone the evolution of the scientific computing demand. As an alternative, a new world-wide opportunistic model, based on the allocation of the computational tasks on federated distributed resources, was recently developed within a series of e-Infrastructure European projects. Such model, exploits the aggregated compute power of DCIs through the use of appropriate middleware and tools (the so called Grid Computing (GC)). The GC model has fostered the evolution into the modern e-infrastructures. It has enabled, in fact, the concurrent execution of distributed programs on a large number (over hundreds of thousands) of processors mainly for applications made of decoupled or loosely coupled tasks and has allowed the production of a large volume of results in reduced time intervals. Within the GC model the generic users can either access, among the already implemented applications, those of their interest or can port on the e-infrastructure the applications for personal use (though this requires some additional skills and support).
The use of e-infrastuctures fosters the sharing of HW and SW and the development of cooperative endeavours. Within this federated model, in fact, users not only can get an on-demand allocation of the available computing time but they can also set common requirements, share in a bottom up fashion data and programs, complement each others' expertise, establish virtual communities, etc. The e-infrastructures developed for that purpose and related software tools are the ground on which various VOs and VRCs originated and have performed inter-disciplinary collaborations.

In order to cope with the multi-discipline and multi-scale ab initio (from first principles) nature of most of the modern molecular and materials computational applications and usecases, the opportunistic model is better upgraded to a synergistic one allowing an a-la-carte variegated combination of codes and competences participated by the members of a community (or different communities). The synergistic model, in fact, meets the wishes of the most recent trends in computational science because it allows to assemble applications of a higher level of complexity, combine different packages in a single procedure and have a flat selected access to the machines of highly heterogeneous platforms.
In other words, the synergistic model encompasses much more than the simple feature of aggregating a large amount of computing resources and users for massive distributed computing. It targets, in fact, the more radical objective of changing the way of using and managing research oriented computing resources by fostering:
- an integrated use of different and distributed computational platforms;
- a synergy among complementary types of software and expertise (including programs, measured quantities and databases);
- a service oriented organization of the Virtual Research Environment
- a rewarded active participation of various providers (including users and community members) to the activities of the community.

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It is important here to emphasize that the proposed synergistic model of the CMMST VRE strongly relies on the possibility of evaluating the QoS and the QoU and base on them a credit economy rewarding resource and service providers. This enhances the sustainability of a community by calling both for introducing a metric suited to rank services and for developing tools facilitating collaborative activities.

Baseline of the project: the implementation of the synergistic credit based model

The above mentioned motivations (developed during the participation of the COMPCHEM VO to EGEE III and EGI-Inspire projects) led to the launch of the CMMST VRC at the Community Forum of Helsinki (May 2014) and to its presentation at the XSEDE 14 Conference held in Atlanta (July 2014). The CMMST VRC took the decision of assembling the present VRE proposal and such message was taken by EUCHEMS (http://www.euchems.eu/divisions/computational-chemistry.html, the association of European chemists) following the sponsorship of its Computational Chemistry Division Council in Instanbul (September 2014), by the ECTN Association (Administrative Council meeting held in Krakow, September 2014, see also http://ectn-assoc.cpe.fr/news/letter/2013/03/1403_201306.htm), by the COST CMST domain (Meeting held in Bled, September 2014, see also http://www.cost.eu/), by the Theoretical Chemistry and Computational Modelling Erasmus Mundus consortium and by the thematic projects MoSGrid and Scalalife plus DRAG (the already mentioned consortium of SMEs and Academic spinoffs).
The fact that the synergistic model fosters the sharing of expertise and products among the members of different communities (especially to the end of tackling multi-scale problems of higher complexity for which individual competences are insufficient) in a trustable objective way once the related metric for monitoring the activities, evaluating their quality and defining the proper terms of exchange for credits is agreed by the community, strongly encourages community members to step up to the level of becoming proactive service providers. Actually, CMMST VRE service providers can be of different types. They can offer, in fact, ordinary and specialistic hardware and software, support the design and development of new algorithms and applications, assist and help other users in running existing packages, produce and validate new data, design and develop new Grid approaches and disseminate community activities. *This enables the community not only to better carry out production work and perform record breaking computations but also to feed new research and development ideas on which grounding future evolution of research and innovation*.
Such mission aims also to overcome the fragmented nature of the CMMST domain, within which a poor interoperability among related software and data leads to the consequence of waisting a significant amount of time in scarcely significant computations and the to reach the critical mass necessary to take the grand challenges associated with the vast amount of extra compute time made available by the e-infrastructure.

Accordingly, the baseline of the project is the assemblage of a synergistic VRE leveraging on standardized, highly or fully automated collaborative protocols enabling the:

- *provision of support and training to the users and a task for experiencing ways of sustainability;*
- *simplification of the procedures to access (and possibly select) the compute resources and the assemblage of the applications;*
- *validation of the adopted and/or developed procedures;*
- *development of advanced data management and commons features for the provision of services of the CMMST communities to their members and to the society at large*.

At the same time the adoption of a synergistic model will further enhance the competitiveness of the various scientific laboratories thanks to the collaboration developed within the VRE (the already mentioned collaborative competition) by enhancing the complexity of problems affordable (typically the high level ab initio electronic structure and dynamics calculations, the design of smart energy carriers, innovative materials and biomedical processes, the handling of knowledge for training and education considered in the present project) and the evolution of the quality based credit system into a business model ensuring sustainability.

Preliminary indications on the transdisciplinary performance/research indicators of the impact of the synergistic model have been already pointed out to be accessibility, integrity, and reliability of the collaborative effort (at qualitative level) and number of succesful compilations, number of results retrieved and number of feedbacks produced (at quantitative level) as illustrated in C. Manuali, A. Laganà, “Requirements of the Chemistry, Molecular & Materials Sciences and Technologies community for evaluating the quality of a service”, VIRT&L-COMM.5.2014.14.

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National and international research and innovation activities relevant to the project

Here we describe the national or international research and innovation activities which will be linked with the project;

A key feature of the present CMMST VRE proposal is the large national diffuse nature of the coordinating Institution INSTM (http://www.instm.it/), that is the largest Italy based CMMST consortium of Universities and Research Institutes combining different scientific and technological (science and engineering) communities carrying out research and producing innovation in the field of Atomic, Molecular and Materials sciences and technologies.
Specific research and innovation activities carried out by the Consortium (as illustrated in the above quoted web pages) and linked to the project are: *Designing materials with special properties, Developing Carbon based materials, Studying non equilibrium chemical systems and processes treatments with particular focus onto combustion, atmosphere, lasers, chemical plasmas, spacecrafts, Investigating Chemistry under extreme conditions, Assembling new technologies with chemical with particular focus onto formation of ionic species relevant to plasma, laser, interstellar, high atmosphere, surface chemistry, vapour deposition and microlithography, Modeling polymeric systems and soft matter, Computing Electronic structure of inorganic materials with particular focus onto catalytic effects and innovative materials design.*
For the above mentioned fields INSTM is also the Italian partner in the "Sustainable Technology for Resource Efficiency by the Process Industry" and "Critical Row Materials" European projects projects developed by the European Federation of Chemical Industries (Cefic) for the Horizon 2020 Public Private Partnerships (PPP). INSTM is also partner in ERIC (European Research Institute on Catalysis), EIMM (European Institute on Molecular Magnetism) and ECNP (European Center for Nanostructured Polymers). From its foundation date (1992) to present INSTM has either managed or been partner of over 200 national and international projects with related activities having led to the publication of over 4000 papers of which over 60% excellent in the field of nano- and Micro-systems.
In the specific field of the VRE activities INSTM operates the INSTM-CST compute platform coordinated by Prof. Orlando Crescenzi (Dip. Scienze Chimiche, Università di Napoli Federico II) with the support of Vincenzo Barone (Network M3-Village), Maurizio Casarin (Departmental Centers), Antonio Laganà (Grid and Cloud Computing), Claudio Zannoni (Cineca and supercomputer centers). The goal of INSTM-CST is to support the broad spectrum of computational research activities carried out by its Research Units and manage the related e Infrastructure nodes in **Pisa**, **Padova** and **Napoli** Research. Links to the European DCI is taken care by the NetSC-UP (Networked Scientific Computing - University of Perugia) node that interoperates with the EGI Virtual Organizations and Research Communities (https://www.egi.eu/community/vos/) as well as with IGI (Italian Grid Initiative). NetSC-UP computational resources consist of three clusters with a total of about 1000 cores.
For the CMMST-VRE proposal liaisons with several International initiatives of the partners are mentioned in the Excellence subsection of section 1. In particular, on the ICT side EGI (and some of its National Grid Infrastructures) and PRACE (and some of its large scale facilities) are international compute e-infrastructures that extend significantly the size of the e-infrastructure available to the project. At the same time the. computational international activities systematically carried out by INFN, MTA-SZTAKI, ENEA and other participants (see related enclosed member profiles) which are major actors of European excellence in managing e-infrastructures add further lustre to the project activities and operations. At the same time, on the CMMST side, the participation to the project of the most recently approved Actions of the COST CMST domain with their networks counting each more than 100 high level EU researchers (plus some non EU associated ones) and the size of the ITN TCCM Joint PhD and Master programmes attracting about 50 young researchers each year from overall the world, generates a continuous stream of new blood into the objectives of the VRE. Finally the large size of ECTN and EUCHEMS Associations membership together with that of COMPCHEM, MOSGRID and SCALALIFE make highly impacting their frequent international computational initiatives.

Networking, Service and Joint Research activities for a synergistic interdisciplinary CMMST VRE

Here we describe and explain the overall approach and methodology, distinguishing, as appropriate, activities indicated in the relevant section of the work programme, e.g. Networking Activities, Service Activities and Joint Research Activities;

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As already mentioned the world-wide opportunistic model, based on the allocation of the computational tasks on federated distributed resources, recently developed within a series of e-Infrastructure European projects, already exploits the networked compute power of the DCIs. The synergistic model proposed for the present CMMST VRE project not only exploits the concurrency of a large number of processors and aims at producing a large volume of results in reduced time intervals but also pivots the activities of the communities of interest on a selective sharing of HW and SW and the development of competitive-cooperative endeavours. This makes it easier to cope with the difficult, multi-discipline and multi-scale ab initio (from first principles) nature of most of the modern molecular and materials computational applications and usecases and to adopt an a-la-carte utilization of codes and competences. In order to disclose such a new operating scenario allowing:
- the integrated use of networked facilities;
- the targeted offer of higher level services (software, expertise, measurements and knowledge);
- the exploitation of innovative research and market oriented applications;
- the quality based crediting of community activities;
the activities of the researchers of the user communities are meant to provide on the e-infrastructure (out of their advances in CMMST research) the services illustrated in SA1, SA2 and SA3 (which vary their target from enhancing methodological research to technological applications in materials and pharmacology/biotechnology). At the same time the activities of ICT researchers and technicians are meant to carry out further JRA activities targeted to develop more appropriate e-infrastructure instrument specific of the considered scientific area. Such complementariety of JRA ICT and SA CMMST activities is driven by the NA activities which match the respective achievements and contributions by further enhancing so far the synergistic nature of the project. The partnership of research teams in this proposal constitutes, in fact, a core balanced with respect to the target scientific communities and the ICT technological competences able to guarantee not only a balanced management of the various activities bu also their widest dissemination and outreach.

For this reason, as already mentioned in the introductory section (1.0) of the proposal, the assemblage of a specific VRE will represent the true leap forward in excellence of the CMMST communities because related Networking Activities will enhance the possibility of an effective co-operation among their members and other relevant stakeholders. NA activities will in fact offer the proper ground enabling both SAs to offer a user friendly access to state-of-the-art e-infrastructures, use of high quality ICT and CMMST services, and support excellent research and JRAs to develop quantitative and qualitative improvements of the e-infrastructures.

NA - Networking Activities

Here we describe how the Networking Activities will foster a culture of co-operation between the participants and other relevant stakeholders.

As just mentioned, in the synergistic model it is of paramount importance to set up an adequate human collaboration network. The setup involves connecting the researchers of the user communities to the researchers and technicians dealing with the e-Infrastructure. The collaboration among research teams is, in fact, the winning instrument for involving the target scientific communities and will guarantee the widest dissemination and outreach of the project's activities.

This is, indeed, a strong commmitment of the present project that aims at extending networked computing to the major CMMST communities of Europe. To this end the VRE will has agreed with EGI and the associated NGIs the present support and the possibility of making a bid for the further use of their networking resources (together with a more intensive usage of the resources of some particularly well equipped partner) if the program is succesfull. In particular, the extension will be concerned with the largest European education and innovation networks (ECTN and COST CMST, respectively). The institutional participation of such networks, together with that of the general Association of the European chemists (EUCHEMS), will give more momentum to the individual participation of a significant fraction of its members to several aspects including the competition for computing time grants on the PRACE supercomputer network. Yet, they are an ideal test ground for the extension of distributed computing to the CMMST communities at large especially if one considers the recent moves of EGI with respect to PRACE itself and to XSEDE.

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In the present VRE project, in order to support the necessary setup and operation, we shall activate the following (a.) management and coordination, (b.) validation of the procedures, (c.) sustainability, business model and expansion of the community as detailed below.

NA1

WP01: Management and coordination

This activity will set up the structure of the project Management Committee by having in mind also the long term organization of the CMMST VRE. The CMMST VRE, in fact, will be articulated into the following three different lines of service: ab initio electronic structure and nuclei dynamics simulations, complex molecular systems and processes modelling, knowledge management for e-learning in molecular sciences (with the complex molecular systems and processes being articulated into three different application areas smart energy carriers, supramolecular effects and condensed matter, pharmacology and medicinal chemistry). This will require a significant effort of codes porting and adapting due to the higly fragmented nature of the software patrimony of the CMMST communities. For this reason the coordination and management effort to be taken care of in the present WP01 by INSTM will leverage on the presence of the WP leaders in the MC for the governance of the project and on the gathering of all the partner experts in the specific TBs in order to spot and solve the technical problems as soon as they arise. The TBs are, in fact, the substructures of the VRE whose leaders are appointed by the MC and that play the important role of being a regular discussion forum in which, if interested, each member Institution should name a competent representative. Regular TB meetings will be held at the biannual open conference organized by the project consortium. Additional meetings can be held (either f2f or in teleconference) at any time whenever the MC needs advice or the TB coordinator (or one fourth of the TB members) believes it appropriate. The TB meetings can also be attendend by other members of the partner groups, by the external advisors, by the representatives of the stakeholders and by members of any other CMMST communities interested in the project.

The project WPs are the substructures devoted to the carrying out of the tasks concerned with some specific subobjectives of the project and produce related deliverables. Formal meetings of each WP mwmbers will be also held regularly at the biannual open conference of the project consortium. Such meetings may be attendend by the external advisors and by the representatives of the stakeholders (EUCHEMS, ECTN, ITN TCCM Joint doctorate). Additional WP meetings (either f2f or in teleconference) will be held whenever the WP coordinator (or one fourth of the members) believes it appropriate. During the WP meetings the work done will be reported, discussed and evaluated in order to propose to the MC (through the WP Leaser) modifications of the strategy and check the project roadmap.

The MC is the governance body of the project and is made of all the WP leaders. The MC will meet quarterly (either f2f or in teleconference) in order to review the work done, to analyse progress made in carrying out the tasks and producing related deliverables, to take the necessary decisions and to prepare as well detailed quarterly reports and action plans. The MC meetings may be attendend as auditors by the external advisors and by the representatives of the stakeholders (EUCHEMS, ECTN, ITN TCCM Joint doctorate).

NA2

WP02: Usec cases dissemination and training

This WP is devoted to the organization of a community-wide implementation of the procedures to be adopted for the CMMST VRE and its training initiatives. This activity plays a central role because it will allow both to better test the portability of the e-infrastructure instruments developed for other communities and to single out the peculiarities and the specificities of the e-infrastructure instruments developed for the CMMST VRE innovative and/or optimised approaches in which the design and use of higher level of complexity ab initio molecular simulations, of more realistic studies of new materials in biology and medicine, of global modeling combustion and atmospheric pollution, of data and knowledge distributed storage for molecular training and education. These elements will provide the ground for comparing and assessing the different solutions. The activities implementation and assessment will be carried out at two levels. The first level is for the procedures already well established in EGI for wich tests will have to be performed in order to make the extension efficiently used by the largest number of new users (and user sites). The second level of tests will be performed on the features most relevant to the CMMST communites and related applications.

To carry out this assessment activity, experts in the field of computational procedures applied to the different areas of the CMMST-VRE will be brought together. In this way, we shall be able to rank the available

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software tools and protocols to be included in the offer of service and joint research activities. In addition, the assessment efforts will help to keep the CMMST-VRE platform continuously updated in terms of state-of-the-art procedures. Such developments will be disseminated among the users.
The number and periodicity of events together with the quality ranking of the resource sites and of the proactive users will be adopted as an indicator of the state of advancement of this objective.

NA3
WP09: Sustainability, business model and engagement of new communities
Establish adequate mechanisms for making the activities of the CMMST communities sustainable is the ultimate goal of the VRE. For this reason the WP09 will leverage both on the outcomes of previous EGI activities (like the specific pay per use Virtual Team) and on the requirements of a cluster of SMEs and spinoffs already established within the CMMST communities. Such cluster of SME, launched during a joint strategic initiative ("COST Actions: A Great Opportunity as Incubators for Molecular Science and Technology" Conference, held in Brussels (Belgium) on 27 and 28 March 2014 (http://www.cost.eu/events/actionsincubators)) as a joint event organized by COST CMST, ECTN and Eureka, will represent the proper test field and the source of know how for developing a suitable business model. As a matter of fact, sustainability measures will be designed and adopted with the cooperation of the participating SMEs by taking as a reference the activities of the already mentioned stakeholders. The key NA activity of this type (the present one) will consist in the transformation of the credit system proposed for the CMMST VRE into a proper business model that will be experimented by targeting selective applications of the various WPs .

1.4 Ambition

Here we describe the advance our proposal would provide beyond the state-of-the-art, and the extent the proposed work is ambitious.

According to the goals of the project, the proposed synergistic model does not only represent the only viable solution to the further enhancement of the excellence of the CMMST communities through a proper orchestration of their network but it also provides a new modern approach to the organization of computational research.
The full exploitation of the ingredients put forward in order to assemble the VRE (QoS run time evaluation, selection of the networked resources, a-la-carte workflow combination of application codes, evaluation of QoU, creditization of the use of the resources and of the work done on behalf of the community, transformation of the credit system into a business model) pave, in fact, the way for a passive filtering approach to making the computational research assessable in an objective way for a research community and targets its sustainability thanks to the link to SMEs.
The matter empowering the present proposal was debated at the EGI Community Forum (Helsinki, May 2014), at the XSEDE Conference (Atlanta, July 2014) and at the EUCHEMS Chemistry Congress (Instanbul, September 2014). It is planned to be further discussed next June at the International Conference of Computational Science and its Applications, Banff, Canada,and at the Quantum reactive Scattering, Salamanca, Spain. If approved a kick off meeting of the project will be hosted the next September by the European Conference on Computational Chemistry in which the outcomes of a preliminary experiment carried out with the PRACE installation at CINECA and suggested by the paper C. Manuali, A. Costantini, A. Lagana', M. Cecchi, A. Ghiselli, M. Carpene', E. Rossi, Efficient Workload Distribution bridging HTC and HPC in Scientific Computing, Lecture Notes Computer Science 7333, 345-357 (2012) will be analyzed and proposed for extension to XSEDE.
This will also be tackled as Joint Doctorate Thesis of the already mentioned ITN TCCM Erasmus^{+} PhD school that is planned to make the CMMST VRE its technological platform for enhancing molecular and materials sciences computations by training new generations of researchers.
A further ambition of the project is the interaction with the Virtual Education Community of the ECTN Association (http://ectn-assoc.cpe.fr/news/letter/2013/03/1403_201306.htm) for which the CMMST VRE will provide not only the environment suited to support distributed e-learning but also the technological channel for establishing a virtuous circle of continuous improvement of molecular and materials sciences knowledge. This is in fact the key feature of the shared usage of Learning objects that will not only improve the remote availability of teaching materials but also enhance personal (self)learning and the collaborative qualification of the e-materials used by the educators.
Finally, the key ambition of the project is to work out an effective business model by leveraging on the

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already mentioned credit system after adapting its scheme as as a result of the SME joint efforts in WP9.

Here we describe the innovation potential which the proposal represents by referring, where relevant, to products and services already available, e.g. in existing e-Infrastructures.

The innovative potential of the proposal lies mainly in the adoption of the synergistic model proposed as a new approach to the use of the DCI both on the technological and on the human side. It is, indeed, in the spirit of the synergistic model proposed for the CMMST-VRE to use QoU to value the contribution of proactive users and to use as well QoS to value the quality of the services provided both to the community members and to possible customers. In this way one can leverage on collaboration in order to fuel a regular stream of research, design, implementation and validation of new solutions and on competition to improve the offered services.
An innovative potential of this approach is, in fact, not only to continuously enrich the involved communities of new competences and technological solutions as interoperable components for addressing real-like problems but also to foster a (possibly) continuous extension of the services to different fields of applications in which the understanding of molecular processes is fundamental.
This innovative factor (see C. Manuali, N. Faginas Lago, A. Lagana', GriF: Empowering Scientific Calculations on the Grid in International Workshop on Science Gateways, R. Barbera, G. Andronico and G. La Rocca (IWSG 2010), Consorzio COMETA, Catania (IT), 13-18 and the more recent Laganà A., Manuali C. and Costantini A. (2013) Grid Computing in Computational Chemistry. In: Reedijk, J. (Ed.) Elsevier Reference Module in Chemistry, Molecular Sciences and Chemical Engineering. Waltham, MA: Elsevier. 30-Jun-14) of the proposed CMMST-VRE will not only solidly ground new continuous advances in research and development, but will also prompt the tackling of further higher complexity scientific challenges, the development of new ICT technologies and the implementation of new services. In fact, the activation of the collaboration channels associated with the adoption of the synergistic model in addition to make different infrastructures (like EGI, XSEDE and PRACE in which CMMST is already involved) interoperate, allows to better evaluate the QoU (see C. Manuali, A. Lagana', GRIF: A New Collaborative Framework for a Web Service Approach to Grid Empowered Calculations, Future Generation of Computer Systems, 27(3), 315-318 (2011)) of the various types of CMMST users among:

a) passive users formulating new computational requirements while using in a passive way the e-infrastructure
b) developpers producing new software or updating the old one for use by the other members of the communities;
c) active users formulating new requirements for computing tools, workflows and web portals and software designers producing them;
d) experimentalists and computationists producing CMMST data and related standard formats to feed scientific and educations databases.

making it realistic to design a versatile true general purpose new generation of collaborative distributed simulators.

To this end the project plans to exploit the outcomes of the activities carried out by COMPCHEM, Gaussian and CHEM.VO.IBERGRID within EGI-Inspire in terms of community building and sets up a coordinated effort with the Computational Chemistry division of EUCHEMS. A further ambition of the project is to collect the inheritance of the presently disappearing COST CMST domain and related actions and spinoffs. The networking aspects of those actions will be given additional value by the use of the VRE as is also the case of some computational CMMST projects like che MoSGrid and Scalalife.

As mentioned before, the rewarding of the users' contribution to the community activities based on quality evaluation of the services provided is a key added value of the synergistic model proposed for the CMMST VRE. It fosters, in fact, the sharing of expertise and products among the members of the community (especially to the end of tackling multi-scale problems of higher complexity for which individual competences are insufficient but including also education for which little scientific recognition is attached and most of the materials are strongly (almost uniquely) linked to the author) in a trustable objective way once the related metrics of monitoring the activities, evaluating their quality and assigning related credits is agreed by the community and strongly encourages some members of the community to become proactive service providers by utilizing their own products and those of the other members of the community. The use of the credit system paves the way to a commercial interaction with the market (see C. Manuali, A. Lagana', A Grid Credit System Empowering Virtual Research Communities Sustainability, Lecture Notes Computer

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Science, 6784, 397-411 (2011)) by assimilating Service suppliers and proactive users to producers and customers. Service suppliers can offer ordinary and specialistic hardware and software, support the design and development of new algorithms and applications, assist and help the users in running existing packages, produce and validate new data, design and develop new Grid approaches and disseminate community activities and therefore possible sources for revenues. This ensures to the community not only a better accomplishment of production work but also feeds new research and development on which grounding future evolution of sustainable research and innovation.

2. Impact

Thanks to the already described increased reliability and use easiness of the synergistic system that allows a better access to discovery as well as access and re-use of data supported by the orchestration of the e-infrastructure, we expect to measure among the members of the CMMST communities

- a highly effective collaboration between researchers that will show up in the
  - Number of cooperative use-cases implemented on the VRE
  - Number of programs ported on the e-infrastructure
  - Number of programs embedded into automated protocols
  - Number of agreed standards adopted or released for data sets
  - Number of joint publications

- a higher efficiency and creativity in research that will show up in the
  - Number of publications
  - Number of new algorithms produced for the e-infrastructure
  - Number of invitation to conferences

- a higher productivity in research applications that will show up in the
  - Number and attendance of assessment events
  - Number and attendance of training events
  - Tutorials/demos made available
  - Usage of the adopted e-Infrastructures

- a higher productivity in innovation applications that will show up in the
  - Number of applications used by third bodies
  - Number of learning

- a higher productivity in education applications that will show up in the
  - Number of learning objects produced
  - Number of contribution to e-tests

Such metric will allow the project members to evaluate to what extent one is able to accelerate innovation in return for an integrated access to distributed digital research resources, tools and services across disciplines and user communities and enable researchers to estimate the efforts required to process structured and qualitative data in virtual and/or ubiquitous workspaces.

This will contribute to increased take-up of collaborative research and data sharing by new disciplines, research communities and institutions. In particular it will contribute to design a strategy for unifying the attack to the market of CMMST based co-developed and co-operated (by researchers, technology and e-infrastructure providers, and possibly commercial vendors) computational services in at present particularly dynamical fields (like Nanostructured materials, Life Science and medicinal chemistry) aiming at building for them a common European research e-infrastructure.

Further effort will be also paid to devise additional quality parameters derived from Quality of Service (QoS) and Quality of User (QoU) criteria (see C. Manuali, A. Laganà, “Requirements of the Chemistry, Molecular & Materials Sciences and Technologies community for evaluating the quality of a service”, VIRT&L-COMM.5.2014.14) allowing a detailed monitoring of both the properties and the fate of the submitted jobs

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and subjobs, an evaluation of the characteristics of the different Grid Service (wrapper), an analysis of the behaviour of the users and of performances of the computing elements.

2.1 Expected impacts

Here we describe how our project will contribute to the expected impacts set out in the work programme, and expected impact. The section describes the innovation capacity of CMMST-VRE and the potential for integrating and disseminating new knowledge. The list of expected impacts from CMMST-VRE follows.

Expected Impact 1: Increased access and usage of e-Infrastructures by Research communities.

CMMST-VRE aims to provide a complete set of tools and applications suited for the Computational Chemistry and Material Science research community allowing easier access and usage of the e-infrastructure for their purposes. Table X gives an indication of the project outputs that CMMST-VRE is expected due to the increasingly access and usage of the e-infrastructure for sample as well as high level applications.

Expected Impact 2: produce innovative scientific results and services

The exploitation of the available e-infrastructure will enable the Computational Chemistry and Material Scinece researches to study and develop several innovative solutions and, where possible, related innovative materials thanks to the possibility of utilizing different computing platforms and tools.

Expected Impact 3: using standards and standard metadata

One of the main problems of existing solutions in some areas, such as the use and re-use of available stored data, is the dependence on proprietary solutions. CMMST-VRE will harmonise the information carried out by the different Computational chemistry communities involved in the project by adopting (de facto) standard metadata and attempt to avoid building data silos due to lack of interrelatedness and ad-hoc interfaces. CMMST-VRE activities will focus on reusing e.g. the semantics (already provided in widespread terminologies/ontologies) that are exposed and interlinked among the databases already in use (see Table XX).

Expected Impact 4: **Quality-based internal economy**.

As already mentioned, the optimal selection of the compute resources based on the QoS parameter (associated with the satisfaction of the quality requirements issued by the users) and the rewarding of the users based on the QoU parameter (associated with the quality of their contribution to the community activities) are the key added value of the synergistic model proposed by CMMST-VRE. The mentioned quality parameters foster, in fact, the sharing of expertise and products among the members of the community (especially to the end of tackling multi-scale problems of higher complexity for which individual competences are insufficient) in a trustable objective way once the metrics of monitoring the related activities, the evaluation of their quality and the assignment of the corresponding credits are agreed by the community.

Summary of the project outputs and related targets:

Description of output	Intended targets
Science gateway for CMMST based on WS-PGRADE and gUSE	Providing easy access to networking, computing, data, software and user interfaces
Applications to predict the catalytic behavior of a material in a reaction (based on data from the new Erasmus Mundus service)	Improved scientific modelling code; Opening the applications to communities via the VRE
Relativistic DFT code for simulation of SuperHeavy Elements and metals	Porting of the code into the e-infrastructure enviroment and opening of the aplication to the community
Implementation of an Open Source Automated tool to build potential energy surfaces.	Implementation of a code to be used by the community as a tool to generate PES. The application will be open to the community.
Software of the SMARTCATS combustion community	Software for the generation, manipulation and management of detailed gas phase kinetic

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	mechanisms and Software for the analysis and reduction of detailed gas phase kinetic mechanisms. These codes should have a tight coupling to the database of objective 8.1. Their implementation on the grid will enable also more complex interactions between the implementations
Software for the management and simulation of potential energy surfaces	Implementation of a code to be used by the community as a tool to generate PES. The application will be open to the community
Codes for the computation of vibrational state-to-state energy transfer and reactive cross sections and rate constants in diatom-diatom collisions	Porting of the code into the e-infrastructure enviroment and opening of the aplication to the community
Porting on the e-infrastructure software devoted to the simulation of the module of an innovative experimental prototype governing the catalytic transformation of CO2 into CH4 through massive calculations performed by varying initial conditions.	Porting of the code into the e-infrastructure enviroment
Workflows, procedures for Ionic liquids modeling. Postprocessing and preprocessing codes for setting up the simulation	Force fields rationalization and automatization
Alghorithms and codes for free-energy calculations, analysis tools	Massively parallel approach in a weak scaling fashion
High-throughput virtual screening against G protein-coupled receptors	Significantly increased throughput and unprecedented easy access to powerful software (in web browser)
Computational enzymology service	Improved, partly generalized workflow for accurate multiscale simulation of catalytic activity of enzymes and related effects (point mutations, nuclear quantum effects)
Drug-receptor Binding Free energies (BFE) using full atomistic detail (explicit solvent)	Fast BFE determination using non-equilibrium alchemical simulations
Efficient quantum mechanics / molecular mechanics (QM/MM) simulation codes	High accuracy simulation on medium to large size simulation systems
Virtual environment for Learning and assessment of General Chemistry and Material and Matter Sciences	Permanent education Platform and Standard Certification of competences and skills related to Chemistry and Matter and Material Sciences

Summary of the project databases and related targets:

Databases and metadata	Intended targets
Database and data management tools in the Erasmus Mundus network	Virtual tool to join all the information (synthesis, characterization and catalytic results) to join the different data acquired in different laboratories and for different students; Opening the data for use by another member of the Erasmus Mundus network
Database for primarily gas phase kinetics and thermodynamics. The primary users of this database will be combustion (SMARTCATS), atmospheric and astrophysical modeling where the primary kinetic data is in the gas phase	A detailed kinetic database for experimental and modeling data needed by the combustion community. For the modeling community this includes all gas phase kinetic and thermodynamic data needed for detailed, reduced and global combustion mechanisms used in 0D, 1D, 2D and 3D calculations

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GLOREP (Grid Learning Object REPository) is a federation of distributed repositories implemented for storing, identifying, localizing and reusing Learning Objects (LOs) related to Chemistry and other Sciences.	The shared database, accessible by all federated servers, stores a map of the federation and an index of its content. The servers are peer entities and each server is responsible for its data, shared among the federation. The database contains the identifiers and addresses of all servers and the information about their status. The database also contains the metadata of all the objects belonging to the federation.

Project results, KPIs and the expected impacts of EINFRA-9:

Expected impacts of EINFRA9	Project results and KPIs
I1. To access advanced federated services tailored to user needs, thus supporting research innovation and efficiency through multidisciplinary scientific collaboration, supported by a robust strategy for training and dissemination.	• Increase access and usage of the e-infrastructures by scientific communities • Improve efficiency in the resource usage • Increase the number of users from project partners and external community researchers PKYs • Number of research communities using the developed Science Gateway **7/10/12** • Number of applications used by the user communities directly integrated with the project products **6/10/12** • External Research Communities using the products developed in the project **3/5/7**
I2. To produce innovative scientific results based on the use cases put forward by the communities.	• Publications of innovative results in the science related journals and magazines • Presentations given to the specific field-related conferences KPIs • Number of publications from partners **2/3/4** • Presentations specific area-related conferences and related contribution **20/30/40**
I3. To significantly widen the effective exploitation of complex data across communities by creating and making publicly available a set of value-added products built upon infrastructures and technological solutions supported by EC.	• Increase data sharing and collaboration between research communities thanks to the adoption of standards and standard metadata for the easy share among community databases • Offer the capability to easily share, discover, use and reuse the results of experiments in form of data sets and related information. • Increase discoverability of services through a service registry and marketplace KPIs • Number of use cases where open data can be published, discovered, used and reused among communities **3/5/7**

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	• Number of services included in the service registry **5/15/20** • Number of contribution to standards coming from project developments: **3/5/7**
I4. To address the following societal challenges: a. Climate action, environment, resource efficiency and raw materials, e.g. protecting the environment, sustainably managing natural resources, water, biodiversity and ecosystems b. Secure societies - protecting freedom and security of Europe and its citizens, e.g. to enhance the resilience of our society against natural disasters	• Increase access and usage of the e-infrastructures by scientific communities • Improve efficiency in the resource usage • Increase the number of users from project partners and external community researchers PKYs • Number of research communities using the developed Science Gateway **7/10/12** • Number of applications used by the user communities directly integrated with the project products **6/10/12** • External Research Communities using the products developed in the project **3/5/7**
I5. To identify and address the needs of large-scale (pan-european and world-wide) initiatives, e.g. ESFRI projects or others (e.g. SKA, EPOS, GEM,E-ELT) , extending the applicability of the platform to new communities to ensure long-term sustainability.	• Discover community requirements and collect feedback • Identify community specific services as well as general services to made available to the public KPIs • Number of external large-scale communities engaged **5/8/10** • Number of external large-scale communities that have adopted CMMST-VRE products by the end of the project **2/5/8**
I6. To exploit I1-I5 to develop innovative ways for engagement with cutting edge science of communities at large.	• Identify deneral e-infrastructures services and related providers • Identify community specific applications and tools • facilitate the interaction between users and resource provides by the provisioning of some operational tools • define proper pilot scenarios used for service validation activities, dissemination and demonstrations KPIs • Number of production sites supporting the project **15/25/50** • Number of applications used by the user communities directly integrated with the project products **5/10/12** • Number of communities and stakeholders contacted **50/80/100** • Number of knowledge transfer related events organized **20/30/40**
I7. Increasing the competitiveness and improving	• Strengthening the competitiveness and growth of

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innovation in EU.	companies by developing innovations • meet the needs of European and global markets by delivering such innovations to the markets. KPIs • Number of business cases elaborated **2/5/7** • Number of open source components made available to internal and external communities **5/12/20**

Barriers and obstacles

The impacts expected to be achieved by the CMMST-VRE results may be limited by a number of barriers and obstacles that exist on the way. The main barriers and obstacles identified so far are:

- The utility of advanced innovations delivered by CMMST-VRE will depend on intensive engagement with leaders in research communities and on their teams' cooperation during co-design, co-development and evaluation. The CMMST-VRE project will promote such communication among the partners and targeted communities in order to sustain their commitment.

- CMMST-VRE will make an intensive use of standards, from e-infrastructure usage to knowledge transfer among users. Unlikely, some (de facto) standards that will be adopted during the project lifetime (e.g. Cloud computing) are rapidly evolving ant it might be difficult to track these changes. However, the presence and experience of CMMST-VRE partners in both open standard bodies and in open source communities will minimize such a barrier.

- Limited capability for SMEs to obtain digital credentials to access e-infrastructures: The current EGI authentication mechanism requires the potential user to be affiliated to a university or research centres recognised by the EUGridPMA, thus making it very difficult for a potential researcher from the private sector to obtain a valid digital certificate. The science gateway for CMMST would mitigate this obstacle, thus simplifying collaborations with the industry.

- Different priorities for SMEs: this may limit the impact of the activity carried out by the CMMST-VRE among internal and external communities. The project will coordinate the efforts and the relations among SMEs and research communities promoting the opportunities to create awareness.

- CMMST-VRE will deliver products that will provide foundations for end users and science developers alike to exploit the provided e-infrastructures. Changes in EC support for what regards future e-infrastructure developments can be an obstacle to the adoption or consolidation of the project outcomes. As an example, the decreased EC support to European infrastructures leads to the forced adoption of other, non-European, solutions.

2.2 Measures to maximise impact

VREs are expected to result in a community (or set of communities) enhancement of (a) collaboration, (b) creativity, efficiency and productivity because designed to increase reliability and accessibility of resources and reliability, accessibility and re-usability of data (this is particularly true for fragmented communities such as the CMMST ones). Moreover, in the case of the CMMST VRE the built-in feature of adopting the synergistic model will lead to an even larger enhancement of collaboration, creativity, efficiency and productivity thanks to the possibility of:

- rewarding development, collaboration and servicing offered by the members of the community in terms of credits

- supporting sustainability via the transformation of credits into a better use of the community resources (including the financial ones).

These features will accelerate innovation in research via their user driven character and enable researchers to work in virtual and/or ubiquitous workspaces. They will contribute to increased take-up of collaborative research and data sharing by new disciplines, research communities and institutions. As a result, over time

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VREs will build an increasing number of generic services delivered by e-infrastructures and domain specific services co-developed and co-operated by researchers, technology and e-infrastructure providers. This will make dissemination, communication and exploitation activities crucial for the long-term sustainability of the project. These activities, in fact, will target project partners and external researchers, as well as any scientific or industrial body interested in intermediate and final results of the project. Accordingly, a structured plan for dissemination of results and exploitation will be developed and implemented during the project in order to support an effective sharing of the results within all relevant actors, the wide pan European user communities, as well as across other research and business communities.

In this respect, the possibility of converting credits into financial resources, will further enhance sustainability and the possibility of establishing relations with commercial vendors.

2.3 Dissemination and exploitation of results

Here we provide a draft plan for the dissemination and exploitation of the project's results by considering measures to be implemented both during and after the project.

Dissemination and exploitation of project's results will play a special role in the project: WP02 will take care of such aspect by setting-up the strategies to guarantee the maximum impact and sustainability beyond the project lifetime. Moreover, WP02 and WP03, in coordination with the other scientific and technological WPs, will collect and analyze the requirements coming from the project partners developers and will liaise with the project technical management to ensure that the requirements are adequately prioritized in the development technical plans, thus maximizing the interoperability with the existing e-infrastructures.
Besides the technical effort to streamline the adoption of the CMMSR-VRE products by other communities **a sustainable exploitation of the outcomes is only assured if the research communities use them**. Any networking strategy addressed to expanding the user base of CMMST-VRE products among research communities needs to take into consideration the organizational possibilities and constrains of the research sector. The Consortium here counts on the strong support of the different and well established research institutions plus, as well, of a pool of SMEs which will act as conduit of the new services towards those communities outside the project initiative.

About exploitation and business opportunities, WP09 maily composed by the SMEs participating in the project, will establish and maintain a set of exploitation activities in a structured and systematic way in order to provide appropriate business models to bring the services outcomes to the market and ensure a profitability and a financial sustainability of the project.

The results of the CMMST-VRE activities (knowledge or products) will be the property, either individual or collective, of the partners who created them; the software developed will be open source and will adhere to a Creative Commons CC-BY type of license.
Articles resulting by the project activities may be submitted to peer-reviewed scientific journals; the project will define appropriate policies to ensure either green or gold open access to them.

Several dissemination and **outreach actions** will rely on some regular activities of both the project and on some initiatives undertaken by the communities stakeholders EUCHEMS, ECTN, ITN Consortium, etc.
As to regular activities of the project the main ones are the planned biannual conferences of the CMMST VRE aimed at managing the activities of the project workpackages. During such conferences, in addition to the mormal activities of the project, tutorials, workshops and training sessions devoted to dissemination will be held, as typical of the EGI conferences. Moreover, i twill be attempted to synchronise at least one biannual conference with an important initiative of the stakeholders (eg the conference of the Computational chemistry division of EUCHEMS (in 2015), of the International Conference of Computational Science and its Applications, of the Distributed Computing Workshop of ITN TCCM, of the ECTN (or other thematic specific) conferences in one of the following years (exact details will be given only after the related planning will have been consolidated).
The other biannual conference will be given a more market oriented bias by asking the SMEs participating to the project (see WP09) to organize CMMST oriented entreprenurship related events. This will enhance the possibility for the VRE of singling out what type of professional services can support its financial sustainability after the funding period.

Specific more focused training initiatives will be located during other specialistic conferences along the tradition of the 2014 training CMMST VRC grid event for molecular sciences held in March 2014. The

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presence of the project at other thematic conferences will be assured by reporting on the related work carried out by the members of the CMMST VRE. In particular the participation to the EUCHEMS conferences will assured the targeting of the project dissemination activities to different sectors (professional chemists, chemical industries, business representatives, politicians, public insitutions managers). At the same time the participation to ECTN activities will assure the targeting to the educational market. Moreover the participation to more focused schools and workshops (like those of the COST actions) will assure access to the technology transfer more variegated market. This will drive the assembling of specific e-learning materials by WP08 for Learning objects and self assessment sessions especially in the fields of operation of WP05 and WP07 which are already operating in contact with EUDAT and ELIXIR

Here we describe the proposed communication measures for promoting the project and its findings during the period of the grant.

The communication activities of the project will include the actions outlined in the dissemination plan drafted in the above section, but are not limited to it. CMMST-VRE Communications will build on the added values, lessons learned and relationships established to become a VRC during the EGI-InSPIRE project. The effort will be subdivided in two main areas: internal communications within the CMMST community and external communication to new users and potential stakeholders.

The internal communication activities aim to reinforce connections between the CMMST stakeholders as a way to promote effective synergies and build a sense of appreciation within the community itself. The key to accomplish this goal will be to coordinate and maintain efficient communication channels open between all the parties: members of the consortium, user communities, resource providers and competence centres. The main channels of internal communication will be established through a website where the CMMST activities as well as problem solving and brainstorming will be made available to the partners by means of:

- an easy to use web site offering content delivery in multiple formats as well as public and private areas;
- a newsletter published quartely containing reports and activity related WP and TB documents;
- an electronic magazine collecting results of research and experiences.

External communications will focus on disseminating the successes and outputs of the project to potential new stakeholders, such as new user communities, new resource infrastructure providers and new industry partners. This will be accomplished through targeted documentation and publications on national and international journals produced in cooperation among different members and WPs for specific goals. Event attendance will also play a role in the outreach activities to new stakeholders. Part of this external communications effort aimed at attracting new users will be directed to inform the wider, general audience (especially within the stakeholders) about the project's impacts and benefits. For this purpose use of the EUCHEMS (http://www.euchems.eu/news/euchems-newsletter.html) and ECTN (http://www.ec2e2n.info/) means of dissemination that guarantee an extremely broad external communication will also be made.
As a complement of the mentioned communication activities, the project will support scientist proficient in the use of e-infrastructures services for their research who will travel to events specific to their own field to present the achievements of CMMST-VRE to their peers. This activity has been pioneered within the EGI-InSPIRE project under the definition of Research Champions programme and will be reused in the present context.

2.4 Consortium as a whole

Here we describe the consortium, how it will match the project's objectives and how do the members complement one another (and cover the value chain, where appropriate)? In what way does each of them contribute to the project? How will they be able to work effectively together?

The Consortium combines a fairly large set of ICT technology experts, HW and SW providers and users together with several CMMST researchers belonging to about 40 different institutions. Among the ICT experts the main ones are the leaders of WP02 (EGI.eu, the manager of the European Grid Infrastructure), of WP03 (INFN a leading European community expert in grid cloud computing), MTA-SZTAKI (expert in gateways and workflows) and the Centre for Parallel Computing (CPC) of the University of Westminster (expert in running scientific experiments on computing infrastructures). CPC and INFN know how bridges ICT competences with the CMMST ones of the experts which couple scientific interests with a high level of

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ICT competence. This is, indeed, the case of ENEA and INSTM. Within the consortium the two expertise are combined at various levels and for different CMMST and ICT aspects as well illustrated by the enclosed user profiles. The CMMST community has in fact a large tradition in developing computational applications and in managing its own local platforms. As already mentioned in the proposal this peculiarity of the CMMST communities turns out to be a strength when considering distributed platforms and represents a solid cultural background for establishing the synergistic model. Moreover, the fact that CMMST methodologies have at present reached such a high level of accuracy and multiscale nature to be suited for carrying out realistic simulations of several technological applications makes the proposed VRE suitable an extended adoption of a credit economy and its conversion into a business model.
This is testified by the significant number of SME partner of the consortium and for their variegated activities ranging from materials to biomedical, energy, education etc. applications.

2.5 Coompute resources

The core compute resources committed to the project are those of the block of the partners of the project offered either as part of the EGI high-throughput platform or as platform of individual institutions.
A second block is the one offered by the members of the project external to EGI (like ENEA and INSTM as well as those of other resource providers including SMEs).
The third one is a block of resources for which during the project lifetime MoUs will be signed following either an application or a bid.

Belong to the first block the EGI high-throughput platform is a global high-throughput data analysis infrastructure, linking hundreds of independent research institutes, universities and organisations delivering top quality computing resources. As of January 2015, EGI offers more than 370,000 CPU cores of installed computing capacity interoperating through the Unified Middleware Distribution and supporting about 1.8 million computing jobs per day. Within this platform resources are allocated to 'Virtual Organisations' (VOs). Each VO represents a scientific community and the resources these communities have access to among those of the production infrastructure. The computational chemistry community operates in EGI through 6 VOs and several regional VOs (like the VO of Central Europe).
To the same block belong the INFN Resources. The INFN divisions involved in CMMST-VRE are CNAF (located in Bologna), Bari, Catania, Padua. All five sites have leading national expertise in the field of distributed computing, have a long experience in the development of software services for e-Infrastructures and are actively contributing to several EU and international projects. In particular, CNAF is the INFN National Center for Research and Development in informatics and hosts the INFN National Computing Center (called "Tier-1"), managing more than 15 TB of disk space, about 18 TB of tape space, about 15.000 CPU cores, and serving more than 20 international scientific collaborations. Padua, Bari and Catania are all national medium sized centers ("Tier-2") with several hundreds of terabytes of disk space and thousands of CPU cores each. All INFN centers are connected through the high-speed GARR-X network and to international networks via multiple 10 Gigabit links. Also belonging to that block MTA SZTAKI that operates a cloud infrastructure based on OpenNebula (that is part of the EGI Federated Cloud), the Westminster Campus Desktop Grid of CPC (2000 desktop computers connected in a BOINC-based desktop grid), IBERGRID, NGI LT and CESNET NGIs (as mentioned in the enclosed LoS).

To the second block belong the resources of ENEA and INSTM which are large Institutions of specific CMMST competences operating on different platforms as indicated in the related LoS and which are ready to make their reources and know how available for the project.

Finally to the third block belong CINECA (for PRACE, see LoS) as well as other Computer centers and research institutions (see also in this case some LoS) wich are ready to commit resources once the project is approved by signing specific MoUs. As an example we quote here:

Świerk Computing Centre (CIŚ) is situated at National Centre for Nuclear Research (NCBJ) in Świerk near Warsaw and is a High Performance Computing centre which provides computational resources and expertise in parallel computing and big data processing for activities performed at NCBJ especially IT support for Polish nuclear energy and related fields of science and technology such as computational fluid dynamics, nuclear physics, high energy physics,

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astrophysics, medical imaging, complex systems and big data analyses. CIŚ also hosts an EGI certified GRID computing site and is a Tier2 site for CMS (Compact Muon Solenoid) and LHCb experiments. Computational resources currently available at CIŚ consist of 13760 cores, 83456 GB RAM and disk space of more than 3PB. Cluster is equipped with the QDR+FDR Infiniband and 10Gbps interconnect. For the needs of the LHC experiments, we provide 320 computing cores, 1280 GB RAM and more than 300 TB of storage space. The theoretical performance of CIŚ cluster is 285 TFLOPS.

CRO NGI resources are currently mainly used by users from computation chemistry field. In the long term we foresee significant increase in resource needs from this community. Top applications used on the infrastructure are: Abinit, Gaussian and Turbomole. Besides for deployment and maintenance of applications, CRO NGI experts helped users in preparing scripts needed for optimal utilization of grid resources. CRO NGI infrastructure currently consists of more than 1800 processor cores, 36 GPUs and 110 TB of disk storage on five grid sites. In addition there is an EGI FedCloud site with 160 processor cores. In the following years we plan to expand the infrastructure significantly, at least by the order of magnitude
SZTAKI

Section 4: Members of the consortium

The CMMST-VRE participants are described in the following sections.
Besides the consortium members, a significant number of external parties considers CMMST-VRE activities and their expected results very important. This is testified by the several Letters of Support to the project received by the CMMST-VRE project coordinator. They are summarized in the following list and have been included in Annex III.

CMST-VRE received Letters of Support from:

1) Sanzio Bassini, Director of SCAI (Supercomputing Applications and Innovation) Dept., CINECA Interuniversity Consortium, Italy
2) Brane Leskosek, Head of the Slovenian ELIXIR node, Slovenia
3) Jorge Gomes, IBERGRID and Portuguese NGI representative, Portugal
4) Jan Jona Javoršek, SLING deputy manager of the Network administration centre of Jožef Stefan Institute, Slovenia
5) Miroslav Ruda, Grid Dept. Manager, CESNET and MetaCentrum NGI, Czech Republic
6) Ivan Maric, University Computing Centre University of Zagreb, Croatia

4.1. Participants (applicants)

4.1.1 INSTM

Description of the legal entity
INSTM (http://www.instm.it/) is the largest Italy based CMMST consortium of Universities and Research Institutes combining different scientific and technological (science and engineering) communities carrying out research and producing innovation in the field of Atomic, Molecular and Materials sciences and technologies. From the date of its foundation (1992) INSTM has either managed or been partner of over 200 national and international projects with related activities having led to the publication of over 4000 papers of which over 60% excellent in the field of nano- and Micro-systems.
Research lines of the consortium are:
Design materials with special electric and magnetic properties with particular focus onto microelectronics, optoelectronics and photonics. Develop Carbon based materials with specific

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focus onto deposition on non conventional materials, Study non equilibrium chemical systems and processes treatments with particular focus onto combustion, atmosphere, lasers, chemical plasmas, spacecrafts, Investigate Chemistry under extreme conditions investigations with particular focus onto high pressure and/or high temperature reactions, Assemble new technologies with chemical with particular focus onto formation of ionic species relevant to plasma, laser, interstellar, high atmosphere, surface chemistry, vapour deposition and microlithography., Model polymeric systems and soft matter, Compute Electronic structure of inorganic materials with particular focus onto catalytic effects and innovative materials design.
The Perugia node (NetSC-UP, Networked Scientific Computing - University of Perugia) consists of the following groups: CDK (Computational Dynamics and Kinetics) University of Perugia, TCIC (Theoretical and Computational Inorganic Chemistry) University of Perugia, HPC (High Performance Computing) University of Perugia, CNR ISTM (Institute of Molecular Science and Technologies).

Key people

Antonio Laganà [M] He is Professor of Chemistry at the University of Perugia and is at present member of the Italian Qualification Committee for University Professors in Chemistry, chair of the Standing Virtual Education Community of ECTN Association, of the Computational Chemistry Division of EUCHEMS. He has been member of the domain committee (and previously of the technical committee) of COST CMST, Director of the Department of Chemistry of the University of Perugia, Director of the University of Perugia Centre for Computer Science and Services, President of the Italian Interdivisional Group of Computational Chemistry.His scientific interests have progressed from the very beginning on a double track: a) high performance computational technologies for molecular science applications and b) development of theoretical and computational approaches for gas phase and molecular dynamics of both simple and complex systems.
For this he has designed and implemented specific numerical algorithms and computational procedures necessary for the assemblage of ab initio accurate complex simulations. These codes have been restructured to efficiently run on massively parallel computers and distributed concurrent environments.
In addition, a problem solving environment has been designed to allow the management of an a priori molecular simulator on the grid. Educational aspects of these research lines are being pursued by developing web based computer assisted teaching and learning and virtual chemical laboratories.
Most of the mentioned investigations have been started or developed during his visits to laboratories of international research centres (like CECAM (Orsay and Lyon), ECSEC (Rome), LANL (Los Alamos), TRIUMF (Vancouver), CALTECH (Pasadena), FORTH (Crete)) and of Universities (like Cambridge, Barcelona, Manchester, Salamanca, Bristol, Nancy). Other important collaborations have been established with some national research laboratories and Universities and with the local Department of Mathematics and Computer Science as well. The research activity of Prof. Laganà has resulted in the publication of about 400 papers in scientific Journals, the authoring or editing of 9 books, the organization of several national and International Schools as well as the delivery of numerous scientific seminars at various institutions and communications at national and international conferences.

Gaia Grossi [F] She is full professor of Inorganic and General Chemistry. Her main skill is the formal derivation of quantum scattering equation and Hyperspherical harmonic expansions. She has developed numerical techniques for basis transformation in few body angular momenta.

Piero Casavecchia [M] He is full professor of Physical Chemistry. His main skill is the management of crossed molecular,beams experimental apparatuses for single collision reactions. He is teacher of Chemical Kinetics. He is member of the editorial board of ChemPhysPhysChem

Nadia Balucani [F] She is Associate professor of Inorganic and General Chemistry. Her main skill is the management of crossed molecular,beams experimental apparatuses for single collision differential cross sections. She is coordinator of the Astrochemistry activities

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Fernando Pirani [M] He is full professor of Inorganic and General Chemistry. His main skill is the management of gas molecular,beams experimental apparatuses for total cross sections. He is member of the Institute of Structure of Matter

Simona Cavalli [F] She is Associate professor of Inorganic and General Chemistry. Her main skill is the formal derivation of quantum scattering equation and Hyperspherical harmonic expansions and the development of numerical techniques for dealing with reactive systems.

Andrea Lombardi [M] He is Doctor in Chemistry, His main skill is the development of codes for classical and semiclassical state to state collision probabilities in gas phase reactive and non reactive systems

Stefano Crocchianti [M] He is Doctor in Chemistry, His main skill is the development of codes for simulation of pollutants production in the atmosphere

Carlo Manuali [M] He is Doctor in Computer science and responsible for the Perugia compute node, His main skill is the management of networked compute systems

Sergio Rampino [M] He is Doctor in Chemistry, His main skill is the development of codes dealing with relativistic systems.

Relevant publications, and/or products, and/or services

- A priori modeling of chemical reactions on computational grid platforms: workflows and data models, Chemical Physics 398, 192-198 (2012), DOI 10.1016/j.chemphys.2011.04.028; 3.33 IF
- M. Bartolomei, F. Pirani, A. Lagana', A. Lombardi, A full dimensional Grid empowered simulation of the CO2 + CO2 processes J. Comp. Chem. (ISSN:0192-8651), 33, 1806–1819 (2012); 4.58 IF (Q1)
- A. Lagana', E. Garcia , A. Paladini, P. Casavecchia, N. Balucani, The last mile of molecular reaction dynamics virtual experiments: the case of the OH (N=1-10) + CO (j=0-3) -> H + CO2 reaction, Faraday Discussion of Chem. Soc. 157, 415 - 436 (2012); doi: 10.1039/c2fd20046e; 5.00 IF
- A. Costantini, R. Murri, S. Maffioletti, A. Lagana', A Grid execution model for Computational Chemistry Applications using the GC3Pie framework and the AppPot VM environment, Lecture Notes Computer Science 7333, 401-416 (2012)
- S. Tasso, S. Pallottelli, M. Ferroni, R. Bastianini, A. Lagana', Taxonomy management in a Federation of Distributed Repositories: a chemistry use case, Lecture Notes Computer Science 7333, 358-370 (2012)

Relevant previous projects or activities

- FP7-INFRA-2007 Enabling Grid for E-Science III (EGEE III): UNIPG (INFN) computational chemistry cluster, member
- FP7-INFRA2010-1.2.1 European Grid Initiative: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe (EGI-Inspire): COMPCHEM VO coordinator
- FP7-SPACE-2009-1 Planetary Entry Integrated Models (Phys4entry) EChem-TC-Valorisation of EChemTest testing centers (504854-LLP-2009-GR-KA4-KA4MP)
- PRIN 2008: Teoria misure e simulazioni di processi, dinamiche ed interazioni molecolari, coordinatore di unità operative EChem-TC-Valorisation of EChemTest testing centers (504854-LLP-2009-GR-KA4-KA4MP)

Relevant infrastructure to the proposed work

NetSC-UP (Networked Scientific Computing - University of Perugia) node of its CST taking care of the links with EGI, PRACE and XSEDE, establish collaboration with related Virtual Organizations and Research Communities. NetSC-UP computational resources consist respectively of three clusters of 240, 392 and 388 cores interconnected via a switch infiniband 40Ghz and gigabit Ethernet cupper UTP, 2 nodes E4 7116 Supermicro motherboard remote management and

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console IPMI 2.0, 24Gb RAM DDR3-1333, 16 dual processor Intel Xeon E5670, 2.40Ghz, 4 core, 12Mb cache, both interfaced to a NVIDIA Tesla S2050 1U, 4GPU Fermi S2050, 3Gb RAM per GPU, 16 core double precision Intel

4.1.2 ARCTUR

Description of the legal entity
Established in 1992, Arctur has progressed to become the main Slovenian commercial supplier of HPC (High Performance Computing) services and solutions. Arctur has its own HPC infrastructure to be used as the technological foundation for advanced HPC and Cloud computing solutions and innovative web services in a distributed, high-redundancy environment. The company has extensive experience in server virtualization and deployment, integration of disparate IT-systems, IT support of project-management and server farm leverage for the deployment of Software as a Service (SaaS), specialised for small and media enterprises (SME).
Understanding the importance of continuous progress, Arctur has its own R&D department, registered with the Slovenian Research Agency (ARRS). Arctur is involved in joint R&D projects with research institutes, universities and other R&D organizations from EU and globally, currently we are partners in two FP7 projects from I4MS initiative: Fortissimo and CloudFlow. The research areas covered are directly implemented in various real-life solutions and products, e.g. web and mobile applications, easy to use interfaces for HPC, ICT security and Cyber Physical Systems. Other research areas include applied mathematics, numerical simulations, advanced statistics, and HPC/Cloud computing.

Key people
Tomi Ilijaš [M] is founder and president of Arctur and he holds a BSEE degree from Ljubljana University. Mr. Ilijaš is an entrepreneur with focus on Hi-Tech innovation and has shared his knowledge and experience to many start-ups and spin-offs in the region. Recently he is researching new business models in HPCaaS and successfully breaking the barriers in bringing HPC to manufacturing SMEs.

Martina Murovec [F] is COO of Arctur and holds a Bachelor's in business and management from University of Primorska. Ms. Murovec has an extensive experience in managing international projects in multicultural environment and leading virtual project teams.

Marko Kobal [M] is Arctur's CTO. He holds a degree in Computer Sciences from Ljubljana University. In last years, Mr. Kobal is intensively involved in High Performance Computing and Cloud Computing, development of algorithms based on applied mathematics, and research in the area of code parallelization. He will lead Arctur's contribution to the technical work.

Relevant publications, and/or products, and/or services
- HPC Puppet: a system for automated running of users' solutions on preconfigured HPC infrastructure.

Relevant previous projects or activities
- Fortissimo (FP7-2013-NMP-ICT-FoF): Fortissimo is a collaborative project that will enable European SMEs to be more competitive globally through the use of simulation services running on a CloudHPC infrastructure.
- CloudFlow (FP7, FoF-ICT-2013.7.1): CF will enable the remote use of computational services distributed on the cloud, seamlessly integrating these within established engineering design workflows and standards.
- NU.SIM.O (National Research & Infrastructures Scheme, 2009 - 2011): Project included development of market-oriented application for numeric simulations in composite materials industry, including setting up of a HPC infrastructure.

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Relevant infrastructure to the proposed work
Arctur's HPC infrastructure is a high-performance, on-demand and scalable HPC environment that was built, configured and optimized for speed and performance.
Compute power available to the project:

- 10 TFlops of processing speed
- IBM iDataPlex dx360 M3 (dual socket) servers
- Intel Xeon X5650 processors (6 cores @ 2,66 GHz)
- 32 GB RAM per server
- 1008 CPU-cores and 2,66 TB RAM

Storage:
Arctur provides Lustre high-performance parallel distributed file system to support large scale cluster computing. Current version used is 2.2. Lustre storage system is built from a high-availability configured MDS node and 20 OSS nodes, providing both high capacity and high IOPS for demanding IO operations
Network:
Arctur's infrastructure has Infiniband QDR 40 Gbps internode connectivity to ensure the highest performance levels with low latency to meet the needs of your most demanding software. Our data centre is strategically positioned on the national fiber-optic backbone, with redundant high speed Internet connections to ensure that data can be quickly uploaded to and downloaded from our environment.
Data Centre:
In the Arctur Data Centres, we offer hosting of virtual and physical servers, colocation for all server types as well as rack space hosting. Efficiently cooled and secured locations with redundant electrical and internet sources offer high availability (>99.98%). We have two Data Centres, one in Ljubljana (central Slovenia) and one in Gorjansko (west Slovenia), connected with dark fibre. This ensures the distribution of data and the possibility of a geographically independent colocation.

4.1.3 CCWE

Description of the legal entity
The University of Westminster is a public research university in London, United Kingdom. Westminster's academic activities are organised into seven faculties and schools, within which there are around 45 departments and 65 research centres. Westminster had an income of £170.4 million in 2012/13, of which £4.5 million was from research grants and contracts. The University of Westminster will be represented in the CMMST consortium by the Centre for Parallel Computing (CPC). The Centre has two missions. First, it is a centre of excellence in high-performance parallel computing. Second, it collaborates and supports research communities and teams within and outside the University to create and run scientific experiments on computing infrastructures. The Centre's major research activities incorporate research in Distributed Computing Infrastructures, particularly in cloud computing and desktop and service grids. As high-performance computing and data intensive applications are gaining strategic importance in all research disciplines it is crucial that CPC supports inter-disciplinary activities. CPC elaborated first, the Grid Execution Management for Legacy Code Applications (GEMLCA) next, the SHIWA Submission Service to enable execution of legacy code applications as services. CPC made a major contribution to the development of Coarse-Grained Interoperability (CGI) to support sharing workflows of different workflow systems. The CGI concept uses these services and the repository framework designed and implemented by CPC. Examples of the repositories based on this framework are the SCI-BUS Portlet Repository and the SHIWA Workflow Repository. The latest research focuses on workflows execution on the cloud using workflow and workflow system virtualisation.

Key people
Prof. Dr Gabor Terstyanszky [M] is a Professor in Distributed Computing at the, University of Westminster. His research interests include distributed and parallel computing, cluster and Grid computing. He supervised several European projects, such as: COPERNICUS, COST, WINPAR, HPCTI, and SEPP as local coordinator. He had a leading role in the FP7 EDGeS, DEGISCO, EDGI, SHIWA, SCI-BUS, ER-flow research projects. He published more than 130 technical papers at conferences and journals. He was member of programme committees of several conferences and workshops.

Dr Tamas Kiss [M] is a Reader in Distributed Computing, and a principal researcher at the CPC. He holds a PhD in Distributed Computing. His research interests include distributed and parallel computing, cloud, cluster and grid

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computing. He has been involved in several FP research projects such as CoreGrid, EDGeS, EDGI, SHIWA, and SCI-BUS, and FP7 support action projects such as DEGISCO, ER-flow and IDGF SP. He led and coordinated the application support activities and work packages in these projects. Currently, he is Project Coordinator of the FP7 CloudSME Project developing a cloud-based simulation platform for manufacturing and engineering SMEs. He co-authored one book and more than 80 scientific papers in journals, conference proceedings and as book chapters.

Relevant publications, and/or products, and/or services

- P. Kacsuk, T. Kiss and G. Sipos: Solving the Grid Interoperability Problem by P-GRADE Portal at Workflow Level, in Future Generation Computing Systems: International Journal of Grid Computing: Theory, Methods and Applications, Vol. 24, Issue 7, July 2008, pp 744-751,
- G. Kecskemeti, G. Terstyanszky and P. Kacsuk: Virtual Appliance Size Optimisation with Active Fault Injection, in IEEE Transactions on Parallel and Distributed Systems, October 2012, Vol. 23, No. 10, pp. 1983-1995,
- G. Kecskemeti, G. Terstyanszky, P. Kacsuk and Zs. Nemeth: Increasing Virtual Appliance Delivery Efficiency Through Minimal Manageable Virtual Appliances, in IEEE Transactions on Services Computing. 2013, ISSN 1939-1374
- G. Terstyanszky, T. Kukla, T. Kiss, P. Kacsuk, A. Balasko and Z. Farkas: Enabling scientific workflow sharing through coarse-grained interoperability, in Future Generation Computer Systems, http://dx.doi.org/10.1016/j.future.2014.02.016
- T. Kiss, P. Greenwell, H. Heindl, G. Terstyanszky, N. Weingarten, Parameter Sweep Workflows for Modelling Carbohydrate Recognition, Journal of Grid Computing, volume 8, number 4, pp 587-601, DOI: 10.1007/s10723-010-9166-8, 2010

Relevant previous projects or activities

FP7 research projects on cloud and grid computing:

- CloudSME: Cloud-based Simulation Platform for Manufacturing and Engineering, Project Coordinator, contract no. 608886
- SCI-BUS: Scientific Gateway Based User Support, contract no. 283481
- SHIWA: Sharing Interoperable Workflows for Large-Scale Scientific Simulations on Available DCIs
- EDGI: European Desktop Grid Initiative
- ER-flow: Building an European Research Community through Interoperable Workflows and Data

Relevant infrastructure to the proposed work

- Cloud cluster - cloud resource of 32 nodes with sixteen cores using the OpenStack middleware
- GPU cluster - 10 CPU nodes and 20 GPU
- Westminster Campus Desktop Grid - 2000 desktop computers connected in a BOINC-based desktop grid

4.1.4 CHFI

Description of the legal entity

The Department of Chemistry "Ugo Schiff" ranks among the largest Departments of the University of Florence. Presently, the academic staff consists of more than 90 scientists involved in teaching duties in Bachelor and Master degree courses of several Schools, including the School of Mathematical, Physical and Natural Sciences, the School of Human Health, the School of Agricultural Sciences and the School of Engineering. The research interests are distributed over a fairly high number of chemical areas, the most relevant for the present project are Theoretical and Computational Chemistry, Molecular Spectroscopy, Nanotechnology and Drug Design. The Chemistry Department run the Doctorate in Chemical Sciences. Many of the people of the unit of Firenze involved in the present project are also associated to the LENS (Laboratorio Europeo for Non linear Spectroscopy),a European reference point for research with light waves.

Key people

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Prof. Gianni Cardini [M] Born in Firenze il 17/07/1956. Gender: Male. He obtained the Laurea in Chemistry from the University of Firenze the 17/07/1981. From September 1983 to May 1985 he worked in the Chemistry department of the University of Lethbridge (Alberta, Canada) with Prof. S.F.O'Shea and from July 1987 to April 1988 in the Chemistry Departement of the Univerity of Pennsylvania with Prof. M.L. Klein. Gianni Cardini obtained the PhD in Chemistry on September 1989. He become Researcher in the Chemistry Department of the University of Firenze the 31st of May 1990. From 1/02/2000 to 30/12/2004 has been Associate Professor in Chemical Physics, Department of Chemistry University of Firenze. He has been in charge as president of the consiglio di corso di laurea in Chemistry for the period 2003-04/2005-06. From 30/12/2004 is full Professor of Chemical Physics in the Chemistry department of the University of Florence. From November 2007 to 2009 has been the coordinator of the PhD program in Chemistry. He was Visiting Professor at the University of LiLLe I (2012). Gianni Cardini has published more than 100 paper on computational and theoretical chemistry on first class journals.

Dr. Riccardo Chelli [M] Born in Pelago, Italy, 28 April 1969. Gender: Male; Citizenship: Italian.; Title: PhD in Chemistry. 1996: Degree in Chemistry at the University of Firenze(Italy). 2000: PhD in Chemistry at the University of Firenze. 2004: Visiting researcher at the Dept. of Chemistry of the University of California, Irvine (USA)(laboratory of the Prof. Shaul Mukamel). 2000- 2009: Postdoctoral position at the Department of Chemistry of the University of Firenze. 2009-Today: Permanent researcher at the Department of Chemistry of the University of Firenze.Research Interests and Scientific Activity: Development of numerical schemes for the phase-space sampling and to compute chemical-physical properties via computer simulations. Theoretical aspects of nonequilibrium thermodynamics. Development of polarizable force fields for computer simulations. Molecular modeling of systems of biochemical and biophysical interest. Dynamical and structural properties of isolated molecules, molecular clusters and condensed phases via molecular mechanics/dynamics and quantum mechanical calculations. Development of models for the interpretation or the prediction of optical spectra.

Prof. Piero Procacci [M] Born in 1961. Citenzenship: Italian. Gender: Male. Marital status: Married. Education: June 1986 Master in Chemistry (Italian "Laurea") Florence University; February 1993 Doctorate in Chemistry Florence University. Employments:January 1988 - August 1989, Associate Researcher,IBM corporation, Kingston NY (USA); July 1993 - June 1994, Postdoctoral Fellow Columbia University, Dept. of Chemistry, New York, (USA); October 1994December 1996, Postdoctoral Fellow CECAM, Ecole Normale Superieure, Lyon (FRANCE); January 1997 - Sept 2001 Lecturer at Florence University, Chemistry Dept. Sept 2001 – Associate Professor at Florence University Chemistry Dept. Research: Dynamical and structural properties of condensed phases; Molecular dynamics of biological systems; Molecular dynamics tools (integrators and polarizability FF); Anharmonic properties of molecular crystals.

Relevant publications, and/or products, and/or services

- J. Chem. Theory Comput. 2014, 10, 953
- J. Chem. Theory Comput. 2014, 10, 42
- J. Chem. Phys. 2014, 140, 064104
- J. Comput. Chem. 2010, 31, 1106.
- J. Chem. Theory Comput. 2011, 7, 1109

Relevant previous projects or activities

- PRIN 2007
- ISCRA projects (CINECA): CHOSM, AIMSUP, MOLD2D

Relevant infrastructure to the proposed work

- 2 linux clusters 8 nodes each
- IBM Bladecenter H, 12 blades PWR6 JS22 (Type 7998) (OS AIX)

4.1.5 CHRO

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Description of the legal entity

La Sapienza University of Rome, founded in 1303 by Pope Boniface VIII, is one of the oldest universities in the world and a high performer among the largest universities in international rankings.

Sapienza offers a vast array of courses including degree programmes, PhD courses, one to two year professional courses and Specialization Schools in many disciplines, run by 63 Departments and 11 Faculties. In the year 1934-, at the Royal University of Rome was already possible to complete degrees in Chemistry, Mathematics, Physics, Natural Sciences and double majors in Maths plus Physics. The Department of Chemistry is now part of the Faculty of Mathematical, Physical and Natural Sciences and promotes scientific research thanks to researchers working in different areas : analytical chemistry , physical chemistry , industrial chemistry , inorganic chemistry and organic chemistry. The current Department of Chemistry of the Faculty of Natural Sciences is thus an organisation that coordinates a research and teaching community of about 120 staff members. The Ph.D. program consists of a 3-years research program. This is the largest of the Chemistry Schools within the complex University system now operating in the area of Rome and of its immediate environments. The theoretical chemistry group of this department which has been dealing for many years with a broad variety of theoretical problems and computational tasks related to the study of elementary dynamical processes which occur in a molecular gas has always been very active in many research fields ranging from high quality ab-initio computations to biophysical modeling.

Key people

Enrico Bodo [M]

Education

- 2013: Qualification for associate professor in Inorganic Chemistry and in Physical Chemistry (Abilitazione Scientifica Nazionale)
- 2004-2011. Collaborator and short term visitor at ITAMP (Harvard Smithsonian Center for Astrophysics) (Cambridge Massachusetts, USA).
- 2004-today: Lecturer at the university of Rome La Sapienza in the Chemistry Department.
- 2002-2004: PostDoc in the theoretical chemistry group of Prof. Gianturco at the University of Rome "La Sapienza".
- 2001: Visiting Fellow at ITAMP (Harvard Smithsonian Center for Astrophysics) (Cambridge Massachusetts, USA).
- 1999-2001: PhD in Chemistry, at the University of Rome La Sapienza – Dissertation title: The Lithium chemistry in the early Universe: quantum treatment of interactions and dynamics.
- 1998: Laurea (Master's Degree) in Chemistry at the University of Rome "La Sapienza" (magna cum laude).

Organization and teaching activities

- 2014 Coordinator and project leader of an European PRACE computational grant for a total of 27,000,000 hours.
- 2013 Coordinator and project leader of an European PRACE computational grant for a total of 18,000,000 hours.
- 2011 Coordinator and project leader of a research grant of 80000 Eur and two post-Doc contracts at the University of Rome La Sapienza.
- 2004-today Holder of various courses for undergraduates in the Master Degree in Chemistry at the University of Rome.

Marco D'Abramo [M]

Education and Research

- 2014-today: Rita Levi Montalcini fellow, Senior associate researcher (RTD/B), Dept. of Chemistry, Sapienza University.
- 2013: Qualification for associate professor in Physical Chemistry (Abilitazione Scientifica Nazionale)
- 2013-2014: "FIRB giovani" fellowship (Head of the computational unit), CINECA, Italy.
- 2009-2011: Staff Scientist at Cancer National Research Center, Madrid, Spain.

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- 2007-2009: PostDoc in the group of Prof. M. Orozco, joint IRB/Universitat de Barcelona, Spain.
- 2004: HPC-europa Fellow at Barcelona Supercomputer Center, Barcelona, Spain.
- 2004-2007: PhD in Chemistry, at the University of Rome La Sapienza
- 2003: Laurea (Master's Degree) in Chemistry at the University of Rome "La Sapienza".

Organization and teaching activities

- 2014-today Holder of courses for undergraduates in the Master Degree in Geological Sciences at the University of Rome.
- 2013-2014 Head of the computational unit of the FIRB project.
- 2004-2007 Teaching assistant for Master in Bioinformatics (Sapienza University)

Relevant publications, and/or products, and/or services

- MoDEL (Molecular Dynamics Extended Library): a database of atomistic molecular dynamics trajectories. Meyer T, D'Abramo M, et al., Structure. 2010, 18, 1399-409.
- FlexServ: an integrated tool for the analysis of protein flexibility. Camps J, Carrillo O, Emperador A, Orellana L, Hospital A, Rueda M, Cicin-Sain D, D'Abramo M, Gelpí JL, Orozco M. Bioinformatics. 2009 2, 1709-10.
- Amino-acid anions in organic ionic compounds. An ab-initio study of selected ion pairs, A. Benedetto, E. Bodo*, L. Gontrani, P. Ballone and R. Caminiti, J. Phys. Chem. B, 118, 2471, (2014).
- A Prototypical Ionic Liquid Explored by Ab-initio Molecular Dynamics, E. Bodo*, S. Mangialardo, P. Postorino, A. Sferrazza, and R. Caminiti, J. Chem. Phys. 139, 144309 (2013)
- Structural properties of 1-alkyl-3-methylimidazolium bis{(trifluoromethyl)sulfonyl}- amide ionic liquids:X-ray Diffraction Data and Molecular Dynamics Simulations E. Bodo, L. Gontrani, R. Caminiti, N. V. Plechkova, K. R. Seddon and A. Triolo, J. Phys. Chem. B, 114, 16398, (2010).

Relevant previous projects or activities

- On-going Project: Amino-acid anions in organic compounds: exploring the boundary of room temperature ionic liquids (financed by "La Sapienza")
- MoDEL (Molecular Dynamics Extended Library): a database of atomistic molecular dynamics trajectories. http://mmb.pcb.ub.es/www/node/564
- Prace project No. 2013091962 Amino-acid anions in organic compounds: charting the boundary of room temperature ionic liquids.
- Prace project No. 2012071279 Ab initio molecular dynamics of lanthanides in protic ionic liquids
- HPC-Europa2 project no. 982: "Free-energy landscape of Intrinsically Disordered Protein regions".

Relevant infrastructure to the proposed work

Local cluster of the Department of Chemistry (12 nodes, mixed architecture CPU-GPU)

4.1.6 CHSA

Description of the legal entity

The main legal entity will be the Department of Chemistry and Pharmacy of the University of Sassari, Italy. The activities of the Department address research in various fields of chemistry and physical chemistry, and provide teaching at both graduate and post-graduate level.

This Department produces, every year, about 100 original articles in international peer-reviewed journals. The research groups working in this department have a strong tradition in the fields of computational chemistry, organic and inorganic synthesis, and pharmaceutical research. In particular, simulations on nanoporous materials have been performed since the advent of modern computers. All this generates a stimulating and productive environment for cutting-edge research.

Key people

Prof. Pierfranco Demontis [M], is a highly acclaimed and well recognized expert on the development of classical force fields for microporous materials for the study of adsorption, diffusion and other properties in zeolites.

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In the group, composed by Prof. Giuseppe B. Suffritti (male), Dr. Andrea Gabrieli (male), Dr. Marco Sant (male), and Dr. Federico G. Pazzona (male), there are experts in first principles calculations on a wide variety of problems, classical molecular dynamics and Monte Carlo computations, and coarse-grained models like Cellular Automata. Finally, the group has an extensive knowledge of various computing platforms (multicore, GPGPU), of code development and porting, and of cluster administration and maintenance.

Relevant publications, and/or products, and/or services

- A. Gabrieli, M. Sant, P. Demontis, and G. B. Suffritti, "Fast and efficient optimization of Molecular Dynamics force fields for microporous materials: Bonded interactions via force matching", Microporous Mesoporous Mater., 197 (2014), 339;
- P. Demontis, J. Gulín-González, M. Masia, G. B. Suffritti, "Distributions of single-molecule properties used for studying dynamical heterogeneities in nanoconfined water" The Journal of Physics: Condensed Matter, 26 (2014), 155103;
- Malay K. Rana, Federico G. Pazzona, Giuseppe B. Suffritti, Pierfranco Demontis, Marco Masia, "Estimation of Partial Charges in small Zeolite Imidazolate Frameworks from Density Functional Theory Calculations", J. Chem. Theory and Comput. 7 (2011), 1575;
- A. Gabrieli, M. Sant, P. Demontis, and G. B. Suffritti, "Development and Optimization of a New Force Field for Flexible Aluminosilicates, Enabling Fast Molecular Dynamics Simulations on Parallel Architectures", J. Phys. Chem. C 117 (2013), 503;
- B. Zheng, M. Sant, P. Demontis, G. B. Suffritti, "Force Field for Molecular Dynamics Computations in Flexible ZIF-8 Framework", J. Phys. Chem. C , 116 (2012), 933.

Relevant previous projects or activities

- EU-India Collaborative Project "AMCOS: Advanced Materials Computational Study" in the context of the Seventh Framework Program (233502);
- ESF research project "SIMU": "Challenges in Molecular Simulations: Bridging the time-scale and length-scale gap", coordinated by CECAM, Lyon, France

Relevant infrastructure to the proposed work

The research group has access to the CPU based computational resources of the host institution: a blade cluster formed by tents of multiprocessor computers (hundreds of computing cores) arranged for parallel computation via first-class InfiniBand technology, with a storage capacity of more than 25 Terabytes.

4.1.7 SZTAKI

Description of the legal entity

MTA SZTAKI is one of the largest IT research institutes in the Central European region with 250+ employees. Among its other achievements, the institute plays a key role in Grid and Cloud computing related research, development, and training as the founding member of the Hungarian Grid Competence Centre (2003), the International Desktop Grid Federation (2010) as well as the Coregrid (2004-2008) and the S- CUBE (2008-2012) European Networks of Excellence.

The mission of the Laboratory of Parallel and Distributed Systems (LPDS) in MTA SZTAKI is two-fold in Grid and Cloud research. The first goal is to provide high-level services together with customizable scientific gateways based on workflows (gUSE/WS-PGRADE) for the most widespread e-Infrastructures and platforms based on Grid, Cloud, cluster and volunteer computing technologies. The second main aim is to offer middleware solutions (SZTAKI Desktop Grid, One-click deployment tool) and technologies for interoperability (3G Bridge, Data Avenue) that enables easy-to-deploy, transparent, and scalable platforms for scientific and business applications involving large amount of data.

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The laboratory has been working as a project member in all phases of the European Grid infrastructure project (EGEE/EGI) serving as a regional training/application porting centre and Virtual Team leader.
CoreGrid, SEE-GRID, DEGISCO, SCI-BUS) the laboratory provides knowledge transfer, and targets new user communities from science and industry. The laboratory has long running experience in establishing and operating production-level Grid and Cloud infrastructures for different purposes and partners; national (HUNGRID, SZTAKI cloud), regional (SEE-GRID, EDGI), global (EGI, EDGeS, DEGISCO), and application specific (CANCERGRID, agINFRA).
The institute is certified according to the ISO 9001:2008 standard, and has significant scientific management experiences as coordinator in national projects (SuperGrid, HAGRID, WEB2GRID) and in EU FP7 projects (EDGeS, EDGI, DEGISCO, SHIWA, SCI-BUS and IDGF-SP) and as WP leader of several projects since the EU 5th Framework Programme (DATAGRID, CANCERGRID, SEE-GRID, CloudSME, etc).

Key people

Prof. Dr. Peter KACSUK [M] is the Director of the Laboratory of the Parallel and Distributed Systems in the Computer and Automation Research Institute of the Hungarian Academy of Sciences. He received his MSc and university doctorate degrees from the Technical University of Budapest in 1976 and 1984, respectively. He received the kandidat degree (equivalent to PhD) from the Hungarian Academy in 1989. He habilitated at the University of Vienna in 1997. He received his professor title from the Hungarian President in 1999 and the Doctor of Academy degree (DSc) from the Hungarian Academy of Sciences in 2001. He served as full professor at the University of Miskolc and at the Eö tvö s Lóránd University of Science Budapest. He has been a part-time full professor at the Cavendish School of Computer Science of the University of Westminster. He has published two books, two lecture notes and more than 300 scientific papers on parallel computer architectures, parallel software engineering, Grid and Cloud computing. He is editor-in-chief of the Journal of Grid Computing published by Springer. He coordinated the following Hungarian Grid projects: SuperGrid, HAGRID, WEB2GRID. He coordinated the following EU FP7 projects: EDGeS, EDGI, SHIWA and currently coordinates SCI-BUS.

Dr. Zoltan Farkas [M] has been a research fellow at the Laboratory of the Parallel and Distributed Systems in the Computer and Automation Research Institute of the Hungarian Academy of Sciences since 2002. He received his M.Sc. and Ph.D. from the Eotvos Lorand Science University of Budapest in 2004 and 2013, respectively. His research interests include grid computing, interoperability solutions, using standards and portal technologies. Within the Enabling Desktop Grids for e-Science (EDGeS) project he has created the core component of the grid interoperability solution, the 3G Bridge. Currently he is heading the portal team at MTA SZTAKI LPDS, and is contributing to a number of EU-funded projects (SCI-BUS, CloudSME). He is a co-author in more than 30 scientific papers in journals and conference proceedings on grid computing.

Relevant publications, and/or products, and/or services

- Akos Balasko, Zoltan Farkas and Peter Kacsuk: Building science gateways by utilizing the generic WS-PGRADE/gUSE workflow system. Computer Science Vol. 14., No. 2., pp 307-325, 2013
- Peter Kacsuk, Gabor Terstyanszky, Akos Balasko, Krisztian Karoczkai, Zoltan Farkas: Executing Multi- workflow simulations on a mixed grid/cloud infrastructure using the SHIWA and SCI-BUS Technology. Advances in Parallel Computing, Volume 23: Cloud Computing and Big Data, pp 141-160, 2013
- Kassian Plankensteiner, Radu Prodan, Matthias Janetschek, Thomas Fahringer, Johan Montagnat, David Rogers, Ian Harvey, Ian Taylor, Ákos Balaskó, Péter Kacsuk: Fine-Grain Interoperability of Scientific Workflows in Distributed Computing Infrastructures. In Journal of Grid Computing, Volume 11, Issue 3, pp 429-455, 2013
- Akos Balasko, Zoltan Farkas, Peter Kacsuk: Building science gateways by utilizing the generic WS-PGRADE/gUSE workflow system. In Computer Science journal, Vol. 14, No. 2, 2013

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- Peter Kacsuk: P-GRADE portal family for Grid infrastructures. Concurrency and Computation: Practice and Experience journal, Volume: 23, Issue: 3, 2011, pp. 235-245, 2011.

Relevant previous projects or activities

- Scientific Gateway Based User Support (SCI-BUS), FP7, 2011-2014
- Cloud based Simulation platform for Manufacturing and Engineering (CloudSME), FP7, 2013-2015
- VIALACTEA - The Milky Way as a Star Formation Engine, FP7, 2013-2015
- Building a European Research Community through Interoperable Workflows and Data (ER-FLOW), FP7, 2012-2014
- agINFRA, I3, 2011-2013

Relevant infrastructure to the proposed work

MTA SZTAKI is operating a cloud infrastructure based on OpenNebula, which is part of the EGI Federated Cloud. A part of these resources can be used for CMMST VRE purposes.

4.1.8 CSIC

Description of the legal entity

The Spanish National Research Council (CSIC) is the largest public institution dedicated to research in Spain and the third largest in Europe. Belonging to the Spanish Ministery of Economy and Competitiveness, its main objective is to develop and promote research that will help bring about scientific and technological progress, and it is prepared to collaborate with Spanish and foreign entities in order to achieve this aim. The CSIC has 70 fully own institutes or centres distributed throughout Spain. In addition, it has 53 Joint Research Units with universities or other research institutions. The group is formed by people belonging to two of these Research Units, one with Autonoma University of Madrid and the second with University of Salamanca, with the institute of Fundamental Physics (IFF).

Key people

Dr. Octavio Roncero [M] has a permanent position in CSIC since 1991. His main research activity concerns with quantum dynamics of molecular procceses such as molecular collissions (inelastic and reactive) and photodissociation. In this subject he has more than 100 publicationin in international journals of higher impact in the field of Molecular Physics or Physical Chemistry. He is the main author of several programs such as madwave3 for quantum dynamics.

Dr. Alfredo Aguado [M] has a permanent position in the Autónoma Universtiy since 1998. His main research activity concerns with highly correlated ab initio methods and fitting of multidimensional potential energy surfaces.

He has more then 80 publications in internationals journals of the higher impact in the field. He is the main author of a series of programs developed to fit multidimensional potential energy surfaces with different number of atoms and symmetries, GFITNC (N=3,4,5).

Relevant publications, and/or products, and/or services

- Coordinate transformation methods to calculate state-to-state probabilities with wave packet treatments", S. Gómez-Carrasco and O. Roncero, J. Chem. Phys. 125 (2006) 054102
- "Differential cross sections and product rotational olarization in A+BC reactions using awave packet methods: H+ + H2 and Li + HF examples", A. Zanchet, O. Roncero, T. González-Lezana, A. Rodríguez-López, A. Aguado, C. Sanz-Sanz and S. Gómez-Carrasco, J. Phys. Chem. A, 113 (2009) 14488
- "Dynamically biased statistical model for the ortho/para conversion in the H2+H3+ → H3++ H2 reaction", S. Gómez-Carrasco, L. González-Sánchez, A. Aguado, C. Sanz-Sanz, A. Zanchet and O. Roncero, J. Chem. Phys. 137 (2012) 09303

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- "A new accurate and full dimensional potential energy surface of H5+ based on a triatomics-in-molecules analytical form", A. Aguado, P. Barragán, R. Prosmiti, G. Delgado-Barrio, P. Villarreal and O. Roncero, J. Chem. Phys. 133 (2010) 024306
- MADWAVE3 program for reactive scattering, and GFITNC programs for potential energy surface fittings.

Relevant previous projects or activities

- COST Action CM-1401 'Our Astrochemical History", financed by EU, period 2014-2018
- Participation as RRHH member of "Gas and Dust from stars to the laboratory: exploring the NanoCosmos" Sinergy project (I-ERC/2050), financed by ERC, period 2014-2020
- "Molecular Astrophysics", ref. CSD2009-00038, financed by Spanish Goverment, period 2010-2015

Relevant infrastructure to the proposed work

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4.1.9 ECTN

Description of the legal entity

The European Chemistry Thematic Network Association, is a non-profit making association registered in Belgium and is an outcome of six years of network activity (1996-2002). The Association was created to provide a sustainable future for the European Chemistry Thematic Network. Higher education institutions, national chemical societies and chemical and software companies comprise our members. There are currently over 120 members of the network coming from 30 different European countries and with associate members world-wide. Expert European groups work on a range of topics and produce reports with a real European dimension. These reports and recommendations are available on our website. A multi-lingual series of tests, that can be used for certification / validation of competence in chemistry at various levels is now available on Internet. Associated E-learning facilities have been produced. The purpose of the tests is to validate the competence of all citizens, irrespective of their learning path.

The aims and objectives of the Association are:

- To implement, consult or supervise programs for the assessment of skills and knowledge in science and engineering, with the emphasis on chemistry.
- To undertake education and training programs, especially those concerning innovative approaches and technologies.
- To operate as a consultant or assessor in programs concerning education and training.
- To provide certification of achievement when assessments have been carried out under appropriate conditions.
- To cooperate with established professional or other associations in the furtherance of its objectives.
- To extend the reach of all aspects of education in science and engineering beyond national borders.
- To provide a European framework for first-cycle degrees in chemistry.

Key people

Anthony SMITH [M] since 1996, director of International Relations at CPE Lyon, has been the co-ordinator of the **European Chemistry Thematic Network Association** (ECTN), which is a network with 160 members in around thirty European countries that aims to promote chemistry education and assessment in Europe. He has taken care of the realisation of a European area for lifelong learning and of development of the European Higher Education Area in order to promote employability and the growth of an entrepreneurial spirit. He has been particularly committed in developing the schemes of employability of graduate chemists will in order to produce a series of portraits of the careers of bachelor chemists and examples of good practice of industry as well as. He has also developed the internet based tests in chemistry and chemical engineering. The test have been produced in English and further developed and translated in to several languages from the initial English version. Along this line he has prompted the creation of a virtual campus for chemistry and chemical engineering learning objects

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Relevant publications, and/or products, and/or services

- Innovative Methods of Teaching and Learning Chemistry in Higher Education, I.
- Eilks and W Byers Eds., RSC Publishing (2009), ISBN 978 -1-84755-958-6
- N Faginas Lago et al, Lect. Notes in Comp. Science, 6019, 29-40 (2010).
- http://ectn-assoc.cpe.fr/network/ec2e2n/docs/WP08_ResultsStudyAboutUniversityTeachingStaffCourses.pdf
- http://www.intensiveschool.eu
- M.A. Rida and others, "Synthesis and X-ray structures of RuCpClL [L = (eta(1)-PPh(2)py)(2) and eta(2)-triphos] and [RuCp{eta(3)- (PPh2)(3)CH}][PF6]. The first eta(3)-(PPh2)(3)CH complex of Ru(II)", J ORGMET CH, 628(1), 2001, pp. 1-10

Relevant previous projects or activities

- ECTN 1: 1996-2000,
- ECTN 2: 2000-2003,
- ECTN 3 : 2003-2006 "The New Generation of Chemists"
- European Chemistry and Chemical Engineering Education Network, Project number:155975-LLP-1-2009-1-FR-ERASMUS-ENWA www.ec2e2n.net
-
- 526259-LLP-1-2012-1-FR-ERASMUS-ENW; **Project Title:** European Chemistry and Chemical Engineering Education Network 2.

Relevant infrastructure to the proposed work

Cluster of 95 computers
ECTN Newsletter, cpe Lyon

4.1.10 EGI.eu

Description of the legal entity

The Stichting European Grid Initiative (also referred to as "EGI.eu") is a not-for-profit foundation established under Dutch law to coordinate and manage the European Grid Infrastructure (EGI) federation on behalf of its members: National Grid Initiatives (NGIs) and European International Research Organisations (EIROs). EGI.eu offers a variety of services to the wider EGI community such overseeing infrastructure operations, coordinating user community support, working with technology providers, representing EGI in collaborative projects, steering strategy and policy development, organising flagship events and publicizing the community's news and achievements. EGI.eu and its members provide EGI, a pan-European infrastructure of publicly funded computing, storage and data resources to support excellent research and innovation in Europe. Building on over a decade of investment by national governments and the European Commission, EGI supports more than 22,000 researchers across many scientific fields with a wide range of technical services such as high-throughput data analysis, federated cloud, federated operations and community building.
EGI aims at contributing to the realization of an integrated European network of centres of excellence, for the implementation of the Knowledge Commons, meaning the capability to easily share and access knowledge, training facilities, open source software, and other digital assets necessary for Open Science.

Key people

Dr. Tiziana Ferrari [F] is Technical Director of EGI.eu, and the project director of the EGI-InSPIRE FP7 project. In her function of Technical Director she is ultimately responsible of the EGI technical infrastructure and user engagement activities. She has been involved in Grid operations since 2007 contributing to the coordination of operations for the Italian Grid infrastructure and contributed to the definition of the European Grid Infrastructure governance model and to the establishment of its headquarters in Amsterdam. She holds a PhD in Electronics and Data Communications Engineering from the Universita' degli Studi in Bologna.

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Yannick Legré [M] is the director of EGI.eu since February 2014. Formerly he was a senior research engineer at the French National Scientific Research Centre - Grid and Cloud Institute (CNRS-IdGC). He holds a Master of Science in Information Technology (MScIT) and a degree in Law (LL.L). Over the last 15 years, Yannick has been involved in more than 30 projects in the areas of healthcare and biomedical research, as well as biodiversity and environmental research, such as the ENVRI & CReATIVE-B projects. Yannick has successfully coordinated several EC, NATO and nationally funded projects. He has also been a co-founder and the president of the international HealthGrid association, and the director for International Relations of a French SME.

Dr. Sara Coelho [F] works in the EGI.eu communications team implementing and leading on many aspects of the the communications strategy for the organisation and the EGI-InSPIRE project. She has been a part of the EGI.eu team since 2010 and has been involved in all aspects of the organisation's communications activities including copy writing, website maintenance, production/design of promotional materials, community building and event organisation. Alongside a PhD in Geology, she has an MSc in Science Communication and her previous experience includes working as a reporter for Science and the UK's Natural Environment Research Council.

Dr. Gergely Sipos [M] works as Technical Outreach Manager for EGI.eu since 2010. He received his MSc degree and Ph.D. in information engineering from the University of Miskolc, Hungary in 2003 and 2010 respectively. Since 2003 he has been involved in several European Grid research and development projects. Between 2005-2010 he was involved in the EGEE, EGEE-II, EGEE-III, ICEAGE and SEE-GRID EU projects. He was the deputy leader of the "Training and induction" work package and the coordinator of the Application Porting Team of the EGEE series of projects. Within EGI he coordinates the User Community Support Team of EGI.eu, the user engagement of the National Grid Initiatives, and supports scientific communities to achieve better results by the European Grid Infrastructure.

Małgorzata Krakowian [F] is Senior Operations Officer EGI.eu and has worked in operations since 2006, collaborating with the EGEE2, EGEE3, EGI-InSPIRE, ENVRI, FedSM and PL-Grid projects. She holds a Master degree in Applied Computer Science and finished post-diploma studies in Project Management (IT project management, International project management). Malgorzata coordinates EGI Production Infrastructure by supervising the operational status and advancement of global and national operational services, contributing to the definition of the operations integration technical roadmap and supervising its progress.

Relevant publications, and/or products, and/or services

- Validation of Grid Middleware for the European Grid Infrastructure; David, M.; Borges, G.; Pina, J. et alt.; Journal of Grid Computing, DOI: 10.1007/s10723-014-9301-z, May 2014
- Resources and Services of the EGEE Production Infrastructure; Ferrari, T.; Gaido, L.; Journal of Grid Computing, June 2011, Volume 9, Issue 2, pp 119-133, DOI: 10.1007/s10723-011-9184-1, June 2011.
- Answering the Cost Assessment Scaling Challenge: Modelling the Annual Cost of European Computing Services for Research, Matti Heikkurinen, Sandra Cohen, Fotis Karagiannis, Kashif Iqbal, Sergio Andreozzi, Michele Michelotto, Journal of Grid Computing, May 2014, DOI: 10.1007/s10723-014-9302-y
- EGI: Implementing service management in a large scale e-Infrastructure, Sy Holsinger, Sergio Andreozzi, Proceedings of the IEEE Network Operations and Management Symposium (NOMS) Conference, 2014, Krakow, Poland, DOI: 10.1109/NOMS.2014.6838371
- EGI: an Open e-Infrastructure Ecosystem for the Digital European Research Area, Sergio Andreozzi, Sy Holsinger, Damir Marinovic, Steven Newhouse, Proceedings of eChallenges e-2012 Conference, Lisbon, Portugal, ISBN: 978-1-905824-35-91

Relevant previous projects or activities

- EGI-InSPIRE (http://www.egi.eu/about/egi-inspire/) is a 56 month 25 MEuro FP7 EU project aiming to support science and innovation by providing a lasting operational model for e-Science for coordinating the infrastructure and for delivering integrated services that cross national borders.

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EGI-InSPIRE is responsible of continued technical support to existing European research collaborations as well as of engagement with new research communities and community building in the private and public sector. The project was responsible of developing the European Grid and Cloud infrastructure into a platform that relies on externally sourced software technologies. Processes for software quality validation and verification, software distribution through public repositories and staged rollout were defined. EGI-InSPIRE was also responsible of providing user-facing services for discovery and distribution of community-specific code and a training marketplace federated training activities carried out by the members of the EGI collaboration.

- ENVRI (Common Operations of Environmental Research Infrastructures) is a PF7 EU project responsible for developing tools to share, use and access software promoting multi-disciplinary science for environmental researchers. In ENVRI EGI.eu was in charge of participating to tool development and technical user support to the Research Infrastructures in the areas of security, distributed high throughput computing, data management and cloud.
- BioVel (Biodiversity Virtual e-Laboratory) is a FP7 EU project (Contract no.: RI-283359) supporting biodiversity research using large amounts of data from cross-disciplinary sources. BioVeL offers researchers the possibility of using computerised 'workflows' (series of data analysis steps) to process data, be that from one's own research and/or from existing sources. EGI.eu contributed to the sustainability discussions taking place in the project by providing input about its own sustainability plans and understanding which components within BioVeL need to be sustained. In WP7 'Services access, operation and management', EGI.eu provided technical support and consultancy to partners in the project, from porting their existing applications exposed through a web service on a single host, to running their applications on the e-infrastructure.
- BioMedBridges (Building data bridges from biology to medicine in Europe) is a FP7 project (Contract no. 284209) forming a cluster of the emerging biomedical sciences research infrastructures (BMS RIs) and construct the data and service bridges needed to connect them.
    - The missions of the BMS RIs stretch from structural biology of specific biomolecules to clinical trials involving thousands of human patients.
    - Most serve a specific part of the vast biological and medical research community, estimated to be at least two million scientists in Europe across more than 1000 institutions from more than 36 ESFRI Member States and Associated Countries.
    - Each of them brings together its own large community of users to build a coordinated infrastructure. This process has already had a major impact on coordination of national infrastructures within each member state.
    - Essentially all BMS RIs are distributed infrastructures, with nodes in many European member states.
- DCH-RP (Digital Cultural Heritage Roadmap for Preservation) was a coordination action supported by EC FP7 e-Infrastructures Programme, launched to look at best practice for preservation standards in use. The project aim to harmonize data storage and preservation policies in the digital cultural heritage sector; to progress a dialogue and integration among institutions, e-Infrastructures, research and private organisations; to identy models for the governance, maintenance and sustainability of the integrated infrastructure for digital preservation of cultural content. EGI.eu was in charge of collecting requirements and defining test infrastructures.
- Civic Epistemologies (Development of a Roadmap for Citizen Researchers in the Digital Culture, conrtact no. RI-632694) is about the participation of citizens in research on cultural heritage and humanities. ICT are powerful drivers of creativity, but specific technical know-how is still generally lacking in the creative industries sectors. In addition, humanities scholarship is not yet taking full advantage of ICT to engage with wider audiences. New skills are needed to enable the cultural sector to grasp employment and commercial opportunities. In the project EGI.eu is responsible of defining business models for the support of citizen science in digital cultural heritage.

Other projects:

- eScienceTalk: Supporting grid and high performance computing reporting across Europe, Project Coordinator, RI-260733
- e-Fiscal: Financial Study for Sustainable Computing e-Infrastructures, RI-283449
- ENVRI
- HelixNebula, The ScienceCloud: Big science teams up with big business, RI-312301

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- ER-Flow
- FedSM: Implementing Service Management in Federated e-Infrastructures, RI-312851
- CloudWATCH: A European cloud observatory supporting cloud policies, standard profiles and services, RI-610994

Relevant infrastructure to the proposed work

- The European Grid Infrastructure (EGI) is a publicly funded e-infrastructure put together to give scientists access to more than 530,000 logical CPUs, 200 PB of disk capacity to drive research and innovation in Europe. Resources are provided by about 350 resource centres who are distributed across 56 countries in Europe, the Asia-Pacific region, Canada and Latin America. EGI also federates publicly funded cloud providers across Europe for the implementation of a European data cloud to support open science.
- EGI also provides central support services for quality verification and validation of open source software, technical support, helpdesk, an application database that for the registration of ported applications available for reuse.
- EGI Federated Cloud: The EGI Federated Cloud is a seamless grid of academic private clouds and virtualised resources, built around open standards and focusing on the requirements of the scientific community. The result is a new type of research e-infrastructure, based on the mature federated operations services that make EGI a reliable resource for science.
- Federated operations: brings together the operational tools, processes and people necessary to guarantee standard operation of heterogeneous infrastructures from multiple independent providers, with a lightweight central coordination.
- EGI is committed to contribute to the open science commons, including the knowledge commons aiming at making knowledge, competences and support services openly available to the whole European Research Area. This is concretely realized through a network of community-driven centres of excellence. EGI aims at providing – together with other key players – a European federation of Centres of Excellence providing services relevant to all the digital assets needed to support European eScience. For more information about the Open Science Commons vision see: http://go.egi.eu/osg

4.1.11 EHU

Description of the legal entity

The University of the Basque Country was founded in 1975. It is an institution with 45,000 students, 5,000 world-class of academic staff and state-of-art facilities. I was labeled as "Campus of International Excellence", highest quality award, by the Spanish Minister of Education. The University of the Basque Country is the main research institution in the Basque Country, carrying out 90% of the basic research made in the territory and taking advantage of the good industrial environment that the region constitutes. The University of the Basque Country is very active at international level and from 2007 has been awarded with more than 130 projects from different research fields.

Key people

- **Dr. Ernesto Garcia** [M] is full-professor in the Department of Physical Chemistry.
- **Dr. Maite Martinez** [F] is associated professor in the Department of Heat Engines and Machines.
- **Dr. Amaia Saracibar** [F] is assistant professor in the Department of Physical Chemistry.

In our group, we have developed several programs to study the reactive collisions of elementary reactions. We have developed methodologies for formulating global potential energy surfaces and to solve the classical and quantum equations of motion of the atoms during the collision. Cross sections and rate coefficients have been calculated for several tri and tetraatomic reactions.

We have experience (since 2005) in High Throughput Computing, using the production grid of EGEE (now EGI).

We have experience in High Performance Computing, using the MareNostrum machine at Barcelona Supercomputer Centre.

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We have experience in support chemistry programs in IBERGRID.

Relevant publications, and/or products, and/or services

- E.Garcia et al, "The effect of the intermolecular potential formulation on the state-selected energy exchange
- rate coefficients in N2-N2 collisions", Journal of Computational Chemistry 35, 722-736 (2014)
- E.Garcia et al, "The last mile of molecular reaction dynamics virtual experiments: the case of OH(N=1-10) + CO(j=0-3) reaction", Faraday Discussions 157, 415-436 (2012)
- E.Garcia et al, "An innovative computational comparison of exact and centrifugal sudden quantum properties of the N+N2 reaction", Physical Chemistry Chemical Physics, 14, 1589-1595 (2012)
- E.Garcia et al, "Capture and dissociation in the complex-forming CH+H2 → CH2+H, CH+H2 reactions", Physical Chemistry Chemical Physics 13, 3421-3428 (2011)

Relevant previous projects or activities

- COST-D37/002/06: "QDYN: Quantum dynamics engine for GRID enable molecular simulators" (Action D37 "GRIDCHEM: Grid Computing in Chemistry")
- COST-D23/003/01: "SIMBEX: A metalaboratory for the a priori simulation of crossed molecular beam experiment" (Action D23, "METACHEM: Metalaboratories for Complex Computational Applications in Chemistry")

Relevant infrastructure to the proposed work

- Access to the production GRID of EGI via the COMPCHEM Virtual Organization.

4.1.12 EKUT

Description of the legal entity

The Eberhard-Karls Universität Tübingen (EKUT) is one of the leading German research universities with both, a long academic tradition and excellent reputation in research. It is consistently ranked among the top ten of German universities and has a strong focus on biomedical sciences (ranked as the number one biology department in Germany by German Science Foundation (DFG)). In 2012 it was awarded the title of one of Germany's 'universities of excellence'. EKUT was the first university in Germany, and one of the first world-wide, to offer dedicated interdisciplinary curricula in Bioinformatics. In 2001 EKUT was awarded one of five DFG-funded centers of excellence in Bioinformatics. The Centre for Bioinformatics Tübingen consists of over twenty partners from five different departments of EKUT and on-campus Max Planck Institutes. In 2011, the Quantitative Biology Center was established as a central core facility for bioinformatics and as a center consolidating research in high-throughput methods, biological management, bioinformatics, and modeling under one roof.

Key people

Dr Jens Krüger [M] obtained his PhD in chemistry from the University of Paderborn and worked as postdoc at the National Yang-Ming University, Taipei. He is currently working on his habilitation at the Applied Bioinformatics Group of the EKUT. His research interests focus on multiscale simulations of ion channels, scientific workflow management and science gateway technology. Within the MoSGrid project, he was responsible for the workflow development and portal work packages. The work was continued within the FP7 project SCI-BUS, including collaborations on science gateway solutions for the Quantitative Biology Center Tübingen and the Karlsruhe Institute of Technology.

Relevant publications, and/or products, and/or services

- J. Krüger, R. Grunzke, S. Gesing, S. Breuers, A. Brinkmann, L. de la Garza, O. Kohlbacher, M.

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Kruse, W.E. Nagel, L. Packschies, R. Müller-Pfefferkorn, P. Schäfer, C. Schärfe, T. Steinke, T. Schlemmer, K. Warzecha, A. Zink and S. Herres-Pawlis: The MoSGrid Science Gateway – A Complete Solution for Molecular Simulations, Journal of Chemical Theory and Computation 2014, 10 (6), 2232–2245, DOI: 10.1021/ct500159h.
- M. Avbelj, O. O. Wolz, O. Fekonja, M. Benčina, M. Repič, J. Mavri, J. Krüger, C. Schärfe, M. Delmiro-Garcia, G. Panter, O. Kohlbacher, A. N. R. Weber, R. Jerala: Activation of lymphoma-associated MyD88 mutations via allostery-induced TIR domain oligomerization, Blood 2014,. DOI:10.1182/blood-2014-05-573188.
- K. Hildebrandt, D. Stöckel, N. M. Fischer, L. de la Garza, J. Krüger, S. Nickels, M. Röttig, C. Schärfe, M. Schumann, P. Thiel, H. P. Lenhof, O. Kohlbacher and A. Hildebrandt: ballaxy: web services for structural bioinformatics, Bioinformatics 2014, DOI:10.1093/bioinformatics/btu57.
- O. Niehörster, A. Brinkmann, A. Keller, C. Kleineweber, J. Krüger and J. Simon: Cost-Aware and SLO-Fulfilling Software as a Service, Journal of Grid Computing, 10(3): 553-577, 2012.
- X. G. Zong, S. Krause, C. C. Chen, J. Krüger, C. Gruner, X. C. Cao-Ehlker, S. Fenske, C. Wahl-Schott, and M. Biel: *Regulation of HCN channel activity by cyclic cytidine 3', 5'-monophosphate (cCMP)*, Journal of Biological Chemistry, 287(32): 26506-26512, 2012.

Relevant previous projects or activities
- MoSGrid: Molecular Simulation Grid (BMBF, grant 01IG09006)
- SCI-BUS: Scientific gateway Based User Support (EU FP7, grant RI283481)
- MoSGrid US: Molecular Simulations in a Distributed Environment (XSEDE project TG-CHE140058)
- Quantitative Biology Center (DFG, grant KO2313/6-1)

Relevant infrastructure to the proposed work
The MoSGrid infrastructure supported by the compute centers of the universities of Tübingen, Dresden, Cologne and Paderborn will serve for prototyping of services.

4.1.13 ENEA

Description of the legal entity
ENEA (www.enea.it) is an Italian Government Agency operating on research, innovation technologies and advanced services in the fields of sustainable economic development and energy. It currently employs around 2,600 people located in 11 research centres throughout Italy.
The operational departments involved in the project are: UTICT – Technical Unit for Information Systems and ICT Development; UTTMAT – Technical Unit for Materials Technologies.
UTICT's mission includes planning, development and management of ICT technologies in support to R&D activities of ENEA. In the framework of this general mission, UTICT:
- Guarantees the operation of hardware and software infrastructures for scientific computing, geographical data networks, their connection to national and international networks, local area networks, and related services such as databases, multimedia services, centralized backup services, supporting services to scientific users;
- Carries out R&D activities in the domains of distributed and high performance computing, ultra-high throughput data networks, interoperability of heterogeneous systems such as large scientific instruments and scientific laboratories, and on specific industry-driven applications.

Experience in high performance computing systems and architectures dates in ENEA since its founding, in the 1950s. In recent years a major computing centre was established in Portici (Naples), where currently the CRESCO facility is hosted. The CRESCO project was originally funded by the Italian Ministry of University and Research through the European Regional Development Funds and allowed, in 1998, the set-up of a supercomputer of more than 4,000 cores and 25 Tflops of aggregated power. The infrastructure was recently upgraded through financing

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from ERDF, which allowed a substantial increase in available computing power, currently around 150 TFlops.
All computing facilities in ENEA are integrated within ENEAGRID, a large infrastructure for cloud computing, which is characterized by solid structural components integrated in a user-friendly environment. ENEA started developing its GRID computing infrastructure in 1998. ENEA took part in the EU-funded EGEE/EGI projects, aimed at the set-up of a pan-European GRID computing infrastructure, focusing its activity on providing access to non-standard platforms, such as AIX, by means of a "gateway" approach.
ENEA's HPC and GRID computing environment supports R&D activities of a substantial number of research groups and associated partners, in sectors such as alternative energies, energy efficiency, climate and environment, new materials, manufacturing technologies, transports, security, cultural heritage. The Technical Unit for Materials Technologies (UTTMAT) carries out applied research aimed at developing new materials and components for sustainable energy technologies. It has been active since decades on materials characterization, processing and synthesis; it develops know-how, designs technologies and fabricates demonstration prototypes. The Unit is involved in many EU and Italian projects for industrial research and experimental development activities and manages a large number o experimental facilities. It also offers excellence skills of modelling development and materials design. The Unit head quarters are at the ENEA Casaccia Research Centre in Rome, where the management and all the technical activities are located. In accordance with its operational programme, the Unit coordinates the whole activitiy of the Agency in the field of Materials Science and Technology, where also other Technical Units are involved, mainly those located in Faenza and Brindisi.

Key people
Dr. Massimo Celino [M] is born in Rome in 1967. He studied Physics at the University of Rome "La Sapienza" discussing a thesis on the numerical modelling of charge flows at the depinning transition. He got a PhD in condensed matter physics at the University of Strasbourg "L. Pasteur" (France) in 2002 discussing a thesis on the numerical characterization of amorphous and liquid atomic structure of silicon diselenide materials. From 1996 staff scientist at ENEA, in the Technical Unit for Materials Science. His main scientific interests are in the field of molecular modeling of amorphous and liquid materials via both quantum and classical molecular dynamics tools on high performance computing platforms. He is author of about 70 scientific papers on international journals, and delivered talks and communications to numerous national and international conferences.

Dr. Francesco Buonocore [M] staff scientist of the UTTMAT-SUP, will be researcher in charge of the graphene extraction process and growth mechanisms studies. Born in Pompei in 1970, Dr Buonocore got a MSc degree in Physics in 1997 and a PhD in 2001 at the University of Napoli "Federico II", with thesis in Condensed Matter Physics dedicated to quantum wires theoretical studies, under the supervision of Prof. Giuseppe Iadonisi and Prof. Domenico Ninno. Before moving to ENEA, he worked from 2001 to 2012 in the semiconductor company STMicroelectronics, where, in particular, he developed physical and atomistic models of carbon nanotubes growth mechanisms and carbon nanotube interfaces with metals. He is author of 17 scientific publications on refereed international journals and is co-inventor of three international patents and one Italian patent.

Dr. Filippo Palombi [M] received a Ph.D. in theoretical particle physics from the University of Rome "Tor Vergata". For about ten years he was involved in computational research in the field of Lattice QCD at postdoctoral level (he was an Alexander-von-Humboldt fellow, a DESY fellow, a CERN fellow, and a Marie Curie fellow). He has teaching experience in the course of "Algorithms and Data Structures" at the University of Rome "La Sapienza", Dept. of statistics and information

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engineering. Since two years he is a staff resesearch scientist at ENEA, where he works as a member of the HPC unit and conducts research in complex systems.

Dr. Giovanni Bracco [M] Graduated cum laude in Physics at the Pavia University, Pavia (Italy). ENEA researcher, he is in charge of the ENEA-GRID HPC infrastructure and its management. In his group all the ENEA tools and services for access and use of the ENEA infrastructure have been developed. He is ENEA coordinator for national and international project on GRID infrastructures.

Relevant publications, and/or products, and/or services

- Water driven adsorption of amino acids on the (101) anatase TiO2 surface: an ab-initio study. L.Agosta, G.Zollo, C.Arcangeli, F.Buonocore, F.Gala, M.Celino. Physical Chemistry Chemical Physics 17 (2015) 1556-1561. DOI: 10.1039/c4cp03056g.
- Icosahedral superclusters in Cu64Zr36 metallic glass. J.Zemp, M.Celino, B. Schönfeld, J.F.Löffler. Phys. Rev. B 90, 144108 (2014). DOI: 10.1103/PhysRevB.90.144108
- A first-principle molecular dynamics study of glassy GeS2: Atomic structure and bonding properties. M.Celino, S.Le Roux, A.Bouzid, M.Boero, C.Massobrio. Phys. Rev. B 88, 174201 (2013).
- DFT model of hydrogen desorption from MgH2: the role of iron catalyst. S.Giusepponi, M.Celino. International Journal of Hydrogen Energy 38, 15254-15263 (2013)

Relevant previous projects or activities

- TEDAT - Centre of Excellence for Technologies and Diagnostics in the Transpotrs Sector, funded by the Italian Ministry of Education, Universities and Research, through ERDF 2007-2013;
- DC4CITIES - An environmentally sustainable data centre for Smart Cities, FP7-SMARTCITIES-2013(ICT), Objective ICT-2013.6.2;
- IT@CHA - Italian Technologies for Advanced application in Cultural Heritage Assets, funded by the Italian Ministry of Education, Universities and Research, through ERDF 2007-2013;
- LAMRECOR – Advanced Logistics for the Mobility of People and Wares; funded by the Italian Ministry of Education, Universities and Research, through ERDF 2007-2013;
- SOPHIA, PhotoVoltaic European Research Infrastructure, FP7-INFRASTRUCTURES-2010-1, INFRA-2010-1.1.22: Research Infrastructures for Solar Energy:Photovoltaic.
- COST (European Cooperation in Science and Technology) action MP1103 project : Nanostrctured materials for solid-state hydrogen storage.

Relevant infrastructure to the proposed work

The computing resources currently available in ENEA are x86–64 Linux systems and dedicated systems (e.g. GPU systems). The storage systems are both AFS and GPFS based. The computing resources are distributed across six ENEA research centres in Italy. The main facility is located in Portici (Naples) and includes several HPC Linux Clusters, with an aggregated ~ 10,000 cores.
The most recent cluster, CRESCO4, consists of 38 Supermicro F617R3–FT chassis, each hosting 8 dual CPU nodes. Each CPU, specifically an Intel E5–2670, hosts in its turn 8 cores, for a total number of 4864 cores. These operate at a clock frequency of 2.6 GHz. The system is provided with a RAM memory of 4 GB per core. Computing nodes access a DDN S2A9900 storage system, for a total storage amount of 480 TB. Computing nodes are interconnected via an Infiniband 4xQDR QLogic/Intel12800-180 switch (432 ports, 40Gbps).
UTTMAT. The relevant infrastructure of the UTTMAT are used for qualification of materials and components, syntesis of materials and nanomaterials, syntesis of cellular metallic materials, development of sensor and sensitive materials qualification, a repository of numerical codes for the design and characterization of materials via numerical simulation methods at atomic level.

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4.1.14 EXACT

Description of the legal entity
eXact lab is an innovative SME that provides solutions, training and on-demand access in the High Performance Computing market. We assists our clients in the government and private sector in procuring mission-critical HPC systems and maximizing the effectiveness of existing systems based on their specific HPC requirements. Founded in 2011 as a spin-off of IOM-CNR institute located in Trieste Italy by three researchers with more than ten years experience in the HPC arena the company is rapidly growing and it now composed by a team of six professionals plus a few more consultants.
Members of our team have acquired experience in addressing different aspects of scientific computing, from the deployment of a computational and cloud infrastructure to the tuning of scientific software in a wide range of scientific field.
eXact lab, thanks to its focus on Research & Development (more than 20% of the annual turnover) and its highly skilled team, is also enlisted in the restricted list of the Italian Innovative Start-UP accordingly to Italian law 221/2012.

Key people
Stefano Cozzini [M] Founder of eXact lab and CNR/IOM researcher.
Education and experience: PhD in Physics (1995, University of Padova) More than 15 years of experience in HPC and e-infrastructures. He took part in several European projects and has a consolidated expertise in the management of HPC and e-infrastructure research projects.

Francesco De Giorgi [M] Founder and CEO of eXact lab. Senior software developer.Education and experience: Master in Mathematics. Large experience in installing/porting and managing scientific software on different kinds of computational infrastructures.

Relevant publications, and/or products, and/or services
- R Alfieri, S Arezzini, GB Barone, U Becciani, M Bencivenni, V Boccia, S. Cozzini. The HPC testbed of the Italian Grid Infrastructure, Parallel, Distributed and Network-Based Processing (PDP), 2013
- T Aleksiev, R Potestio, F Pontiggia, S Cozzini, C Micheletti PiSQRD; A web server for decomposing proteins into quasi-rigid dynamical domains, Bioinformatics 25 (20), 2009, 2743- 2744
- S Cozzini, D Vaddi, S Goel, F De Giorgi, SK Dash; Regional Climate Simulations on EU-INDIA Grid Infrastructures: Methodologies and Performance Journal of Grid Computing, 2013, 1-18
- RegCM4: Model description and preliminary tests over multiple CORDEX domains F Giorgi, E Coppola, F Solmon, L Mariotti, MB Sylla, X Bi, N Elguindi, S.Cozzini ... Climate research 936 (52), (2012), 1; 7-29

Relevant previous projects or activities
- openViewSHIP, a FVG regional project to provide Cloud based analysis and remote visualization services for CFD intensive calculation in the area of naval engineering
- Collaboration with NFFA project to setup data repository for nanoscience
- EU-IndiaGRID project (2010-2012)

Relevant infrastructure to the proposed work
Openstack private CLOUD infrastructure available for deployment and as testing facility.

4.1.15 FACH

Description of the legal entity
FACH is the acronym for Dipartimento di Farmacia, University “G. d’Annunzio” of Chieti-Pescara, located in Chieti, Italy. The research in the Department covers various aspects of chemical and

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biological characterization of molecular species. Expertise from people in the group include:

- the management and development of HPC systems, optimization and parallelization of computational procedures, software development both in academic and commercial environments, applied to electron structure calculations, to mixed quantum-classical nuclear dynamics and general purpose molecular science.
- the study of the promotion on natural gas hydrate formation by surfactants, the design and synthesis of conditioners that could promote hydrate formation for storage and transportation.

extraction, isolation, and structural characterization of secondary metabolites from the vegetable kingdom.

Key people

Cecilia Coletti [F] got the PhD in Chemical Sciences (Physical Chemistry) at the University of Perugia. She was a Post Doctoral fellow at the University of Barcelona, at the University of Copenhagen (Denmark) and at the University of Perugia. She is Associate Professor at the Department of Pharmacy of the University of Chieti-Pescara. She has worked on the development of alternative coordinate systems and basis sets to be used for the description of atomic structures or for atoms in fields. She addressed the detailed description of the nuclear dynamics of molecular systems, contributing to the development of novel mixed quantum-classical methodologies and to their application to systems of interest in atmospheric, optical and laser chemistry. More recently, her research interests focus on the accurate investigation of simple systems or of weak interactions using highly correlated post Hartree-Fock methods and on the study of the electronic structure, by quantum mechanical techniques (DFT, post-HF methods).This activity is reported in more than 55 papers published in international journals.

Loriano Storchi [M] completed his degree in Chemistry and got his PhD at the University of Perugia. During these years, he worked mainly as a programmer in various fields dealing essentially with parallelization and optimization of computational chemistry programs. He also worked with the Department of Computer Science at University of Pisa for the "Developing parallel ASSIST codes for chemical applications in the strategic project MIUR (High-performance distributed platform)". Since 2004 he has also worked as scientific consultant and programmer with the following public and private institutions: Molecular Discovery Ltd., UK, developing many commercial programs; Center for Research on Climate and Climate Change of Perugia, optimizing, porting and management in HPC environments of parallel codes for the simulation of convective weather phenomena. From 2010 he has worked as a collaborator of the National Institute of Nuclear Physics for evaluating the computational needs for the Einstein Telescope project using Many-Core (GPU) environment. At the beginning of 2011 he got one-year research grant at the ISTM (CNR) which involved the implementation of methods for sphere and polyhedra packing algorithms and development of relativistic DFT code. Since December 2011 he is researcher at the Department of Pharmacy of University of Chieti-Pescara. Since March 2013 he is also research associated with the INFN and CERN involved in CLOUD Computing and reconfigurable computing for the CMS experiment.

Pietro Di Profio [M] graduated in Chemistry in 1990, then was visiting researcher with the University of California at Santa Barbara (1992), working with prof. Clifford A. Bunton and prof. David F. Nicoli, Particle Sizing Systems, Inc. (Santa Barbara, CA). This research period was dedicated to the knowledge of light scattering techniques and relevant theories (auto-correlation functions, cumulants approach, inverse Laplace transform, etc.) and models employed for modeling supramolecular systems (DLVO, HNC, ecc.). Dr. Di Profio received a PhD in chemistry in 1995, working on supramolecular and micellar systems, and their interactions with biological macromolecules (DNA, enzymes, etc.) for cell transfection and gene therapy. A main current research activity is focused on the study of clathrate hydrates, which forms the basis for the establishment of the Gas Hydrate Facility in the FACH. This activity is currently also being

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outsourced by Gas and Oil companies.

Relevant publications, and/or products, and/or services

- L. Storchi, F. Tarantelli, A. Lagana', "Computing molecular energy surfaces on a grid", Lecture Notes in Computer Science 3980, 675 (2006).
- Di Profio P, Arca S, Germani R, Savelli G. Chem. Eng. Sci., 60 (2005), 4141-4145
- Di Profio, et al., European Patent No. 2 024 077.
- C. Coletti and G.D. Billing "Vibrational energy transfer in molecular oxygen collisions"
- Chem. Phys. Lett., 356 (2002), 14-22
- S. Rampino, L.Belpassi, F. Tarantelli, L. Storchi, "Full parallel implementation of an all-electron four-component Dirac-Kohn-Sham program" J. Chem. Theory Comput., 10, 3766, (2014)

Relevant previous projects or activities

- 2011-2012: PRELIMINARY INVESTIGATION ON THE ADHESION OF METHANE HYDRATE ON PIPELINE SURFACES, AND RELATED KINETIC ISSUES; 'CUBE HYDRATES PROJECT FOR PREDICTION OF HYDRATE FORMATION IN SUBSEA APPARATUS' Commissioned by TEA Sistemi SpA on behalf of Eni SpA
- 2014: THz for Hydrate Prevention - PHASE 2 RdO 0179/2013; Committente Tecnomare SpA
- PRIN 2009 (Research Projects of National Interest) funded by the Italian Ministry of Education and Research, Grant n. 2009W2W4YF "Photons, radicals and charged molecules involved in systems of nano and biotechnological interest"
- Open City Platform (OCP) (funded by the MIUR - National Ministery of Education and Research) intends to research, develop and test new technology solutions that are open, interoperable and usable on-demand on the Cloud, as well as innovative organizational models that will be sustainable over time. The aim of the project is to innovate, with scientific results and new standards the delivery of services by Local Government Administrations (LGA) and Regional Administrations to citizens, businesses and other Public Administrations (PA)
- GRID.IT funded by the MIUR - National Ministry of Education and Research (2002-2005).The goal of this project is to enable ICT platforms for distributed high-performance Computational Grids, oriented to the development of complex multidisciplinary applications and scalable Virtual Organizations in highly dynamic and heterogeneous context. The target technologies covers all the system levels: from the high-speed networks, to the Middleware services, to the programming tools and environment. The proposal contains the development of demonstrators in the fields of Astronomy, Earth Observation Systems, Biology, Computational Chemistry and Geophysics

Relevant infrastructure to the proposed work

- Gas Hydrate Facility: (i) Constant Pressure reactors; (ii) Pressure-drop reactors with optical windows; (iii) Mini-flow-loop pilot.
- Intel Xeon x86_64 clusters
    - 2 x Intel Xeon 4-Core E5-2603 1.8 Ghz
    - 24 x Intel Xeon 6-core E5-2620 2.0 Ghz
    - 8 x Xeon 8-core E5-2650 2.0 Ghz
    - 4 x Xeon 8-Core E5-2650v2 2.6 Ghz
    - # 248 cores
    - ~1 TB RAM
    - InfiniBand
    - SATA / SAS

4.1.16 ICMA

Description of the legal entity

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Málaga University (UMA) follows an educational model to promote competitive, quality teaching which is employment-orientated and accredited in Europe. The University is awarded as an International Campus of Excellence, Andalucia TECH, this Campus model is based on existing strengths and opportunities, and is composed of different entries linked one to each other. Within the last two decades has participated in 96 international projects. At present the Universidad de Málaga counts 37 active European projects belonging to different programmes, with 28 active in FP7. So far 6 projects have been coordinated by Universidad de Malaga and currently, 3 of these projects are FP7 active projects with UMA in the lead.

Key people
M. Olga Guerrero-Pérez [F] (born in Madrid, 1974), is Associate Professor at the Chemical Engineering Department at Málaga University. She has co-authored more than 60 peer-review papers in international Journals, participated in more than 100 international Conferences; and she has edited 3 special issues of Catalysis Today. She has also organized several international conferences and several workshops and seminars. She has supervised 2 Doctoral Thesis and currently she is supervising 3 more; she has also supervised 12 Master and Graduate final projects. She has experience in European networks, for instance, she participated in COST Action D36 as management committee member and actually she is the coordinator of EurasiaCat (https://sites.google.com/site/emeurasiacat/home).

Relevant publications, and/or products, and/or services
- "New Reaction: Conversion of Glycerol into Acrylonitrile", ChemSusChem, 1 (2008) 511
- "On the Nature of Surface Vanadium Oxide Species on Carbons", J. Phys. Chem. C 116 (2012) 20396
- "Performance of NiO and Ni-Nb-O active phases during the ethane ammoxidation into acetonitrile", Catal. Sci. & Tech. 3 (2013) 3173
- "Carbon materials as template for the preparation of mixed oxides with controlled morphology and porous structure", Catal. Today 227 (2014) 233
- Metrics of acrlylonitrile: from biomass vs. petrochemical route", Catal. Today 239 (2015) 25

Relevant previous projects or activities
- "EURASICAT: Advanced Education European-Asian Exchange Program in Materials Science and Catalysis". Erasmus Mundus Action-2 Strand-2 (EMA2/S2). European Commission. Countries involved: Spain, The Neederlands, France, Italy, Poland, Hong Kong, Macao, Taiwan, Singapore. Budject: 1.503.175 €. July 2014-Agoust 2018. M.O. Guerrero Perez project coordinator. European partners of this project: University of Twente (Prof. Guido Mul) NL, Adam Mickiewicz University (Prof. Maria Ziolek) PL, Univerisite Pierre et Marie Curie VI (Prof. Monica Calatayud) FR, University of Trieste (Prof. Paolo Fornasiero) IT, Instituto de Catálisis y Petroleoquímica CSIC (Prof. Miguel Bañares) ES.

Relevant infrastructure to the proposed work
Central Computing Service (ICS) providing support for the implementation of projects and research and training activities.

4.1.17 INFN

Description of the legal entity
The Italian National Institute of Nuclear and Particle Physics (INFN) (www.infn.it) was founded in 1951 and is a governmental research organization which promotes, co-ordinates and funds nuclear, particle and high-energy physics research in Italy.
INFN has been developing all along in house open ICT innovative solutions for its own advanced needs of distributed computing and software applications. It has a remarkable excellence expertise on Grid and Cloud technologies, having fostered and participated, with leadership roles, to many of the large Projects financed by EC that promoted the realization of the European Grid Infrastructure (EGI).

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INFN, in fact, has been one of the main participants to the EGI-InSPIRE activities and its personnel has very high skills and experience in operating large distributed computing infrastructures, coordinating the activities of distributed teams and providing support to system administrators and user communities.
INFN has been the coordinator of the Italian Grid Infrastructure (IGI) and will be the coordinator of a new JRU that is going to be established with INAF (Istituto Nazionale di Astrofisica) and INGV (Istituto Nazionale di Geofisica e Vulcanologia).
INFN is a leader in the development of distributed computing and has recently consolidated EGI-Engage 27 collaborations with the main international Research Centres developing ICT solutions for the scientific world and is a primary partner of many projects funded by the EC through the FP7 program. It has established one of the largest European Grid infrastructures, including more than 56 Data Centres.
The Grid middleware (based on open standards and protocols and high level security technologies) used in almost all the 350 EGI Data Centers was designed, developed and released by the European Project EMI (European Middleware Initiative), where INFN was one of the main partners. INFN itself develops and provides many of the key components for the EGI operations, including the general interface to the computing resources (CREAM), the interface (based on the OGF standard SRM) to access distributed storage (StoRM), used by the main INFN Data Centre (CNAF-Bologna) and other European centres, the Virtual Organizations Membership Service (VOMS), the resources access policies service (ARGUS), the accounting service (DGAS), the Workload Management System (WMS) and an access service to the computing infrastructure based on federated authentication and authorization systems.
Furthermore, INFN has developed an open Cloud IaaS solution, integrated in Grid (WNoDeS: http://web.infn.it/wnodes), that was one of the solutions of the EGI Cloud Task Force, and the Catania Science Gateway Framework (www.catania-science-gateways.it) that is one of the frameworks fostered by EGI.
INFN is participating to national projects (PRISMA and Open City Platform), funded by the Italian Ministry of Education and Research within the Smart Cities and Communities framework, to develop an open source cloud solution to federate different cloud services provided by both public institutions and private companies.
Moreover, INFN is leading a Project proposal called INDIGO-DataCloud (INtegrating Distributed data Infrastructures for Global ExplOitation). INDIGO-DataCloud is aimed at developing a data/computing platform targeted at scientific communities, deployable on multiple hardware, and provisioned over hybrid (private or public) e-infrastructures.
This open source and standard based federated cloud aims at allowing different actors (private companies, academic and research institutions, public sector institutions) to provide efficient, cheap and "standard" services to the various Italian public administrations. Some pilot public administrations are involved in these projects with the role of validating the federated cloud solution by means of application/services/procedures (implemented as SaaS or PaaS) of their interest.

Key people
Davide Salomoni [M] is Director of Technology (Dirigente Tecnologo) at the Italian National Institute for Nuclear Physics (INFN). His role is Manager of the Research and Development team at CNAF (the INFN National Center for research and development on IT technologies), Bologna. His interests are focused on the evolution, scalability, and interoperability of Cloud computing and storage technologies and on low-power architectures. He leads or participates to several national and international projects such as: COKA (an INFN-funded project on the efficient usage of many-core architectures); PRISMA (PiattafoRme cloud Interoperabili per SMArt-government), an innovative project funded by the Italian Ministry of Education and Research (MIUR) and by the Ministry of Economic Development (MISE); EGI (the European Grid Infrastructure); Open City Platform (OCP), a MIUR-funded Smart Cities project in the "Cloud computing technologies" section, where he coordinates the IaaS area. Davide is also the coordinator of the INFN Cloud computing workgroup. He is engaged as well with activities related to technology transfer in Universities, Public Administrations and industries through seminars, courses and lectures. In the past, Davide was manager of the computing farm of the INFN National Computing Center, was engaged in several European projects (such as EGEE, OGF-Europe, SIENA) and was one of the architects and implementors of the Italian Research and Academic Network (GARR), being also the first manager of its network operation center. He worked abroad for several years, assuming the roles of senior scientist at NIKHEF (Dutch institute for research in Astro-Particle Physics, Amsterdam, NL), technical manager of the Dutch internet team at COLT Telecom (Amsterdam, NL), head of the networking group at SLAC (Stanford Linear Accelerator Center,

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Menlo Park, USA). With 25 years of international experience in the fields of networking, distributed computing and scientific computing, Davide has got extensive expertise at both technical and management level in team management, definition of novel services, design and operation of complex networks and of distributed computing infrastructures, in commercial and academic environments. He worked and is familiar with Internet communication protocols, modern programming languages, virtualization technologies and distributed computing frameworks such as Grids and Clouds.

Luciano Gaido [M] got his Degree in Physics "cum laude" in 1988 at the Torino University.He is currently working as Senior Technologist (Primo Tecnologo) at INFN-Torino where he has been the head of the Network and Computing Service for about ten years. He has participated to many EU-funded (European DataGrid, EGEE-I,II,III, EGI-InSPIRE) and national (INFNGRID, IGI) grid projects. In the framework of these projects, he has set up and coordinated the Regional Operations Center for the Italian grid distributed infrastructure. He is currently the Technical Coordinator of the Italian Grid Infrastructure (IGI) and Technical Coordinator of the Open City Platform project funded by the Italian Ministry of Education and Research in the “Cloud computing technologies” section.
He is the Italian representative in the EGI Council and member of the EGI.eu Executive Board. He will also the INFN reference person for the project EGI-Engage, the follow-up of EGI-InSPIRE. Within CMMST-VRE he will collaborate to the WP02 and WP03 activities.

Roberto Barbera [M] was born in Catania (Italy) in October 1963. He graduated in Physics "cum laude" at the University of Catania in 1986 and since 1990 he holds a Ph.D. in Physics from the same University.
Since 2005 he is Associate Professor of Experimental Physics at the Department of Physics and Astronomy of the Catania University and at the beginning of 2014 he got the National Scientific Qualification to act as Full Professor of Experimental Physics of Fundamental Interations. Since his graduation his main research activity has been done in the domains of Experimental Nuclear and Particle Physics.. He is author of several book chapters, more than 250 scientific papers published on international journals, and more than 400 proceedings of international conferences.
At European level, he has been involved with managerial duties in many FP6 and FP7 EU funded projects (agINFRA, CHAIN, DCH-RP, DECIDE, EarthServer, EELA, EELA-2, EGEE, EGEE-II, EGEE-III, eI4Africa, EPIKH, EUChinaGRID, EUMEDGRID, EUMEDGRID-Support, GISELA, ICEAGE, INDICATE, etc.) in Europe, Asia, Africa and Latin America and he’s currently the Technical Coordinator of the CHAIN-REDS4 project. He is also the manager of the GrIDP Identity Federation (http://gridp.garr.it) and he is strongly involved in the establishment of Certificate Authorities, Identity Federations and Open Access Digital Repositories in various regions of the world. He will collaborate to the WP04 activities.

Alessandro Costantini [M] was born in Perugia (Italy) in December 1978. . He graduated in Chemistry at the University of Perugia in 2005 and since 2009 he holds a Ph.D. in Chemistry from the same University. In 2013 he holds a Ph.D. in mathematics and Computer Science from the University of Perugia. Since 2011 he is a Technologist at INFN participating to EU-funded (EGI-InSPIRE) and national (IGI) grid project working on User support to distributed computing GRID platforms and coordinating the support for new communities through consultancy, application poring and disseminationa and training activities. He is currently working in the Open City Platform project funded by the Italian Ministry of Education and Research in the “Cloud computing technologies” section aimed at developing an open source cloud solution for the public administation.

Relevant publications, and/or products, and/or services

- Salomoni D et al., A Cloud-based solution for Public Administrations – The experience of the Marche region. In proceedings of: The 2014 International Conference on Collaboration Technologies and Systems (CTS 2014), Minneapolis, USA, May 2014.
- V. Ardizzone et al., The DECIDE Science Gateway, J. Grid Computing (2012) 10:689–707; DOI 10.1007/s10723-012-9242-3.
- G. Andronico et al., “E-Infrastructures for International Cooperation”, chapter 6 of the book “Computational an Data Grids: Principles, Applications, and Design”, N. Preve (Ed.), IGI Global 2011, DOI: 10.4018/978-1-61350-113-9.
- C. Aifitimiei et al., Design and implementation of the gLite CREAM job management service, Future Generation Computer systems, volume 26, Issue 4, april 2010, pp. 654-667, Elsevier, ISSN:

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0167-739X, DOI: 10.1016/j.future.2009.12.006.
- Venturi, V., Stagni, F., Gianoli, A., Ceccanti, A., & Ciaschini, V. (2007, December). Virtual organization management across middleware boundaries. In e-Science and Grid Computing, IEEE International Conference on (pp. 545-552). IEEE.

Relevant previous projects or activities
- PRISMA: http://www.ponsmartcities-prisma.it
- EGI-InSPIRE: http://www.egi.eu
- EMI: http://www.eu-emi.eu
- WeNMR: http://www.wenmr.eu
- EGEE III: http://eu-egee-org.web.cern.ch/eu-egee-org/index.html

Relevant infrastructure to the proposed work
The INFN divisions involved in CMMST-VRE are CNAF (located in Bologna), Bari, Catania, Padua. All five sites have leading national expertise in the field of distributed computing, have a long experience in the development of software services for e-Infrastructures and are actively contributing to several EU and international projects. In particular, CNAF is the INFN National Center for Research and Development in informatics and hosts the INFN National Computing Center (called "Tier-1"), managing more than 15 TB of disk space, about 18 TB of tape space, about 15.000 CPU cores, and serving more than 20 international scientific collaborations. Padua, Bari and Catania are all national medium sized centers ("Tier-2") with several hundreds of terabytes of disk space and thousands of CPU cores each. All INFN centers are connected through the high-speed GARR-X network and to international networks via multiple 10 Gigabit links

4.1.18 ITMA

Description of the legal entity
Masaryk university (MU) is a public, non-profit educational and research organisation, founded in 1919 as the second Czech university. At present it comprises nine faculties with over 200 departments, institutes and clinics and is the second largest university in the Czech Republic. The Central European Institute of Technology (CEITEC) was established in 2009 as an independent institute of Masaryk University focused solely on research. It was created within the framework of the CEITEC project by four leading Brno universities and two research institutes – likewise based in Brno – who joined forces in order to establish a supraregional centre of scientific excellence combining life sciences, advanced materials and nanotechnologies.

Key people
prof. RNDr. Jaroslav Koča, DrSc [M] is as a director of CEITEC and head of Computational Chemistry Group (CCG) at CEITEC. He received his doctorate degree (DrSc) in chemistry at MU in 1993 and he is full professor at MU since 1995. His research interests are mathematical and computer assisted chemistry and biochemistry, information technology in chemistry and biochemistry, methods for analysis of conformational potential energy surfaces and energy landscapes of chemical reactions using molecular mechanics and quantum chemistry techniques. He is author of 6 monographs, 1 textbook, over 140 journal full text papers cited more than 2100 times, H-index 31.

RNDr. Petr Kulhánek, PhD. [M] is a member of CCG at CEITEC. He received his PhD in organic chemistry at MU in 2006. He is interested in application of computational techniques in simulation of chemical and biochemical processes, especially in the free energy calculations. He is author or coauthor of 26 scientific papers cited more than 285times, H-index 12.

Relevant publications, and/or products, and/or services
- Mones, L.; Kulhanek, P.; Simon, I.; Laio, A.; Fuxreiter, M. The Energy Gap as a Universal Reaction Coordinate for the Simulation of Chemical Reactions. J Phys Chem B 2009, 113, 7867–7873.

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- Strelcova, Z.; Kulhanek, P.; Kmunicek, J.; Koca, J.; Matyska, L. Implementation and Testing of Multiple Walkers Approach Based Free Energy Calculations in the Grid Environment. In Proceedings of GCCP; Bratislava, 2009; pp. 29–36.
- Kmunicek, J.; Kulhanek, P.; Strelcova, Z. Applicability of Free Energy Calculations Using High-Throughput Grid Approach. In Data driven e-Science: use cases and successful applications of distributed computing infrastructures (ISGC 2010); Lin, S. C.; Yen, E., Eds.; Springer: New York, 2011; pp. 459–474.
- Tvaroska, I.; Kozmon, S.; Wimmerova, M.; Koca, J. Substrate-Assisted Catalytic Mechanism of O-GIcNAc Transferase Discovered by Quantum Mechanics/Molecular Mechanics Investigation. J. Am. Chem. Soc. 2012, 134, 15563–15571.
- Tvaroska, I.; Kozmon, S.; Wimmerova, M.; Koca, J. A QM/MM Investigation of the Catalytic Mechanism of Metal-Ion-Independent Core 2 Beta 1,6-N-Acetylglucosaminyltransferase. Chem.-Eur. J. 2013, 19, 8153–8162.

Relevant previous projects or activities
Participation in the EGEE-I project as a member of CESNET (currently the Czech NGI).

Relevant infrastructure to the proposed work
- PMFLib – A Toolkit for Free Energy Calculations, which consists of computer libraries and utilities suitable for variety of potential of mean force calculations such as the string method and metadynamics suitable for the mechanistic studies of enzymatic reactions by means of ab initio simulations.
- Computational clusters (ca 1000 CPUs), which are shared with computational infrastructure operated by the Czech NGI. These resources will be used during adaptation of PMFLIb to the virtual environment built by the project.

4.1.19 JUELICH

Description of the legal entity
Forschungszentrum Juelich manages one of the most important supercomputing center in the world, operating supercomputers of the highest performance class in Europe. It acts synergistically with renowned hardware and software vendors like IBM, Intel and ParTec, to meet the challenges arising from the development of exaflop systems. As a member of the German Gauss Centre for Supercomputing, it has coordinated the construction of the European research infrastructure "PRACE - Partnership for Advanced Computing in Europe" back in 2008. Forschungszentrum Jülich is an active node of the Centre Europeen de Calcul Atomique et Moleculaire, (CECAM). The node is active in the fields of Computational Chemistry, Soft Matter Research and Materials Sciences. It has a strong focus on methods, algorithms and codes for computer simulations using high performance parallel computer architectures. Forschungszentrum Jülich has recently recognized the relevance of HPC-based applications for human biology by establishing an **Institute of advanced simulation "Computational Biomedicine" (IAS-5/INM-9),** involved in this EU project. Forschungszentrum Jülich and its institutes are involved in several areas of research within the Human Brain Project, the European Union FET Flagship Initiative to understand the human brain using simulation. Some of the deliverables of CMMST-VRE will be beneficial to the Human Brain Project, which is expected to last for ten years.

Key people
Paolo Carloni [M] has a joint appointment as full professor in Theoretical Biophysics at RWTH-Aachen University and is Director of the "Computational Biomedicine" Institute at Forschungszentrum Jülich. His research focuses on molecular simulations and bioinformatics approaches applied to molecular biophysics, molecular medicine and structural genomics. He has published more than peer-reviewed 220 papers and edited one book. He has given more than one hundred seminars and colloquia delivered throughout the world at the major universities, research and industrial laboratories and professional meetings. In addition, he has organized a dozen of international conferences. He has supervised the PhD thesis of 35 international

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students. He is currently leading the Molecular Dynamics working group of the Human Brain Project from the EU.

Relevant publications, and/or products, and/or services

- Musiani F., Rossetti G., Capece L., Gerger T. M., Micheletti C., Varani G., and Carloni P., Molecular Dynamics Simulations Identify Time Scale of Conformational Changes Responsible for Conformational Selection in Molecular Recognition of HIV-1 Transactivation Responsive RNA. Journal of the American Chemical Society 2014, 36 (44): p. 15631–15637
- Arcella A., J. Dreyer, E. Ippoliti, I. Ivani, G. Portella, V. Gabelica, P. Carloni, M. Orozco, Structure and Dynamics of Oligonucleotides in the Gas Phase, Angewandte Chemie 2014. DOI:10.1002/anie.201406910.
- Li J., G. Rossetti, J. Dreyer, S. Raugei, E. Ippoliti, B. Lüscher, P. Carloni, Molecular simulation-based structural prediction of protein complexes in mass spectrometry: The human insulin dimer, PLOS Computational Biology 2014. 10(9): e1003838
- Zhang C., D. Knyazev, Y. Vereshchaga, E. Ippoliti, T. H.Nguyen, P. Carloni, P. Pohl, Water at hydrophobic interfaces delays proton surface-to-bulk transfer and provides a pathway for lateral proton diffusion. Proc. Natl. Acad. Sci. USA 2012, 109: p. 9744-9749.
- Tomatis P.E., Fabiane S.M., Simona F., Carloni P., Sutton B.J., and Vila A.J., Adaptive protein evolution grants organismal fitness by improving catalysis and flexibility. Proceedings of the National Academy of Sciences of the United States of America, 2008. 105(52): p. 20605-20610.

Relevant previous projects or activities

- Organization of sponsored conferences in the field: CECAM 2013 on “Frontiers of computational biomolecular spectroscopy and mass spectrometry”; CECAM Workshop 2015 on “Computational approaches to chemical senses”.
- Grants for funds and computing resources include:
    - PRACE Grants for computing 5 ~156,330,000 core-h (last 5 years)
    - JARA-HPC Grants for computing 16 ~13,069,000 core-h (last 5 years)
    - DFG:
        - “ERA-Chemistry: Design and synthesis of biologically inspired ion-conducting nanopores”, 2014
        - “Computer-aided design of immunotoxins for a potential anti-cancer therapy”, 2014
        - “Copper binding to the physiological form of the alpha-synuclein protein”, 2013
        - “Interaction of the anticancer drug cisplatin with its cellular partners: Insights from molecular simulation”, 2012
        - “Molecular basis of odorant ligands recognition: a computational study”, 2011
        - “Ion Permeation in the Single Channel of the Bacterial Porin NanC: an integrated in silico and in vitro approach”, 2010
    - FET Flagship Initiative: Human Brain Project (WP6.3 Molecular Dynamics Simulations, 2013
    - Illy Fellowship “In silico Toxicology: Inhibiting Acrylamide Action”, 2012

Relevant infrastructure to the proposed work

- Infrastructure of Forschungszentrum Juelich, which includes access and computational resource allocations on two of the largest supercomputers in Europe, JUQUEEN (http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUQUEEN/JUQUEEN_node.html) and JUROPA (http://www.fz-juelich.de/ias/jsc/EN/Expertise/Supercomputers/JUROPA/JUROPA_node.html).
- Other smaller clusters with partitions equipped with GPUs, provided by Forscungszentrum Juelich.

4.1.20 MAUP

Description of the legal entity

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MASTER-UP is a spinoff company sprout off the Chemistry and Computer Science areas active since 2004 in the field of computer science tools for Molecular science innovation. Particular fields of activity of MASTER-UP are reaction dynamics calculations. Cloud and Grid distributed computing for Molecular Sciences. Meter and nanometer virtual reality. Electronic tests on chemical knowledge sessions management. Scientific conferences and training events organization. This SME is mainly based on research and development with strong links with academic research groups. The small structure of MASTER-UP allows direct exchange between the company leaders and young researchers, which represents an enormous advantage to the link among the SME and partners involved in this project.
These links have fostered new ideas for scientific research as well as providing underpinning science for new technologies. This proposal provides new opportunities to expand and deepen the connections between academic institutions and industrial partners, by allocating and funding specific for interactions with partners.

Key people
Dr. Maria Noelia Faginas Lago [F] works as Manager and scientific coordinator for MASTER-UP since 2004. Within MASTER-UP she coordinates the scientific partner involved inside MASTER-UP defining and executing technical projects that result sustainable for Chemistry scientific communities.
Dr. Faginas-Lago received her MSc degree and Ph.D. in Chemistry from the University of Salamanca (Spain) and the University of Perugia (Italy) in 1999 and 2002 respectively. Since 2004 she has been involved in several research and development projects. From 2006 she is the President of the Board of MASTER-UP and organizes its scientific activities. From 2009 she is an active member of the EChemTest® and leader of the Working Group taking care of the Computational Chemistry Library (Level 4).
From 2011 she is Editor of the Virt&l-Comm, the international e-magazine on electronics which originates from the joint effort of the Virtual Organization (VO) COMPCHEM, of the organization European Chemistry Thematic Network (ECTN) which takes care of the management of information technologics and the contents. Virt&l-Comm is aim to provide a service of free publishing for different fields such as innovation, research, teaching/learning.

Dr. Leonardo Pacifici [M] is a shareholder of Master Up since its creation. Now, it works as a secretary for the spin off. He graduated in 1999 in Chemistry at the University of Perugia and received his Ph.D in 2003 under the supervision of Prof. Laganà working on grid-based molecular simulators. Since 2004 he has been involved in many national and international scientific projects. He is now a post-doc at the Department of Chemistry, Biology and Biotechnologies of the University of Perugia.

Relevant publications, and/or products, and/or services
- S. Rampino, N. Faginas lago, A. Laganà, F. Huarte-Larranga, An Extension of the Grid Empowered Molecular Simulator to Quantum Reactive Scattering" J. Comput. Chem. 2012, 33, 708–714. DOI: 10.1002/jcc.22878 (2012)
- M. Alberti, L. Pacifici, M. Verdicchio, N. Faginas Lago, A. Lombardi, A. Costantini, High Level Ab Initio study of the N2+N2 Reaction channel, J. Comp. Chem. Volume 34, Issue 31, pages 2668–2676, 2013
- Costantini, O. Gervasi, C. Manuali, N. Faginas Lago, S. Rampino, A. Laganà.
- COMPCHEM: progress towards GEMS a Grid Empowered Molecular Simulator and beyond, J. Grid Computing, 8, 571 (2010).

Relevant previous projects or activities
- Organization of International Conference on Computational Science and its applications and related training events held in Suwon, Korea (2009), Perugia, Italy (2008), Kuala Lumpur, Malaysia (2007), Glasgow, UK (2006), Singapore (2005).
- Organization of the Chemistry and Material Science applications on Grid Infrastructures first edition (Trieste, 2008), (Trieste, 2010). Training grants of the Umbria region 2009, 2010, 2011.

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- Organization of the Conference "From Astrophysics to Astrochemistry towards Astrobiology" Perugia, 2012
- Organization of the COST CM-0805 The Chemical COSMOS Custody service for the activities related to regional emissions inventory (IRE) and emissions from production activities. Cost Centre Technical Management with ARPA (Regional Agency for Environmental Protection) 2012.
- Installation of the forecasting system of air pollutants at ARPA (Regional Agency for Environmental Protection) headquarters.

Relevant infrastructure to the proposed work

- MASTER-UP runs the Grid node of the COMPCHEM Virtual Organization of the European Grid Infrastructure and the local (Perugia) node of the Italian Grid Initiative.
- MASTER-UP offers cloud services to private companies in different innovative sectors of high societal impact.
- MASTER-UP supports the Italian National test center in administering the European self evaluation EChemTest sessions.

4.1.21 MOLDIS

Description of the legal entity

MOLDIS (Molecular Discovery Ltd) is an SME based in the UK, and has provided software for pharmaceutical discovery for 30 years. The software portfolio is based on the proprietary GRID software that describes molecular interaction fields for both small molecule ligands and macromolecule protein targets. The portfolio covers a range of applications including virtual screening, pharmacophore modelling, docking, binding site analysis and off-target prediction, metabolism prediction and metabolite identification, pKa prediction and ADME modelling. In CMMST-VRE MOLDIS will port it's BioGPS software (part of the FLAP suite) to the grid to enable rapid large scale protein site comparisons using their interaction fields, in a protein-pocket-omics approach. Such an application is of broad interest in the field of pharmaceutical discovery for the prediction of potential off-target effects (drug side effects), and hence will be developed as a service to be commercialised in this context.

Key people

Dr Simon Cross [M] PhD degree in Chemistry, University of Nottingham 1997-2000. He works in the area of Computational Chemistry, and is currently Senior Scientist and Product Manager for Molecular Discovery Ltd where he is also co-developer of FLAP (virtual screening, pharmacophore modelling, docking, 3D-QSAR, water prediction and modelling). In the last few years he developed FLAPpharm for pharmacophore hypothesis generation and modelling, FLAPdock for small molecule ligand docking, and has been involved in the prediction and scoring of water molecules for lead optimisation and selectivity. He is currently involved in the EU IMI project ENABLE as part of the molecular modelling hub, and recently finished an EU FP7 project OPTObacteria where he developed and optimised FLAPdock for the discovery of novel ligands against beta-lactamases.

Relevant publications, and/or products, and/or services

- WIREs Comput Mol Sci 2013, 00: 1-20 DOI 10.1002/wcms.1150
- J Chem Inf Model 2012, 52, 2587-2598 DOI 10.1021/ci3300153d
- Mol Informatics 2014, DOI: 10.1002/minf.201400028
- Curr Med Chem 2013, DOI: 10.2174/09298673113320666032 3

Relevant previous projects or activities

- OPTObacteria (FP7)
- ENABLE (IMI)

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Relevant infrastructure to the proposed work
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4.1.22 MROM

Description of the legal entity
Molecular Links Rome (MoLiRom s.r.l.) is a spin-off Company of the "Sapienza" University of Rome focused on the development of advanced projects in the synthesis, extraction and production of bioactive substances of natural origin and protein based products. MoLiRom main industrial sector is biotechnology.
MROM will contribute to CMMST activity. The unit will support the validation of computational procedures established within the consortium by monitoring the correlation of computational predictions with available experimental data, as well as will use these protocols to perform de novo calculations. In this latter case, experimental data will be provided to assess the reliability of the VRE. The unit will also contribute to dissemination and training activities, i.e. by organizing a training school dedicated to the established VRE platform within the COST Action CM1407 Chaired by Prof. Bruno Botta. The MROM unit will participate to business and sustainability tasks.

Key people
Prof. Bruno Botta [M] is full professor of Organic Chemistry at Sapienza University since 2001 and is a co-founder of the spn-off MoLiRom (http://www.molirom.com/). He has been nominated Deputy Rector for the Internationalization in November 2014 and is the Head of the Dipartimento di Chimica e Tecnologie del Farmaco since 2011. His interest during the years has been focused on the structural elucidation and synthesis of biologically active compounds derived from living plants. Since 20 years, he has been working on the field of plant tissue cultures in combination with chemistry directed toward the understanding of biosynthetic pathways of the compounds under investigation. In last years he dedicated many efforts in developing Hedgehog (Hh) signalling pathway inhibitors as anticancer agents. Prof. Botta established a vast network of national and international collaborations among which it is worth considering the long standing cooperation with recognized world leaders in the synthesis of anticancer drugs, derived both from higher plants and marine natural products. He is author of 130 publications, 5 patents (3 national and 2 international – USA and Europe) and is author and co-author of 10 books. Prof, Bruno Botta is member of several COST Actions Management Committee and is the proposer and Chair of the Action CM1407 "Challenging organic syntheses inspired by nature - from natural products chemistry to drug discovery". He has been responsible of EU and National grants.

Dr. Mattia Mori [M] obtained his degree in Chemistry and Pharmaceutical Technologies at the university of Florence in 2004. He received the PhD degree in Structural Biology at CERM – Magnetic Resonance Center of the University of Florence in 2009 under the guidance of prof. Ivano Bertini. He is now post-doctoral researcher involved in computational medicinal chemistry. Dr. Mori's research activity mainly focuses on the use of computational modeling tools, including (but not limited to) Quantum Mechanics, Molecular Dynamics, Molecular Docking and Chemoinformatics for the design and optimization of pharmacologically active small molecules. In last years, the collaboration with prof. Bruno Botta has led to a growing interest in natural compounds as lead structures for the design of Hedgehog pathway inhibitors and small molecule of pharmaceutical relevance.

Relevant publications, and/or products, and/or services

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- Uccello-Barretta, G., Balzano, F., Aiello, F., Vanni, L., Mori, M., Menta, S., Calcaterra, A., Botta, B. Hydrolytic inhibition of α-chymotrypsin by 2,8,14,20-tetrakis(d-leucyl-d-valinamido) resorc[4]arenecarboxylic acid: a spectroscopic NMR and computational combined approach (2014) Org. Biomol. Chem. [DOI: 10.1039/C4OB01936A]
- Infante, P., Mori, M., Ghirga, F., Alfonsi, R., Aiello, F., Toscano, S., Ingallina, C., Siler, M., Miele, E., D'Amico, D., Canettieri, G., De Smaele, E., Ferretti, E., Screpanti, I., Uccello Barretta, G., Botta, M., Botta, B., Gulino, A., and Di Marcotullio, L. Gli1/DNA interaction is a druggable target for Hedgehog-dependent tumors (2014) EMBOJ, DOI: 10.15252/embj.201489213
- Mascarello, A., Mori, M., Chiaradia-Delatorre, L.D., Menegatti, A.C.O., de Monache, F., Ferrari, F., Yunes, R.A., Nunes, R.J., Terenzi, H., Botta, B., Botta, M. Discovery of Mycobacterium tuberculosis Protein Tyrosine Phosphatase B (PtpB) Inhibitors from Natural Products (2013) PLoS ONE, 8 (10), art. no. e77081.
- Ghirga, F., Quaglio, D., Iovine, V., Botta, B., Pierini, M., Mannina, L., Sobolev, A. P., Ugozzoli, F., D' Acquarica, I. Synthesis of a Double-Spanned-Resorc[4]arene via Ring-Closing Metathesis and Calculation of Aggregation Propensity (2014) J. Org. Chem. 79 (22), 11051–11060.
- Botta, B., D'Acquarica, I., Delle Monache, G., Nevola, L., Tullo, D., Ugozzoli, F., Pierini, M. Nitrosonium complexes of resorc[4]arenes: Spectral, kinetic, and theoretical studies (2007) Journal of the American Chemical Society, 129 (36), pp. 11202-11212.

Relevant previous projects or activities

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Relevant infrastructure to the proposed work

Local cluster
Intel Xeon x86_64 workstation
Intel Xeon CPU E5-2690 @2.9 GHz
# of cores 16
CUDA Quadro6000
CUDA Tesla C2075
RAM 256 GB
Storage 4 TB

4.1.23 POLIMI

Description of the legal entity

Established in 1863 in Milan, and now counting approximately 40,000 enrolled students, Politecnico di Milano (POLIMI) is the largest and most renowned Engineering, Architecture and Industrial Design school in Italy. Politecnico di Milano has always fostered quality and innovation in teaching and research, cultivating a prolific relationship with the economic and manufacturing worlds. As a result, Politecnico di Milano is now ranked as one of the most outstanding European universities in Engineering, Architecture and Industrial Design, and in many areas is regarded as a leading research institution worldwide. POLIMI is in fact involved in many research and training projects with the best qualified European universities. The Department of Aerospace Science and Technology (DAST) gathers 45 faculty members, 70 postdocs and PhD students and 27 members of the technical staff. The group involved in the project works on numerical schemes for kinetic equations and has access to local computing facilities as well as to national HPC nodes.

Key people

Prof. Aldo Frezzotti [M] Born in Rome on February 4th 1952. Gender: male. Graduated cum laude in Physics on March $30th$ 1977 in the University of Milano. From July 1978 to October 1980 he has been working on thermo-physical properties of advanced nuclear fuels in the European Transuranium Elements Institute in Karlsruhe (Germany), within the framework of a EC fellowship.

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From November 1980 to November 1983 he has been working in the research and development center of Alfa Romeo SpA as research group leader on reactive flows simulations. From 1984 to 1992 he has been Assistant Professor of Mathematical Physics in the Department of Mathematics of Politecnico di Milano. From 1993 to 2000 he has been Associate Professor of theoretical mechanics in the Department of Mathematics of Politecnico di Milano. From 2001 to present he is Full Professor of theoretical mechanics in Politecnico di Milano.
He is member of the International Advisory Committee of Rarefied Gas Dynamics and member of the editorial board of CEAS journal. He has published about 70 papers on the kinetic theory of fluids and its applications.

Dr. Gian Pietro Ghiroldi [M] Born in Desenzano del Garda, October 24, 1981. Gender: Male. Citizenship: Italian. Title: PhD in Mathematical Engineering. 2006: Degree in Aeronautical Engineering at the Politecnico di Milano (Italy). 2010: PhD in Mathematical Engineering at the Politecnico di Milano. 2010-2012: Post-doctoral position at the Department of Mathematics at the Politecnico di Milano. 2013-Today: Post-doctoral position at the Department of Aerospace at Politecnico di Milano. Research interest and scientific activity: kinetic theory of gases, rarefied gas dynamics. Numerical schemes for atomistic simulations for parallel high performance computers of classical and hybrid architecture (CPU/GPU). Plasma dynamics in low voltage circuit breakers. Mathematical models and numerical methods for active barriers.

Relevant publications, and/or products, and/or services

- Tantos, C., Valougeorgis, D., Pannuzzo, M., Frezzotti, A., Morini, G.L., International Journal of Heat and Mass Transfer 79, 2014, Pages 378-389.
- Frezzotti, A. , Ghiroldi, G.P., Gibelli, L., Bonucci, A., Vacuum 103, May 2014, Pages 57-67.
- Ghiroldi, G.P., Gibelli, L., Journal of Computational Physics 258, 2014, Pages 568-584.
- Frezzotti, A. , Ghiroldi, G.P., Gibelli, L., Computer Physics Communications 182(12), 2011, Pages 2445-2453.
- Lorenzani, S., Gibelli, L., Frezzotti, A., Frangi, A., Cercignani, C., Nanoscale and Microscale Thermophysical Engineering 11, 2007, Pages 211-226.

Relevant previous projects or activities

- CARIPLO 2005 Project "Models for the behavior of solid and fluids at the micro/nanoscale"
- CARIPLO 2007 Project "Dissipative and failure phenomena in Micro and Nano Electro Mechanical Systems"
- CARIPLO 2009 Project "Interaction between surface in micro/nano devices"
- PRIN 2009: Mathematical Problems of Kinetic Theories

Relevant infrastructure to the proposed work

- The group has access to the following local computing facilities
    - Dual exacore processor ThinkStation equipped with NVIDIA GTX 780 GPU.
    - Linux cluster with 192 cores.
- Access to national HPC facilities is also granted by agreements between Politecnico di Milano and CINECA

4.1.24 RWTH

Description of the legal entity

The Rheinisch-Westfälische-Technische Hochschule Aachen (CHAA) belongs to the largest universities in Germany with a long-standing excellent research tradition. The Chemistry division of the RWTH consists of

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32 professors. Besides the theoretical chemical workgroups, a great number of work groups in organic and inorganic work groups use theoretical methods as well. In today´s chemistry, the close combination of experimental and theoretical methods belongs to the key techniques to advance chemical sciences. At RWTH Aachen, a multitude of chemical groups uses this approach. Within the faculty of mathematics, informatics and natural sciences, an ideal research environment is supported by the German excellence initiative. Moreover, in the profile area of Molecular Science & Engineering (MSE) an ideal interdisciplinary a stimulating research environment has been created.
Within the Jülich-Aachen-Research Alliance (JARA), RWTH is supported by the Forschungszentrum Jülich in research and application of distributed and parallel computation technologies (Jülich Supercomputing Centre (JSC)). The JSC provides with several high performance computing resources and the JUQUEEN System which offers scientists a modern platform for simulations. The JSC contributes significantly to the PRACE initiative (Partnership for Advanced Computing in Europe) and forms in joint activity with the John von Neumann Institut für Computing (NIC), the LRZ, and the Höchstleistungsrechenzentrum Stuttgart (HLRS) the largest and most powerful supercomputer infrastructure in Europe within the Gauss Centre for Supercomputing (GCS).

Key people
Prof. Dr. Sonja Herres-Pawlis [F] is Professor for Bioinorganic Chemistry at RWTH in the Department of Chemistry. She is inorganic chemist with interdisciplinary interest in catalyst development for polymerisation and oxidation reactions. For research, she combines experimental studies in synthetic chemistry with extensive computational studies using quantum chemistry. Her research interests include the use of workflows in quantum chemistry for the full spectroscopic characterisation of compounds. She has several research grants for projects in catalyst development with theoretical methods. She published 90 papers in chemical journals and at conferences, 4 book chapters and 4 patents. She has a lot of expertise in using the quantum chemistry codes on several cluster systems like the ARMINIUS (Paderborn), the SuGI (Köln), the LiDO (Dortmund) and the LRZ (Munich). Besides a number of research prizes and fellowships, she has been awarded the Innovation Prize of Northrhine-Westfalia. She belongs to the founders of the German BMBF-supported project Molecular Simulation Grid (MoSGrid). In this function, she established the quantum chemical subgroup of the MoSGrid community and organised the MoSGrid community management. The Herres-Pawlis group consists of seven PhD students and one Postdoc.

Relevant publications, and/or products, and/or services
- J. Krüger, R. Grunzke, S. Gesing, S. Breuers, A. Brinkmann, L. de la Garza, O. Kohlbacher, M. Kruse, W.E. Nagel, L. Packschies, R. Müller-Pfefferkorn, P. Schäfer, C. Schärfe, T. Steinke, T. Schlemmer, K. Warzecha, A. Zink and S. Herres-Pawlis: *The MoSGrid Science Gateway – A Complete Solution for Molecular Simulations*, Journal of Chemical Theory and Computation 2014, 10 (6), 2232–2245, DOI: 10.1021/ct500159h.
- A. Hoffmann, S. Herres-Pawlis, Hiking on the potential energy surface of a functional tyrosinase model – implications of singlet, broken-symmetry and triplet description, Chem. Commun. 2014, 50, 403 - 405.
- A. Hoffmann, S. Binder, A. Jesser, R. Haase, U. Flörke, M. Gnida, M. Salomone Stagni, W. Meyer-Klaucke, B. Lebsanft, L. E. Grünig, S. Schneider, M. Hashemi, A. Goos, A. Wetzel, M. Rübhausen, S. Herres-Pawlis, Catching an entatic state – a pair of copper complexes, Angew. Chem. 2014, 126, 305 - 310; Angew. Chem. Int. Ed. 2014, 53, 299 - 304.
- A. Hoffmann, C. Citek, S. Binder, A. Goos, M. Rübhausen, O. Troeppner, I. Ivanović-Burmazović, E. C. Wasinger, T. D. P. Stack, S. Herres-Pawlis, Catalytic Phenol Hydroxylation with Dioxygen: Extension of the Tyrosinase Mechanism Beyond the Protein Matrix, Angew. Chem. 2013, 125, 5508 - 5512 ; Angew. Chem. Int. Ed. 2013, 52, 5398 - 5401.
- I. dos Santos Vieira, E. L. Whitelaw, M. D. Jones. S. Herres-Pawlis, Synergistic Empirical and Theoretical Study on the Stereoselective Mechanism for the Aluminium Salalen Complex mediated Polymerisation of rac-Lactide, Chem. Eur. J. 2013, 19, 4712 - 4716.

Relevant previous projects or activities
- MoSGrid: Molecular Simulation Grid (BMBF, grant 01IG09006)
- ER-Flow: Building an European Research Community through Interoperable Workflows and Data

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(EU/FP7/ 312579)
- FOR1405: Dynamics of Electron Transfer Processes within Transition Metal Sites in Biological and Bioinorganic Systems (DFG research unit, leadership and two projects)

Relevant infrastructure to the proposed work
The MoSGrid infrastructure supported by the compute centers of the universities of Tübingen, Dresden, Cologne and Paderborn will serve for prototyping of services.

4.1.25 UCPH

Description of the legal entity
University of Copenhagen is a highly ranked international University with high-quality education. The Department of Drug Design and Pharmacology has strong expertise and track record within drug design, including computational chemistry.

Key people
Dr. David Gloriam [M] is an Associate Professor in computational drug design. He applies state-of-the-art techniques to identify new ligands for a range of targets, and also develops new methods and the major database for G protein-coupled receptors (GPCRDB), which is the largest drug target protein family. Thus, he has an extraordinary profile in database and web server tool development for medicinal chemistry, and a strong community and network of related resources. In 2014, he received a prestigious ERC Starting Grant, which involves the development of additional new bioinformatics and computational chemistry techniques. Gloriam has led several interdisciplinary ligand discovery and optimization projects, and the GPCRDB database development including a range of European labs. He is a management committee member of a EU COST Action.
He received his MSc degree (2003) and Ph.D. in Medicine (2006) from Uppsala University, Sweden. He conducted two postdocs at EMBL-EBI and GlaxoSmithKline, respectively, before joining the University of Copenhagen in 2008.

Relevant publications, and/or products, and/or services
- Isberg, V., .. Gloriam, D.E., Generic GPCR Residue Numbers - Aligning Topology Map While Minding The Gaps., Accepted by Trends in Pharmacological Sciences
- Isberg, V., B. Vroling, R. van der Kant, K. Li, G. Vriend and D.E Gloriam., GPCRDB: information system for G protein-coupled receptors. Nucl. Acids Res. 2014;42:422-425
- Rydberg P, Gloriam DE, Olsen L, The SMARTCyp cytochrome P450 metabolism prediction server. Bioinformatics 2010;26:2988-2989.
- Bourbeillon J..., D.E. Gloriam et al., Minimum information about a protein affinity reagent (MIAPAR). Nature Biotechnol. 2010;28: 650-653
- Taussig M.J..., D.E. Gloriam et al., ProteomeBinders: planning a European resource of affinity reagents for analysis of the human proteome. Nature Methods 2007;4: 13-17

Relevant previous projects or activities
- Received a 2014 ERC Starting Grant, which includes development of new drug design methods
- Head of GPCRDB: The G protein-coupled receptor database (gpcrdb.org)
- Developed SMARTCyp: A widely used software for site-of-metabolism predictions (farma.ku.dk/smartcyp)

Relevant infrastructure to the proposed work
GPCRDB (gpcrdb.org) is a hub for several online servers for bioinformatics, protein modeling and drug design. It includes a suite of analysis and visualisation tools, and is interlinked with other related resources. It leads the development of new server tools within the field of GPCRs, and together with its 20+ history and ~1000 users every month has placed it as the one-stop-shop and portal.

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4.1.26 VILN

Description of the legal entity
The Stichting European Grid Initiative (also referred to as "EGI.eu") is a not-for-profit foundation established under Dutch law to coordinate and manage the European Grid Infrastructure (EGI) federation on behalf of its members: VU MIF is a coordinator and main partner of Lithuanian parallel and distributed computing and e-services network Lithuanian Grid Infrastructure**.** participate actively in the development of computational systems such as **theoretical computer science** (neural networks, software process, semantics of programs, artificial intelligence, retrieval of logical proofs, error-correcting codes, cryptography, discrete algorithms and structures, probabilistic analysis of number-theoretical structures, combinatorial statistics, and randomized algorithms), **applied computer science** (computer vision computational geometry, visualization, speech and signal processing, data structures and algorithms, open queuing networks, message switching systems, information security, electronic signature, **software engineering** (software process, software engineering methods and tools, software quality management, business process modeling, information systems modeling, human–computer interaction), **information and computing technologies** (grid computing, cloud computing, virtualization, service oriented frameworks, Internet technology and information systems). VU MIF provides also service to researchers from each department of Vilnius University and offer IT resources on demand. Cloud computing technology analysis are performed, too.

Key people
Rimantas Kybartas [M] has worked as a lecturer and freelance researcher at Vilnius University since 2011. He performs research in fields of Cloud computing and machine learning. He worked in Bank of Lithuania from 2002 till 2014 years, where performed managing user requirements, engineering and developing treasury management system components (using *Microsoft* .NET, C#, *Oracle* database).
Rimantas obtained Master degree from Vilnius University and finished Ph. D. of computer science (machine learning) studies at this university in 2010. During his studies he was constanntly involved in various scientific projects such as 'Promotion of Socioeconomic Development and Encouragement of Entrepreneurship by Developing Cross-border R&D and Innovation Network in Cloud Computing Area'. He has also expierence developing software in Delphi programming language, managing small projects, programming in C and C++, programming in assembler, software design in UML.

Dr. Jelena Tamuliene [F] worked as senior research fellow since 2004. She performs modelling and investigation of metal nanoparticles and their properties as well as investigations of dendrimers, nuclei basis and their derivatives. She was the coordinator of the LitGrid project and was involved in several e-infrastructure research and development BalticGrid, BalticGridII and InsPire projects. She is Lithuanian NGI International Liaisons.
Jelena received Ph.D. in physics from Institute of Theoretical Physics and Astronomy in 2000. In 2012 she received Master in Business Economy from Vilnius University. She assisted EGI with reviewing existing applications provided by EGI members from the 'Computational Chemistry and Material Sciences' domain, identifying key scientific applications that could benefit from resources and services of the National Grid Infrastructures, and assist the integration of these applications into EGI through the setup of focused technical project in 2012. She has taken part in several Virtual Teams of EGI activities since 2012.

Relevant publications, and/or products, and/or services
- Rimantas Kybartas, Fuzzy Templates for Pair-wise Multi-class Classification, ICPRAM (2) , 2012, p. 564-567;
- Sarunas Raudys, Rimantas Kybartas, Edmundas Kazimieras Zavadskas, Multicategory nets of single-layer perceptrons: complexity and sample-size issues. IEEE Transactions on Neural Networks 21(5): 2010, p. 784-795;
- Rimantas Kybartas, Nurdan Akhan Baykan, Nihat Yilmaz, Sarunas Raudys, Multiclass Mineral Recognition Using Similarity Features and Ensembles of Pair-Wise Classifiers. IEA/AIE (2), 2010, p 47-56

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- K. Paulikas, J. Tamulienė, R. Vaišnoras, G. Badenes, L.M. Balevičius,. Dendrimerų molekulių ertmių prigimties nustatymas naudojant GRID'Ą, Jaunųjų mokslininkų darbai. 2008, Nr. 3 (19), p. 194-201. [CEEOL.; IndexCopernicus];
- A. Juozapavicius, J.Tamuliene, V.Tomkus, S.Lapienis. GRID computing for the space technology research, Space Research Review, 1, 213-219 (2012);

Relevant previous projects or activities

- "Multi-class error estimating pattern recognition methods for security and risk analysis"; (2011-2012), project participant
- EGI-InSPIRE: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe, Project Coordinator, RI-261323
- LitGrid (2005-2006), Project coordinator;
- BalticGrid (2005-2007), project participant;
- BalticGridII (2008-2010), project participan

Relevant infrastructure to the proposed work

Local 1500 core cluster

4.1.27 CSPG

Description of the legal entity

The University of Perugia plays a prominent role in the Italian and the European academic and research environments. The University is 707 years old, has 3 excellence centers, 16 Departments and approximatively 30.000 students. The Department of Mathematics and Computer Science is composed by 11 Full Professors, 19 Associate Professors, 27 Researchers. The Department is part of the EGI Grid Infrastructure with a small cluster since 2004 and the research group manages the COMPCHEM Virtual Organization since then.

Key people

Dr. Osvaldo Gervasi [M] is researcher at the Department of Mathematics and Computer Science since 2001. He teaches Network Architecture, Virtual Reality and Operating Systems. He has been involved in several European research projects: EGEE, EGEE-III, EGI. He leaded the Working Group "SIMBEX: Simulation of Molecular Beam Experiments" in the COST in Chemistry action D23 (Metachem: Metalaboratories for Complex Computational Apllications in Chemistry) and the Working Group "E-science and Learning Approaches for Molecular Science" of the action D37 (Grid Computing in Chemistry: GridChem).

Dr. Sergio Tasso [M] is Aggregate Professor at the Department of Mathematics and Computer Science since 2001. He teaches Simulation, Open and Distributed Systems and Computer Networks: Protocols. He participated to the Working Group "SIMBEX: Simulation of Molecular Beam Experiments" in the COST in Chemistry action D23 (Metachem: Metalaboratories for Complex Computational Apllications in Chemistry) and to the Working Group "E-science and Learning Approaches for Molecular Science" of the action D37 (Grid Computing in Chemistry: GridChem).

Dr. Simonetta Pallottelli [F] is Aggregate Professor at the Department of Mathematics and Computer Science since 2005. He teaches Multimedia Systems.

Relevant publications, and/or products, and/or services

- A. Costantini, O. Gervasi, F. Zollo, L. Caprini, User Interaction and Data Management for Large Scale Grid Applications, (2014) Journal of Grid Computing, V. 12, Issue 3, pp. 485-497, DOI: 10.1007/s10723-014-9300-0
- A. Costantini; E. Gutierrez; J. Lopez Cacheiro; A. Rodriguez; O. Gervasi; A. Laganà (2010). On the

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extension of the Grid Empowered Molecular Science simulator: MD and visualization tools. INTERNATIONAL JOURNAL OF WEB AND GRID SERVICES (ISSN:1741-1106), 141-159 6;
- A. Costantini; O. Gervasi; C. Manuali; N. Faginas Lago; S. Rampino; A. Laganà (2010). COMPCHEM: progress towards GEMS a Grid Empowered Molecular Simulator and beyond. JOURNAL OF GRID COMPUTING (ISSN:1570-7873), 571-586 8;
- A. Laganà , O. Gervasi (2009). A priori molecular virtual reality on EGEE grid. INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY (ISSN:0020-7608), 446-453 110 (2);
- D. Skouteris; O. Gervasi; A. Laganà (2009). Quantum mechanical studies using cylindrical coordinates. The nanotube case study. COMPUTER PHYSICS COMMUNICATIONS (ISSN:0010-4655), 459-465 180;

Relevant previous projects or activities
- EGI-InSPIRE: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe, member, RI-261323
- EGEE III: FP7-INFRA-2007 Enabling Grid for E-Science III. Member. Project reference 222667

Relevant infrastructure to the proposed work
- COMPCHEM Virtual Organization Management on EGEE and EGI Grid Infrastructures for supporting the Computational Chemistry Community Computational needs.
- UNIPG Grid Site Management on EGEE and EGI Grid Infrastructures

4.1.28 IMIP

Description of the legal entity
IMIP is the acronym for Istituto di Metodologie Inorganiche e dei Plasmi, a CNR (Consiglio Nazionale delle Ricerche) Institute, located in Bari, Italy. The research in the Institute concerns elementary processes in gases and plasmas, with molecular ro-vibrational and electronic resolution, while electronically excited levels are considered for atoms. Atom/molecule interactions with different solid surfaces are studied. Kinetic and fluid dynamic codes have been developed by the IMIP researchers for the simulation of different systems like laser-solid interaction, re-entry problems, transport properties in plasma, electrical thrusters, non-equilibrium plasma for fusion applications. The relevant expertise is summarized below: • Molecular Dynamics studies on electron-molecule, molecule-molecule and heterogeneous energy exchange and reactive processes for plasma material processing, astrophysics, aerospace and fusion related applications (negative ion sources, divertor). • implementation of a hybrid bi-dimensional model for the description of the plume of an electric thruster for spatial applications • thermodynamics and transport studies for multi-temperature plasmas • chemical-physical models for high enthalpy supersonic expansions • Monte Carlo models for the solution of kinetic problems in the physics of shock waves, detonations and gas discharge.

Key people
Mr. Fabrizio Esposito [M] was born in Taranto (Italy) in 1966, graduated cum laude in Physics from University of Bari (Italy) in 1994, and received his PhD in Chemical Sciences in 1999 from the same University. He has been researcher in General Chemistry for two years at the Bari University since 1999. He is now researcher of IMIP (Institute of Inorganic Methodologies and Plasmas of CNR, National Research Council of Italy) since 2001. His interests are in the field of computational molecular dynamics, with applications in rovibrational kinetics of air species (reentry of spacecrafts, atmospheric chemical kinetics), in nuclear fusion chemistry (divertor, negative ion production), and in astrochemistry. He is author of more than 40 publications on ISI journals, with about 760 citations (2014)

Ms. Maria Rutigliano [F] was born in Barletta (Italy) on April 30th 1968. She graduated in Physics at the University of Bari in 1993. Since 2001 she is a researcher at the Institute of Inorganic Methodologies and of Plasmas of the Italian Research Council. Its research field is focused on investigation of surface processes, assisted by phonon and/or electronic excitations by Molecular Dynamics Calculations using a semiclassical

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method. Main research results include determination of recombination/dissociation probability and coefficients, reaction energetics, vibrational and rotational distributions, probability for different surface processes, effect on reaction dynamics of surface temperature, modification and site. She has published around 35 papers in high quality peer reviewed journals and has participated as speaker to different international and national conferences.

Mr. Domenico Bruno [M] was born in Napoli (Italy) on August 5th 1970. He graduated cum laude in Physics at the University of Bari in 1997. In 2001 he obtained the Doctorate in Chemistry at the University of Bari. Since 2001 he is a researcher at the Institute of Inorganic Methodologies and of Plasmas of the National Research Council. Main research interests include: 1) Monte Carlo methods for the kinetic simulation of reacting gas mixtures and collisional plasmas under non-equilibrium conditions; 2) kinetic theory of transport processes in these systems. He has published around 60 papers in high quality peer reviewed journals.

Ms. Iole Armenise [F] was born in Bari (Italy) on June 8th 1966. She graduated in Physics at the University of Bari in 1992. In 1996 she obtained the PhD in Chemical Sciences at the University of Bari (final national examination in Pisa). In 1997 she obtained the Post-Graduate Diploma in Fluid Dynamics, Option: Aeronautics & Aerospace, at the Von Karman Institute for Fluid Dynamics, Rhode-Saint-Genese, Belgium. Since November 2000 to October 2002, she obtained a 'Research Fellowship' at ESTEC-ESA, Noordwijk, The Netherlands. Since September 1998 she is a researcher of the National Research Council (at the cscp, now IMIP, Institute of Inorganic Methodologies and of Plasmas). Main research fields include: 1) Gas-Phase state-to-state vibrational kinetics in N2/N/O2/O/NO and CO2/CO/C/O/O2 mixtures; 2) Gas-surface interaction in re-entry problems in air; 3) Hypersonic boundary layers.

Relevant publications, and/or products, and/or services

- F. Esposito, I. Armenise, and M. Capitelli, Chemical Physics 331, 1 (2006).
- F. Esposito, I. Armenise, G. Capitta, and M. Capitelli, Chemical Physics 351, 91 (2008).
- D. Bruno, M. Capitelli, S. Longo, P. Minelli, Direct Simulation Monte Carlo modeling of non equilibrium reacting flows. Issues for the inclusion into a ab initio molecular processes simulator, LECTURE NOTES IN COMPUTER SCIENCE, 3044 383-391 (2004) International Conference on Computational Science and its Applications, S. Maria degli Angeli, Assisi, Perugia (Italy) May 14-17, 2004 (Eds. M.L. Gavrilova, V. Kumar, Y. Mun, C.J.K. Tan, O. Gervasi).
- D. Bruno, M. Cacciatore, S. Longo, M. Rutigliano, Gas-surface scattering models for Particle Fluid Dynamics: A comparison between analytical approximate models and Molecular Dynamics calculations, Chem. Phys. Lett. 320, 245 (2000).
- M. Capitelli, I. Armenise, D. Bruno, M. Cacciatore, R. Celiberto, G. Colonna, O. De Pascale, P. Diomede, F. Esposito, C. Gorse, K Hassouni, A Laricchiuta, S Longo, D Pagano, D Pietanza and M Rutigliano, Plasma Sources Science and Technology 16, S30 (2007).

Relevant previous projects or activities

- Phys4Entry, "Planetary Entry Integrated Models", Call FP7-SPACE-2009-1, project 242311.
- Participation in the project "Piattaforme abilitanti per griglie computazionali a elevate prestazioni orientate a organizzazioni virtuali scalabili", MIUR PNR 2001-2003, FIRB art. 8, contract n.RBNE01KNFP
- Research Contract ESA Platinum Purch.Ord.5401000700 - Prot.CNR IMIP 447 del 02/03/2011 "TRANSPORT PROPERTIES OF HIGH TEMPERATURE COMPONENTS OF SI/C/O PLASMA FROM 100 TO 20000K INCLUDING ELECTRONICALLY EXCITED STATES" – Statement of Work Reference TEC-MPA/2010/883/DG - CUP B91J11000760006
- Scientific cooperation agreement between CNR and Promes/CNRS (Francia) – 2012-2013 "Hydrogen atoms recombination on tungsten for ITER- Experiments and molecular dynamics simulation"
- ESA CCN1 to contract 21790 prot.n.0000739 del 02/04/2012 "Thermodynamics and Transport properties of atomic-Hydrogen Plasmas"

Relevant infrastructure to the proposed work

- one server:

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  - 2 cpu Intel Xeon E5-2695 v2 (12 cores per processor)
  - 256GB RAM
- two coprocessors MIC:
  - Intel® Xeon Phi™ Coprocessor 5110P
  - (8GB, 1.053 GHz, 60 cores per coprocessor)
- one server:
  - intel Xeon E5620 quad core
  - 8GB RAM
- four servers:
  - 2 processors Intel Xeon X5570 quad core
  - 24 GB RAM
- one server:
  - 48GB RAM
  - 2 processors Intel Xeon X5690 esa core

4.1.29 CHMI

Description of the legal entity

The University of Milan, established in 1924, is a public teaching and research-intensive university, the only Italian among the 21 prestigious members of LERU (League of European Research Universities), and an internationally high-ranked university. With a teaching staff of about 2.200 tenured professors and with almost 60.000 students, the University of Milan is the largest university in Lombardy, one of the most dynamic and internationally-oriented EU regions and leader in the Italian economy. The University of Milan has a deserved reputation as one of the European universities that is most seriously committed to research. Research activities are conducted in 31 Departments and 29 Inter-departmental Research Centres and their results are attested by a significant quantity of scientific publications (more than 24.000 in the last three years) and international patent applications. The University's researchers occupy leading positions in numerous research programmes conducted both at a national and international level. Moreover, since years, the University of Milan is focused in the protection and exploitation of the scientific productivity. To this aim it has developed a policy aimed to facilitating and shortening the time and mode of transfer of results from research to market and it has built relationships with different third party (Industry; not profit organization, institutional entity; SME) that it necessary to fill the gap exists between research and market.

Several patent applications, in co ownership with partners, have been filed to protect results developed within European Project. EU programmes represent a major source of funding for the University of Milan, which up to December 2012 has signed 135 contracts with the EU under the 7th Framework Programme (2007-2013), for a total value of € 46.351.414. 10 more projects are currently in the negotiation phase. Research and training at the University of Milan is recognised as being of an extremely high standard (1st place in Italy, 58th in the world by The Leiden Ranking – Universiteit Leiden).

Michele Ceotto is part of the Department of Chemistry, which consists of 87 members, between professors and research staff members (52% of whom are women), 30 technical staff and 19 administrative. It is one of the most productive Chemistry Departments in the country. An impressive collection of state-of-the-art facilities and a commitment to being at the forefront of developing technologies make the Department a centre of excellence for academic research. In addition to the Masters courses in Chemistry and Industrial Chemistry, the Department has two active PhD programmes in "Chemical Sciences" and "Industrial Chemistry" hosts every year ca. 50 PhD students and 50 post-docs.

The University of Milan assists researchers: in accessing EU funds, in the achievement of innovative results and in the exploitation of them by: Negotiating research-related contracts and agreements; Consulting on Intellectual Propriety Rights issues; Supporting University and Divisional research-related planning; Promoting the responsible conduct of research and compliance with regulatory requirements; Supporting Intellectual property protection of innovative results; Promoting exploitation of research results;

The continuous improvement of research administration is based on a constant training of personnel and the access to relevant information through: meetings with national delegates and other EU program representatives; Sharing of good practise on IP management between the major EU universities; Supporting

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the development of the University's knowledge exchange/knowledge transfer activities and its partnerships with key external organizations and facilitating technology transfer within international research projects is also among the main goals of the University of Milan.

Key people

Micheme Ceotto [M]

- 2006 Assistant Professor, Department of Chemistry, Università degli Studi di Milano
- EDUCATION
- 2005-2006 Postdoctoral Fellow, "Center for Biophysical Modeling and Simulation", Prof. G.A. Voth's group, Dept. of Chemistry, University of Utah, Salt Lake City (USA)
- 2005-2000 PhD in Chemistry, University of California at Berkeley (USA); advisor Prof. W. H. Miller, thesis's title: "Semiclassical and Quantum Instanton approximations for thermal rate constants of chemical reactions"
- 2000-1999 Laurea (M.S.) in Physics (110/110), Università degli Studi di Roma "La Sapienza"
- 2000 TMR Researcher, "Consejo Superior de las Investigaciones Cientificas" (CSIC) and "Istituto de Matematicas y Fisica Fundamental" (IMAFF), Madrid (Prof.s Garcia-Vela and Delgado-Barrio)
- 1999-1991 Laurea (M.S.) in Chemistry (110/110 e lode), Università degli Studi di Roma "La Sapienza" (Advisor: Prof. F.A. Gianturco)
- FELLOWSHIPS AND AWARDS
- 2000-2005 University of California at Berkeley (USA): International student fellowship for graduate studies in Theoretical & Computational Physical Chemistry
- 2000-2001 Fellowship by the "Consiglio Nazionale delle Ricerche" (CNR) for studies outside Italy
- 2000 European Union Training and Mobility for Researchers (TMR) Fellowship at the C.S.I.C. (Consejo Superior de las Investigaciones Cientificas) in Madrid
- 1998 Visiting student Fellowship at University of Warwick (UK), Chemistry Dep.
- 1995-1991 I.D.I.S.U. (Regional Institute of University Studies) Annual Fellowship for outstanding GPA in each academic year
- 1995-1991 Tax-free application at the University of Rome "La Sapienza" for outstanding GPA at each academic year
- 1998-1990 Italian National Federation "Cavalieri del Lavoro" Fellowship (20 nationwide each year): full board and lodging during all undergraduate studies
- SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS
- Present: C. Aieta (PhD); R. Bellani (Master); G. Diliberto (Master)
- Past: 2007 D. dell'Angelo, Master Thesis in Chemistry (now postdoctoral fellow at Univ. South Carolina)
- 2008 S. Valleau, Bachelor and Master Thesis in Chemistry (now PhD student at Harvard University)
- 2010 D. Lotti, Bachelor and Master Thesis in Chemistry (now PhD student at Univ. of Zurich),
- 2010 M. Azzola, Bachelor and Master Thesis in Chemistry (Physics student)
- 2010 C. Aieta, Bachelor in Chemistry (Bachelor student)
- 2012 R. Conte, Postdoctoral Fellow (now postdoctoral fellow at Emory University)
- 2013 S. Mandra, PhD Thesis in Physics (now postdoctoral fellow at Harvard University)
- 2013 G. Diliberto, Bachelor in Chemistry (Master student)
- 2013 F.S. Dambrosio, Bachelor Thesis in Chemistry (Physics student)
- 2014 C. Aieta, Bachelor in Chemistry (Master student)
- TEACHING ACTIVITIES
- @ University of California at Berkeley
- Fall 2006-07 Physical Chemistry Laboratory: Statistics and Thermodynamics (undergrad. div.)
- Fall 2002 Biophysical Chemistry: Principles of Thermodynamics (upper division)
- Fall 2001 Quantum Mechanics: Principles of Quantum Mechanics (graduate division)
- Fall 2000 Principles of Chemistry: Principles of chemistry (undergraduate division)
- @ Università degli Studi di Milano
- Since 2007 Theoretical Chemistry: Classical and Quantum Molecular Dynamics (master div.)
- Since 2006 Lab. of Physical Chemistry I: statistical theory of experimental data treatment (undergr. div.)
- Fall 2007-08 Lab. of Physical Chemistry A: software for ab initio calculations (master div.)
- Since 2009 Principles of Physical Chemistry: atoms and Molecule (undergraduate division)

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- Since 2011 Spectroscopy(Part I): Fundamental theory for spectroscopical techniques (und. div.)
- ORGANIZATION OF SCIENTIFIC MEETINGS
- CECAM Workshop:"Many-dimensional quantum dynamics with (non)classical trajectories", June 06/17/13-06/21/13, Lausanne, Switzerland; http://www.cecam.org/workshop-0-884.html
- INSTITUTIONAL RESPONSABILITIES
- 2014, 2010 Master degree Committe member, Ecole Polytechnique Fédérale de Lausanne (EPFL)
- 2012-present Teaching Committee of Chemistry and Industrial Chemistry (Comissione Didattica);
- 2012-present Committee for High schools Orientation (Comissione Orientamento);
- 2012-present Committee for internal evaluation and planning (Comissione Valutazione e Programmazione);
- 2010-2012 Committee of Doctoral School of Chemical Science (Comissione Dottorato)
- 2012-present "Collegio" of Doctoral School of Chemistry
- External examinator for the Department of Chemistry of EPFL (Lausanne)
- 2010 M. Wehrle, Master exam
- 2014 J. Rohrbach, Master exam
- MEMBERSHIP OF SCIENTIFIC SOCIETIES
- 2002- Present American Chemical Society
- 2006-Present Italian Chemical Society
- MAJOR COLLABORATIONS
- A. Aspuru-Guzik (Harvard University): Ab initio calculations for semiclassical dynamics
- W.L. Hase and Y. Zhuang (Texas Tech): Hessian integrators for semiclassical molecular dynamics
- D. Tamascelli (University of Milan): GPU accelerated semiclassical molecular dynamics
- L. Lo Presti (University of Milan): Plane Wave (VASP, QE) and atom-centered (CRYSTAL) DFT calculations of doped TiO2
- L. Falciola and S. Ardizzone (University of Milan): Characterization and photocatalysis of doped titania for photocatalytic enviromental remediation
- G. Cappelletti and P. Fermi (University of Milan): Characterization of nanotexured titania films for outdorr cultural heritage protection
- J. Schrier (Haverford College, USA): Helium Isotope Enrichment by Resonant Tunneling Through Nanoporous Graphene Bilayers
- COMMISSIONS OF TRUST
- 2012 Dataset Papers in Atomic and Molecular Physics
- 2013 Frontiers in Chemistry
- Referee for:
- Ministero dell'Università e della Ricerca; J. Chem. Phys.; J. Chem. Theory and Compu.; J. Phys. Chem.; J. of Material Chemistry; Mol. Phys.; International Journal of Quantum Chemistry; RCS Adv.; Dalton Transactions; Phys. Chem. Chem. Phys.; Chemistry of Materials;

Relevant publications, and/or products, and/or services

- D. Tamascelli, F.S. Dambrosio, R. Conte, M. Ceotto*, "Graphics Processing Units Accelerated Semiclassical Initial Value Representation Molecular Dynamics", J. Chem Phys., 140, 174109 (2014);
- R. Conte, A. Aspuru-Guzik, M. Ceotto*, "Reproducing Deep Tunneling Splittings, Resonances, and Quantum Frequencies in Vibrational Spectra From a Handful of Direct Ab Initio Semiclassical Trajectories", J. Phys. Chem. Lett., 4, 3407−3412 (2013);
- M. Ceotto*, Y. Zhuang and W.L. Hase, "Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme", J. Chem. Phys. 138, 054116 (2013);
- Y. Zhuang*, M. R. Siebert, W.L. Hase, K.G. Kay, M. Ceotto*, "Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations" J. Chem. Theory and Computation, 9 (1), 54-64 (2013)
- M. Ceotto*, G.F. Tantardini, A. Aspuru-Guzik, "Fighting the curse of dimensionality in first-principles semiclassical calculations: Non-local reference states for large number of dimensions", J. Chem. Phys. 135 (21), 214108 (2011)

Relevant previous projects or activities

- 2014-2015: "ab initio Semiclassical Molecular Dynamics", role of the proponent PI, amount 7000€,

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Interdisciplinary Laboratory for Advanced Simulations by CINECA (the Italian Computational Center)
- 2011: INVIDIA (8000 € in GPUs) "GPU accelerated semiclassical molecular dynamics"
- 2013-2009 "Cinque per mille" grant by the University of Milan (40000 €) "Monitoring and environmental remediation of organic and inorganic pollutants from waste waters: a theoretical and experimental approach"
- 2011-2009 Italian Minister of Research (117000 €) "DFT calculations of confined nano-systems"
- 2009-2007 Italian Minister of Research (121000 €) "Quantum-mechanical calculations for gas phase molecular spectra"

Relevant infrastructure to the proposed work
Access to national CINECA HPC facilities.

4.1.30 BBLU

Description of the legal entity
Hosting the BBLU group, National Institute of Chemistry (NIC) is one of the major research institutes in the country and is by far the largest in the field of chemistry and related sciences. Practiced at the institute for about 40 years, computational chemistry has been one of the most respected disciplines, establishing strong tradition of high impact research and featuring a number of renowned scientists. Current expertize of BBLU includes state-of-the art research in computational studies of enzyme catalysis, nuclear quantum effects, hydrogen bonding and solid state chemistry. Parallel computing on reasonably sized clusters has been practiced at the institute for about 20 years. In addition, the institute hosts a number of experimental disciplines that are often combined with theoretical work (including IR and NMR spectroscopy, molecular biology, catalysis, etc.). This provided substantial experience in a collaborative use of simulation techniques, as proposed in the service.

Key people
Dr. Jernej Stare [M], currently Senior Research Associate at NIC
- PhD in Chemistry, 2003
- 2004-2006 postdoc at Center for Nonlinear Studies, Los Alamos National Laboratory, New Mexico, USA: Studies of structure and catalytic activity of titanosilicalite zeolite catalysts, supervisor: Prof. Juergen Eckert
- 2012-2013 visiting researcher at Laboratory of computational chemistry and biochemistry, Swiss Institute of Technology Lausanne (EPFL): Classical and QM/MM simulation of interactions between organometallic cytostatics and proteins, host: prof. Ursula Röthlisberger

Prof. Janez Mavri [M], currently Scientific Counsellor at NIC and head of Laboratory of biocomputing and bioinformatics
- PhD in Chemistry, 1992
- 1993-1995 postdoc at the group of Prof. Herman J. C. Berendsen, Groningen, The Nederlands
- 1995-1996 visiting researcher at the group of Prof. Hans Vogel, Department of Biochemistry, University of Calgary, Canada
- 2003 visiting professor, Universite de Franche-Comte, Department of Molecular Physics, Besançon, France
- 2004 Senior Fulbright Scholar, University of Southern California, Los Angeles, in the group of Prof. Arieh Warshel

Both researchers have substantial experience in the fields of structure and spectroscopy of short hydrogen bonding, thermodynamics and kinetics of enzyme reactions, solid state chemistry, catalysis and nuclear quantum effects by classical and quantum simulation methods. They are also experienced in hosting and organizing workshops and summer schools in their area of expertize.

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Relevant publications, and/or products, and/or services

- M. Repič, R. Vianello, M. Purg, F. Duarte, P. Bauer, S. C. L. Kamerlin, J. Mavri. Empirical valence bond simulations of the hydride transfer step in the monoamine oxidase B catalyzed metabolism of dopamine. Proteins 2014, 82, 3347-3355.
- R. Borštnar, M. Repič, S. C. L. Kamerlin, R. Vianello, J. Mavri. Computational study of the pKa values of potential catalytic residues in the active site of monoamine oxidase B. J. Chem. Theory Comput. 2012, 8, 3864-3870.
- J. Stare, J. Mavri, J. Grdadolnik, J. Zidar, Z. B. Maksić, R. Vianello. Hydrogen bond dynamics of histamine monocation in aqueous solution: Car-Parrinello molecular dynamics and vibrational spectroscopy study. J. Phys. Chem. B 2011, 115, 5999-6010.
- R. Vianello, M. Repič, J. Mavri. How are biogenic amines metabolized by monoamine oxidases?. Eur. J. Org. Chem. 2012, 36, 7057-7065.
- G. Pirc, J. Mavri, J. Stare. Program package for numerical solving time-independent Schrödinger equation for vibrational problems: Inclusion of coordinate dependent reduced masses. Vib. Spectrosc. 2012, 58, 153-162.

Relevant previous projects or activities

- In 2004, Janez Mavri was visiting researcher (4 months with the Senior Fulbright grant) at the Prof. Warshel's group at the University of Southern California, Los Angeles. He adopted the Empirical Valence Bond simulation methodology which is now being practiced at BBLU, resulting in three joint papers with Prof. Warshel and several other publications in the field of enzyme catalysis. In 2013 Prof. Warshel was awarded Chemistry Nobel Prize for his contribution to multiscale simulation methods.
- In 2012-2013, Jernej Stare was visiting researcher (Swiss Rectors' Conference grant) at the Prof. Röthlisberger group at the Swiss National Institute of Technology (EPFL). He adopted the multiscale QM/MM methodologhy, as implemented in the CPMD simulation package, applying it to a compelling problem of interaction between proteins and ruthenium cytostatic drugs.
- The BBLU's main source of funding is the Program Group Grant P1-0012 titled 'Molecular Simulation and Drug Design', financed by the Slovenian Research Agency. Started in 2014, the grant will support the major part of BBLU's research activities for 5 years. As implied by the title, biomolecular simulation of enzyme catalysis is listed as the primary activity of the group. Given that the same scientific content was included in the previous funding period (2009-2013), computational enzymology has a long term support in the national research funding scheme.

Smilarly to the long term program group financing, BBLU received grants for shorter term projects (3-year duration) by the Slovenian Research Agency. BBLU obtained a 3-year (2010-2012) Project Grant J1-2014 titled 'Proton Transfer Dynamics in Biological Systems'; the project tackled problems related to enzyme catalysis, especially in the context of nuclear quantum effects.

Relevant infrastructure to the proposed work

- BBLU utilizes the 1200-core computer center at the National Institute of Chemistry. Given the estimated computing demands, BBLU will only occasionally make use of superior parallel computers, but will also offer CPU surpluses to the members of the community.
- BBLU has proper license for all the software packages required by the proposed service, including GAUSSIAN, CPMD, Q, MOLARIS, VASP, GROMOS, GROMACS, etc.

4.1.31 CHZA

Description of the legal entity

The RBI is Croatia's leading scientific institute in the natural and biomedical sciences as well as marine and environmental research, owing to its size, scientific productivity, international reputation in research, and the quality of its scientific personnel and research facilities. Moreover, the RBI is the leading and internationally most competitive Croatian institute by virtue of its participation in international research projects, such as the IAEA and EC FP5-7 programs funded by the European Commission, NATO, NSF, SNSF, DAAD and other

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international scientific foundations. The primary task of the RBI is to conduct excellent basic research, which is a prerequisite for the fulfillment of the other tasks that the RBI assumes in the development of the Republic of Croatia. The RBI carries out these tasks in collaboration with universities, scientific institutions and other related institutions in Croatia and abroad. There are nearly 900 persons employed at the Institute today. Over 500 of them are scientists and researchers that pursue research in more than 80 laboratories in theoretical and experimental physics, material physics and chemistry, electronics, physical chemistry, organic chemistry and biochemistry, molecular biology and medicine, marine science and the environment, information and computer sciences, laser and nuclear research and development. Due to its manpower and well-organized infrastructure, including a large number of valuable experimental instruments, which comprise 50% of all scientific equipment in Croatia, the Institute is able to maintain its activities at the highest level.

Key people

Dr. Robert Vianello [M] (PhD in Chemistry in 2003): Senior Research Associate at RBI and two-times Marie Curie Fellow, being awarded with individual IEF fellowship (2010–2012) and CIG research grant (2013–2017). Highly experienced with the application of the computational methods of quantum chemistry to systems in the gas- and condensed-phases as well as within the enzyme active sites. Supervisor of 2 PhD and 4 undergraduate students at the University of Zagreb. Frequent invited and plenary speaker at international conferences and workshops. Expert reviewer for established scientific journals in the field of physical-organic chemistry and funding agencies. Very active in science popularization. Chair of the Croatian Chapter within the Marie Curie Alumni Association.

Relevant publications, and/or products, and/or services

- I Despotović, R Vianello*: "Engineering exceptionally strong oxygen superbases with 1, 8-diazanaphthalene di-N-oxides", Chemical Communications 2014, 50, 10941–10944.
- M Pavlin, J Mavri, M Repič, R Vianello*: "Quantum-chemical approach to determining the high potency of clorgyline as an irreversible acetylenic monoamine oxidase inhibitor", Journal of Neural Transmission 2013, 120, 875–882.
- ZB Maksić, B Kovačević*, R Vianello*: "Advances in determining the absolute proton affinities of neutral organic molecules in the gas phase and their interpretation: a theoretical account", Chemical Reviews 2012, 112, 5240–5270.
- R Vianello*, M Repič, J Mavri: "How are biogenic amines metabolized by monoamine oxidases?", European Journal of Organic Chemistry 2012, 7057–7065.
- R Borštnar, M Repič, M Kržan, J Mavri, R Vianello*: "Irreversible inhibition of monoamine oxidase B by the antiparkinsonian medicines rasagiline and selegiline: a computational study", European Journal of Organic Chemistry 2011, 6419–6433.

Relevant previous projects or activities

- Marie Curie Career Integration Grant (FP7–PEOPLE–2012–CIG call) for 48 months of reintegration phase at the Ruđer Bošković Institute in Zagreb (Croatia). Total financial value: 100.000 EUR (excluding salaries); 2013–2017.
- Marie Curie Fellowship for Career Development (FP7–PEOPLE–2009–IEF call) for 18 months stay at the National Institute of Chemistry in Ljubljana (Slovenia). Total financial value: 99.127,60 EUR; 2010–2012.
- Research Grant from the Unity through Knowledge Fund under the Young Researchers and Professionals Program co-financed by the industrial partner APO Environmental Protection Services Ltd. Zagreb. Total financial value: 35.000 EUR (excluding salaries); 2008–2010.
- Member of COST Action CM1103 "Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain". Chair: Dr. Rona Ramsay, University of St. Andrews, United Kingdom.
- Member of the Selection Committee of the NEWFELPRO program – new international fellowship mobility programme for experienced researchers in Croatia (2013 – onwards)

Relevant infrastructure to the proposed work

- CHZA is equipped with its own high-performance LINUX cluster consisting of 12 HP blade servers (240 CPU cores, 768 GB RAM memory, 12 TB disk space), and a full-time access to the Croatian

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University Computing Centre hosting national cluster (800 CPU cores, 5 TB RAM memory, 44 TB disk space) and GRID infrastructures (1400 CPU cores, 10 TB RAM memory, 55 TB disk space).
- CHZA has proper licenses for all of the software packages required by the proposed service, including GAUSSIAN, AMBER, Q, MOLARIS, etc.

4.1.32 KIT

Description of the legal entity
Karlsruhe Institute of Technology (KIT) is the combination of a science and research institution with a University in Germany. Funded by the Federal Republic of Germany and the state of Baden-Württemberg KIT is leading in innovation, research and teaching with a staff of 10000 employees and 25000 students. KIT is a member of the Helmholtz Association of German Research Centres.
The Steinbuch Centre for Computing (SCC) operates the central computing facilities of KIT and provides and supports the campus IT-infrastructure for research at KIT and within the Helmholtz-Association of German research centres. It has solid experience in distributed computing infrastructures (DCIs), as well as in large scale data processing, data storage and archives. Research is focuses on big data, data management and federated identity management and security. SCC runs the German T1 node of the LHC computing grid and recently developed and operetes the largest German university cloud storage for sync-and-share, providing access to more than 350,000 students and 100,000 researchers from 29 different Institutions. In total, SCC administers 22 PB disk (+22 PB tape) storage for a diverse range of scientific experiments on site as well as national and international experiments and collaborations.
SCC successfully participated in several European projects such as CrossGrid, Int.EU.grid, EUFORIA, EGEE-1, EGEE-2 and EGEE-3, EGI-Inspire and is currently contributing to EUDAT. SCC has coordinated the G-Eclipse and MMM@HPC projects.
SCC is a partner in this proposal because it can contribute expertise and resources in the context of the European data infrastructure as provided in EUDAT

Key people
Prof. Dr. Achim Streit [M] is the director of the Steinbuch Centre for Computing (SCC) and at the same time professor for computer science at KIT since mid-2010. He is responsible for the HPC and Big Data activities at SCC – both hardware and systems as well as R&D activities. He is the lead PI of the German Helmholtz Association' project Large Scale Data Management and Analysis (LSDMA), which is about fostering data-intensive science in Germany through Data Life Cycle Labs and generic methods research and which involves in total 11 partners and an annual budget of 3 M€ for 5 years. Prior to KIT, he was leading the Grid and Data activities at the Jülich Supercomputing Centre (JSC) of Forschungszentrum Jülich, Germany. In this role he was very active in several EU infrastructure projects such as DEISA, PRACE, EGEE-2, OMII-Europe, EGI-InSPIRE and ETICS-2 on the managerial level and initiated the EMI and EUDAT projects. He holds a PhD in computer science specialising on scheduling for cluster and distributed systems. He is co-author of more than 70 peer-reviewed publications in peer-reviewed conferences, workshops and journals.

Dr. Christopher Jung [M] Holds a PhD in particle physics and has contributed to the development and operational structure of computing and data management of the CMS and ALICE collaborations. He has lead the GridKa school, a recurring event attended by over one hundred international students presenting a collection of courses and lectures at graduate level with focus on distributed computing and data management. Since 2011 he leads the Large Scale Data Management and Analysis (LSDMA) project a selected portfolio theme of the Helmholtz

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Association in which domain scientists of several universities and research centers closely collaborate with data scientists to enhance the life cycle of scientific data. Dr. Jung actively participated in several national and international projects such as EUDAT, RDA and Physics at the TeraScale.

Relevant publications, and/or products, and/or services

- A. O. Garcia, S. Bourov, A. Hammad, V. Hartmann, T. Jejkal, J. C. Otte, S. Pfeiffer, T. Schenker, C. Schmidt, P. Neuberger, R. Stotzka, J. van Wezel, B. Neumair, A. Streit , Data-Intensive Analysis for Scientific Experiments a the Large Scale Data Facility, Proceedings on Symposium on Large Data Analysis and Visualization (LDAV 2011), IEEE Computer Society Press, 2011, ISBN 978-1-4673-0156-5, pp. 125-126, DOI: 10.1109/LDAV.2011.6092331
- J. Meyer, M. Hardt, A. Streit and J. van Wezel: Archival Services and Technologies for Scientific Data. In: Journal of Physics, 2014, Conference Series 513 062033, DOI: 10.1088/1742-6596/513/6/062033
- C. Jung, M. Gasthuber, A. Giesler, M. Hardt, J. Meyer, F. Rigoll, K. Schwarz, R. Stotzka and A Streit: Optimization of data life cycles. In: Journal of Physics: Conference Series 513 032047, DOI:10.1088/1742-6596/513/3/032047
- A. O. Garcia, S. Bourov, A. Hammad, T. Jejkal, J.C. Otte, S. Pfeiffer, T. Schenker, C. Schmidt, J. van Wezel, B. Neumair and A. Streit: Data Management and Analysis at the Large Scale Data Facility. In: Proceedings of 6th International Conference on Digital Information Management (ICDIM 2011), IEEE Computer Press, 2011, ISBN 978-1-4577-1538-9, pp. 235-241, DOI: 10.1109/ICDIM.2011.6093357

Relevant previous projects or activities

- MMM@HPC: (Coordinated at KIT) User oriented project to bring completely new communities to HPC
- LSDMA (funded by Helmholtz Association): Large Scale Data Management and Analysis; establishing Data Life Cycle Labs (DLCL) optimize community data life cycles and to develop generic solutions;
- EUDAT: Building and operating data services for a pan-European collaborative data infrastructure
- EGI-InSPIRE - Integrated Sustainable Pan-European Infrastructure for Researchers in Europe
- bwDataArchiv: Development of petabyte scale archive services for scientific data for HLRS Stuttgart the LSDF, the LHC Tier-1 (GridKa) and state archives and libraries in Baden-Württemberg.

Relevant infrastructure to the proposed work

- Tier-1 Centre for LHC experiments (GridKa) with > 10,000 cores, 14 PB disk and 18 PB tape
- LSDF - Large Scale Data Facility, supporting data intensive science with 480 cores, 6 PB disk and 8 PB tape – available for all scientific disciplines offering high speed instrumentation storage with integrated computing, archival storage i.e. long-time storage and cloud storage services for 350,000 students and 100,000 researchers.
- Cloud and Data storage for Universities and Institutions in the State of Baden-Wuerttemberg (Germany) based on a federated authentication infrastructure.
- HPC systems with in total more than 25,000 cores

4.1.33 KTH

Description of the legal entity

The Royal Institute of Technology (KTH), established in 1827, is one of Europe's top schools for science and engineering, graduating one-third of Sweden's undergraduate and graduate engineers in the full range of engineering disciplines. Enrolment is about 17,500 students, of which about 1,400 are pursuing PhD studies. In this proposal, KTH is represented by the PDC-Center for High Performance Computing

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Key people
Prof. Erwin Laure [M] is Professor in Computer Science, High Performance Computing, at KTH. He is head of the HPCViz department and director of PDC – Center for High Performance Computing. He is the Coordinator of the EC-funded project "EPiGRAM" investigating programming models for exascale computing with a focus on message passing and PGAS, and actively involved in major European HPC infrastructure projects (EGI, PRACE, EUDAT) for many years. He has been appointed expert advisor by the Swedish Research Council to the PRACE and EGI councils. He holds a PhD in Business Administration and Computer Science from the University of Vienna, Austria. His research interests include programming environments, languages, compilers and runtime systems for parallel and distributed computing, particularly exascale computing.

Dr. Rossen Apostolov [M] received a PhD in Computational Chemistry from Osaka University, and is currently a researcher and application expert in bio-molecular simulations at KTH. He has been working for many years on improving the scalability and performance of life science software. He has served as a Technical Director of the ScalaLife FP7 project and is a reviewer for several journals in the field of computational chemistry and biophysics. His interests include HPC computing, accelerators, as well as best practices for software development.

Relevant publications, and/or products, and/or services
- M. Schliephake, E. Laure, P. Fischer and K. Heisey. Design, implementation and use of mampicl, the multi-algorithm MPI collective library. In Proceedings of the 1st International Applications and Software Conference EASC 2013; Edinburgh, Scotland, UK, 2013.
- M. Schliephake and E. Laure. Towards improving the communication performance of CRESTA's co-design application NEK5000. In Proceedings - 2012 SC Companion: High Performance Computing, Networking Storage and Analysis, SCC 2012; Salt Lake City, US, 2012.
- M. Schliephake, X. Aguilar and E. Laure. Design and Implementation of a Runtime System for Parallel Numerical Simulations on Large-Scale Clusters. In International Conference on Computational Science (ICCS2011), Singapore, June 2011.
- S. Pall, M.J. Abraham, C. Kutzner, B. Hess, E. Lindahl, Tackling exascale software challenges in molecular dynamics simulations with GROMACS, In. Lect. Notes Comp. Sci. in press (2014)
- S. Pronk, S. Pall, R. Schulz, P. Larsson, P. Bjelkmar, R. Apostolov, M.R. Shirts, J.C. Smith, P. Kasson, D. van der Spoel, B. Hess, E. Lindahl, GROMACS 4.5: A high-throughput and highly parallel open source molecular simulation toolkit. In Bioinformatics 29(7), 845-854 (2013)

Relevant previous projects or activities
- EU FP7: Collaborative Research into Exascale Systemware, Tools and Applications (CRESTA), member
- EU FP7: Scalable Software Services for Life Sciences (ScalaLife), Coordinator
- EU FP7: PRACE 1-3IP, Member
- ETP4HPC: Member
- EU FP7: EUDAT, Member

Relevant infrastructure to the proposed work
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4.1.34 EUCH

Description of the legal entity
EuCheMS is a not-for-profit organisation founded in 1970. Its object is to promote co-operation in Europe between scientific and technical societies and organisations in the field of chemistry and molecular sciences. EuCheMS is a consortium of 43 member associations with more than 150,000 chemists operating in

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academia, industry, government and professional organisations in 32 countries across Europe. EuCheMS has several Divisions and Working Groups which cover all areas of chemistry and bring together world class expertise in the underpinning science and development needed for innovation. EuCheMS has a strong network and will mostly contribute to promotional and dissemination activities. EUCHEMS Divisions take care of the thematic activities and several of them interact with the tasks of the CMMST-VRE proposal especially in WP06-WP08. The EUCHEMS Division most involved in the proposal is the Computational Chemistry one that has specific competences also in WP02 – WP05 and has tight relationships with some spinoffs, SMEs and professional organizations.

Key people
Nineta Majcen did her PhD in analytical chemistry and chemometrics, with the emphasis on neural networks in 1996. During the past decade, she is mostly involved in management in her area of expertise and wider at the European level. Amongst other, she was a project leader of an European CARDS project (2004-2007), chair of the Editorial Board of a programme ran by the European Commission JRC; evaluator of various project proposals at the European level. Since 2011 she is the Secretary General of EuCheMS.

Relevant publications, and/or products, and/or services
- MAJCEN, Nineta, RAJER-KANDUČ, Karmen, NOVIČ, Marjana, ZUPAN, Jure. Modelling of property prediction from multicomponent analytical data using different neural networks. Analytical chemistry, ISSN 0003-2700. [Print ed.], 1995, vol. 67, str. 2154-2161.
- N. H. Majcen, EuCheMS Annual Report, Editor
- R. Salzer, P. Taylor, N. Majcen et all, Education and careers of European analytical chemists, Analytical and Bioanalytical chemistry, Springer, October 2014
- N. H. Majcen, Brussels News Updates, Author (monthly publication)
- For the bibliography please see http://splet02.izum.si/cobiss/BibPersonal.jsp?lang=eng&init=t&code=&type=conor

Relevant previous projects or activities
- EC2E2N-2 "Chemistry and Engineering Skills for Europe in 2020" http://www.ec2e2n.net/2/index

Relevant infrastructure to the proposed work
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4.1.35 CSMA

Description of the legal entity
REACTION is a spin-off company from work from the Research Institute for Symbolic Computation and the University of Lund. The company has two mainstays encapsulated in two software systems. The REACTION software system is an automatic generation system for the development and reduction of detailed combustion mechanisms. It's primary use is the generation of fuel mechanisms involving long chain hydrocarbons for liquid fuel combustion. The second system, ANALYSIS++ is an expert system with generalized fuzzy logic machine learning methods. ANALYSIS++ has been used for a variety of domains from quality control in industrial processes, analysis of combustion systems, analysis and reduction of detailed combustion models, analysis of user buyer activity for recommendation systems and revision control analysis in software engineering. The company has also done extensive work in the development of tabulation methods of detailed combustion mechanisms for more efficient use in reactive flow in computational fluid dynamics.

Key people
Edward Blurock [M] is the CEO of REACTION. For this project Edward Blurock will be representing the combustion community through the SMARTCATS CM1404 COST Action by helping in the implementation

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of several important software systems and for the development of a general database of combustion data for the entire community. This newly started Action was a continuation of a previous action, CM901: Detailed Chemical Models for Cleaner Combustion, in which Edward Blurock was one of the founders. Edward Blurock has been working in physical chemistry modeling since his degree in Computational chemistry in 1983 from the University of California at Irvine. As a lecturer and researcher at the Research Institute of Symbolic Computation (RISC), he worked on a wide domain of software modeling: Computer Aided Organic Synthesis (CAOS), automatic generation of detailed combustion mechanisms and quality control for industrial processes. It is at RISC where the development of the ANALYSIS++ and REACTION systems started. Edward Blurock has been involved in numerous industrial cooperations, many of which were FP6 and FP7 projects, by applying the software systems to the combustion and industrial process analysis. Complementing his domain experience in physical chemistry and particularly relevant for this project is his extensive experience in computer science software development which, for example, started in high school as a summer job programmer for a company. After his degree at UCI, he worked at RISC (an institute emphasizing the overlap between mathematics and computer science) and, along side his research with software development, he held classes in artificial intelligence, machine learning, computer algebra systems, LISP and PROLOG. He is now working at department of computer science in Malmö University giving a wide range of classes for undergraduate and masters students, as well as advising on undergraduate projects and masters theses.

Relevant publications, and/or products, and/or services

- Hexadecane mechanisms: Comparison of hand-generated and automatically generated with pathways, Mersin, I. E., Blurock, E., Soyhan, H. S., & Konnov, A., Fuel, 115, 132-144 (2014). DOI:10.1016/j.fuel.2013.06.055
- Development of detailed chemical kinetic models for cleaner combustion, Editors: F. Battin-Leclerc, J. M. Simmie, E. Blurock, ISBN: 978-1-4471-5306-1 (Print) 978-1-4471-5307-8 (Online), Springer, 2013
- JTHERGAS: Thermodynamic estimation from 2D graphical representations of molecules, Edward S. Blurock, , Valérie Warth, Xavier Grandmougin, Roda Bounaceur, Pierre-Alexandre Glaude, Frédérique Battin-Leclerc, Energy, 43, 161–171 (2012).
- Phase Optimized Skeletal Mechanisms for Engine Simulations, Blurock, Edward S., Tuner, Martin, Mauss, Fabian, Combustion Theory and Modeling,14:295-313 (2010).
- Towards cleaner internal combustion engines through groundbreaking detailed chemical kinetic models, Frédérique Battin-Leclerc, Edward Blurock, René Fournet a Pierre-Alexandre Glaude, Olivier Herbinet and Baptiste Sirjean, Chemical Society Reviews, 40 4762-4782 (2011).

Relevant previous projects or activities

- SMARTCATS Action CM1404, Chemistry of Smart Energy Carriers and Technologies: In this project, Edward Blurock, through REACTION, will be representing the 21 countries with 53 participating entities (15 industrial). These are the leaders in combustion science development in Europe. Work package 8 of this action is exactly the domain of this project, namely, Standard definition for data collection and mining toward a virtual chemistry of smart carriers.

Relevant infrastructure to the proposed work

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4.1.36 SRCE

Description of the legal entity

SRCE is coordinator and legal representative of the CRO NGI - Croatian National Grid Infrastructure / Initiative established in 2007. CRO NGI is a common resource of the scientific and academic community and represents the fundamental infrastructure for the scientific research, the application of new technologies

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and the integration of Croatia and Croatian scientists into the European Research (ERA) and European Higher Education (EHEA) Area.(http://www.cro-ngi.hr/).
SRCE provides a modern, sustainable and reliable e-infrastructure for research and education community. This includes computing and cloud services, high performance computing, advanced networking, communication systems and services, middleware, data and information systems and infrastructure.(http://www.srce.unizg.hr/).
Expertise and knowledge have enabled SRCE to actively participate in international, mostly European, projects in the area of Information Technology for more than 30 years.

Key people
Ivan Maric [M] is a Deputy Director and CTO of SRCE and international representative of CRO NGI appointed by CRO NGI Council. He initiated, constructs and build the Croatian academic and research network at the beginning of 1990's. He was and is actively involved in building and governing pan-European e-infrastructures: GEANT and EGI. He is a member of GÉANT Executive Committee and he was a member of the Board of Directors of DANTE. He act as a representative of CRO NGI in the EGI Council.

Dobrisa Dobrenic [M] is Assistant Director of SRCE for Computing and Network Infrastructure and Head of CRO NGI since its establishment in 2007. He was project leader of building Croatian first HPC cluster open for researchers. In 2003-2006 he was head researcher of national project which in 2005 resulted in first computing grid in Croatia. Lately he led project which established first cloud IaaS infrastructure and services for A&R community in Croatia.

Emir Imamagic [M] is a Head of Computer Systems Department of SRCE and Operations manager of CRO NGI responsible for technical development, CA administration, running EGI regional core services, developing and running grid monitoring systems.

Relevant publications, and/or products, and/or services
- Croatian National Grid Infastructure http://www.cro-ngi.hr/index.php?id=1334&L=1
- Here you can find a list of publications: http://www.cro-ngi.hr/za-korisnike/radovi-korisnika/.

Relevant previous projects or activities
- Project EGI-InSPIRE - European Grid Initiative: Integrated Sustainable Pan-European Infrastructure for Researchers in Europe, FP7, RI-261323, 2010-2014;
- Project GN3 plus Multi-gigabit Pan-European Research and Education, FP7, RI-605243,2013-2015;
- Project GEANT3 Multi-gigabit Pan-European Research and Education, FP7, RI-238875, 2009-2013;
- Project EGEEIII - Enabling Grids for E-sciencE phase III, FP7, RI-222667, 2008-2009;
- Project GEANT2 Multi-gigabit Pan-European Research and Education, FP6, RI-511082, 2004-2009;

Relevant infrastructure to the proposed work
- CRO NGI resources are currently mainly used by users from computation chemistry field. In the long term we foresee significant increase in resource needs from this community. Top applications used on the infrastructure are: Abinit, Gaussian and Turbomole. Besides for deployment and maintenance of applications, CRO NGI experts helped users in preparing scripts needed for optimal utilization of grid resources.
- CRO NGI infrastructure currently consists of more than 1800 processor cores, 36 GPUs and 110 TB of disk storage on five grid sites. In addition there is an EGI FedCloud site with 160 processor cores. In the following years we plan to expand the infrastructure significantly, at least by the order of magnitude.

4.1.37 CHBU

Description of the legal entity

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Eötvös Loránd University, the longest continuously serving university of Hungary, was founded in 1635 in the city of Nagyszombat (today Trnava, Slovakia) by Cardinal Péter Pázmány, Archbishop of Esztergom. It serves the interests of high quality education and research, building upon the best European traditions. Its mission is to preserve and enrich national and universal culture, to cultivate science and to pass on academic knowledge, as well as to shape and satisfy the real, long-term needs of Hungarian society and of mankind.

Key people

Dr Attila Csaszar [M] is specialized in first-principles quantum chemical computations on small and medium-sized, organic and inorganic molecular systems with an emphasis on variational nuclear motion computations. Theoretical prediction of vibrational (infrared, near- and far-IR, and Raman), rotational (microwave and millimeterwave), rovibrational and photoelectron spectra; in particular, interpretation of high-resolution molecular spectra. Utilization of spectroscopic networks in improving spectroscopic information systems. Resonances and tunnelling in chemistry. Potential energy and property hypersurfaces. Computation, interpretation and use of harmonic and anharmonic molecular force fields. Large-amplitude internal motions. Structures of molecules in the gas phase as studied by experimental and theoretical methods. Ab initio thermochemistry, including determination of accurate enthalpies of formation and partition functions at elevated temperatures. More than 180 scientific publications with more than 5500 citations and an h-index of 42.

Relevant publications, and/or products, and/or services

- O. L. Polyansky, A. G. Császár, S. V. Shirin, N. F. Zobov, P. Barletta, J. Tennyson, D. W. Schwenke, and P. J. Knowles, High-Accuracy Ab Initio Rotation-Vibration Transitions of Water, Science 2003, 299, 539-542.
- P. R. Schreiner, H. P. Reisenauer, F. C. Pickard, A. C. Simmonett, W. D. Allen, E. Mátyus, and A. G. Császár, Capture of Hydroxymethylene and its Fast Disappearance through Tunnelling, Nature 2008, 453, 906-909.
- A. G. Császár, C. Fábri, T. Szidarovszky, E. Mátyus, T. Furtenbacher, and G. Czakó, The Fourth Age of Quantum Chemistry: Molecules in Motion, Phys. Chem. Chem. Phys. 2012, 14(3), 1085-1106.
- M. Pavanello, L. Adamowicz, A. Alijah, N. F. Zobov, I. I. Mizus, O. L. Polyansky, J. Tennyson, T. Szidarovszky, A. G. Császár, M. Berg, A. Petrignani, A. Wolf, Precision Measurements and Computations of Transition Energies in Rotationally Cold Triatomic Hydrogen Ions up to the Mid-Visible Spectral Range, Phys. Rev. Lett. 2012, 108, 023002.
- J. Tennyson, P. F. Bernath, L. R. Brown, A. Campargue, A. G. Császár, L. Daumont, R. R. Gamache, J. T. Hodges, O. V. Naumenko, O. L. Polyansky, L. S. Rothman, A. C. Vandaele, and N. F. Zobov, A Database of Water Transitions from Experiment and Theory (IUPAC Technical Report), Pure Appl. Chem. 2014, 86(1), 71-83.

Relevant previous projects or activities

- IUPAC Task Group 2004-035-1-100 on “A database of water transitions from experiment and theory”, vice-chair
- FP6 Marie Curie Research Training Network QUASAAR (Quantitative Spectroscopy for Atmospheric and Astriphysical Research), participant
- IUPAC Task Group 2011-022-2-100 on “Intensities and line shapes in high-resolution spectra of water isotopologues from experiment and theory”, vice-chair
- COST action CM1405, Molecules in Motion (MOLIM), proposed chair
- COST action CM1401, Our Astro-Chemical History, MC member

Relevant infrastructure to the proposed work

Local cluster

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4.1.38 NCBJ

Description of the legal entity

National Centre for Nuclear Research was established on 1 September 2011, as a result of the inclusion of the Institute of Atomic Energy POLATOM to the Andrzej Soltan Institute for Nuclear Studies. NCBJ (Narodowe Centrum Badań Jądrowych) deals with basic research in the field of subatomic physics (particle physics and nuclear physics of hot plasma, etc.) and the application of the methods of nuclear physics and nuclear technology development. The Centre creates informatics and laboratory infrastructure necessary to support nuclear power construction program in Poland.

National Centre for Nuclear Research is one of the largest research institutes in Poland. It has the Poland's only nuclear research reactor "Maria". The Centre employs more than 1000 physicists, engineers and support staff. Our faculty is about 70 professors and associate professors and more than 120 doctors.

Research activity of NCBJ concentrates on:

- experimental and theoretical exploration of the most fundamental laws of nature,
- nuclear reactor research and development of nuclear fuel, as well as studies of nuclear
- installations safety,
- studies of hot plasma for fusion energy and developing methods for material modifications,
- research to protect the environment and safety regulations,
- preparing for the role of technical support organizations for Polish nuclear program.
- Other NCBJ activities:
- production and developing of new radiopharmaceuticals (NCBJ is one of the leading
- manufacturer of radiopharmaceuticals in the world),
- production of isotopes for medicine and industry,
- building of subsystems of the largest accelerators in the world,
- production of accelerators for medicine, industry and science,
- manufacturing of specialized equipment for medicine.

Key people

Dr. Renata Mikolajczak [F] PhD, DSc, professor at the National Centre for Nuclear Research, Radioisotope Centre POLATOM. Publications (Scopus 2014): **67**, citations (excl. auto-citat.) **626**; H-index: **15**. **Achievements**: development of technologies for preparation of kits for ^{99m}Tc- labelling, ^{188}W/188Re radionuclide generator, technologies for high specific activity radionuclides production in the nuclear reactor, novel radiopharmaceuticals for clinical practice. Dr Mikołajczak carried out the pioneer works in Poland on the development of peptide based kits for ^{99m}Tc labeling of somatostatin analogues indicated for diagnosis of neuroendocrine tumors and in cooperation with the clinics implemented the peptide receptor radionuclide therapy with ^{90}Y and ^{177}Lu. She is the organizer of multi-center international research teams. Extensively develops collaborations within COST (European Cooperation program of Scientific and Technical cooperation), in the last years Management Committee member of 7 Actions. Currently in: COST TD1004 – Theragnostics Imaging and Therapy: An Action to Develop Novel Nanosized Systems for Imaging-Guided Drug Delivery (2011-2015), leader of WG1 Imaging reporters for theranostic agents and in COST CM1105 - Functional metal complexes that bind to biomolecules (2012–2016). Project partner in International Atomic Energy Agency (IAEA) coordinated research programs and IAEA expert in the field of radiopharmacy. Co-inventor in patents and utility models. Contributor and leader of over 20 research grants.

Awards: Silver Medal at The 61 Belgian and International Trade Fair for Technological Innovation "Brussels INNOVA 2012" for the innovation "ItraPol & LutaPol, ^{90}Y and ^{177}Lu precursors for application in oncological radiotherapy", The World Intellectual Property

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Organization Award (WIPO) for the best invention presented by woman- inventor for „^{99m}Tc-Tektrotyd – peptide based pharmaceutical kit for isotope diagnostics in oncology" and Gold Medal awarded at The World Exhibition on Innovation, Research and New Technologies BRUSSELS INNOVA 2009, 19-21.11.2009, Brussels Expo, Belgium

Dr. Krzysztof Nawrocki [M] Graduated from the Faculty of Physics, Warsaw University, specializes in high-energy physics, astronomy and large-scale information processing. His research interests are focused mainly on high energy physics, astronomy, distributed computing and big data analysis. In years 1995 – 2003 involved in DELPHI experiment and since 2004 in CMS experiment at European Organization for Nuclear Research (CERN). In 2003 he defended his doctoral thesis titled "Study of the decay of b quark to s quark and gluon in the DELPHI experiment". In CMS experiment Krzysztof Nawrocki is working on searching for models beyond the Standard Model of fundamental interactions. He is also working on computing infrastructure the CMS experiment being administrator of Tier2 WLCG (Worldwide LHC Computing GRID) clusters in Poland. Since 2005 Krzysztof Nawrocki is a member of the „Pi of the Sky" experiment searching for optical counterparts of GRB (Gamma Ray Burst) flashes. Since 2002 participating in series of projects aimed at creation of computational grid infrastructure in Europe. Beginning in CrossGrid, through Enabling Grids for E-sciencE, Int.Eu.Grid and PlGrid. He has been one of the key members of the team building Polish part of the Worldwide LHC Computing Grid. Since 2003 he has been working for the National Centre for Nuclear Research. He was one of the founders of Świerk Computing Centre (CIŚ), project carried out at the National Centre for Nuclear Research (NCBJ), which aim is to provide IT support for Polish nuclear energy and related fields of science and technology. Krzysztof Nawrocki is the head of the scientific applications team in CIŚ.

Dr. Adam Padee [M] He studied at the Faculty of Electronics and Information Technology of the Warsaw University of Technology. He graduated in 2002, receiving the highest grade and rector's distinction. His research interests are focused mainly on distributed computing architectures and metaheuristic optimization algorithms. In 2013 he defended with distinction his doctoral thesis titled "Distributed evolutionary algorithms for optimization of data classification in High Energy Physics experiments". In years 2001 – 2012 involved in COMPASS (COmmon Muon Proton Apparatus for Structure and Spectroscopy) experiment which is carried out at European Organization for Nuclear Research (CERN). The experiment is focused on studying the hadron structure and hadron spectroscopy with high energy hadron and muon beams. Adam Padée worked on optimization tools for offline data processing software. He was also responsible for deployment of distributed grid resources for COMPASS and for making COMPASS software work on these resources. His work on both of these fields resulted in creation of a special architecture of evolutionary algorithm which is able to adapt to the dynamic grid structure and is not affected by low bandwidth of WAN connections between the grid clusters. The algorithm has been described in his doctoral thesis and several publications.
Since 2002 participating in series of projects aimed at creation of computational grid infrastructure in Europe. Beginning in CrossGrid, through Enabling Grids for E-sciencE, Int.Eu.Grid and PlGrid, he was involved in creation and deployment of grid middleware, maintenance of the resources and support for the application developers. He has been one of the key members of the team building Polish part of the Worldwide LHC Computing Grid (WLCG), a distributed computing infrastructure supporting Large Hadron Collider experiments conducted at CERN.
Since 2009 he has been working for the National Centre for Nuclear Research. He was one of the founders of Świerk Computing Centre. Currently he is the head of the Computing

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Infrastructure Team, responsible for procurements of new hardware, configuration of the computing environment for scientific applications and everyday administration. His group is also involved in algorithmic support of the application teams as well as developing new methods and working on existing ones to adapt them to large, distributed computing environments.

Relevant publications, and/or products, and/or services

- Polish Contribution to the Worldwide LHC Computing. Building a National Distributed e-Infrastructure – PL-Grid. Scientific and Technical Achievements, pp. 285-300, Springer LNCS, Vol. 7136, ISBN 978-3-642-28266-9 (2.03.2012)
- Computing support for advanced medical data analysis and imaging, W. Wiślicki et. al, Bio-Algorithms and Med-Systems 10(2014)52
- Jan Cz. Dobrowolski, The Chiral Graph Theory, MATCH Commun. Math. Comput. Chem. 73(2015)347-374
- Grażyna Karpińska, Aleksander P. Mazurek, Jan Cz. Dobrowolski, On Substituent Effect on the Benzodiazepinone System, Comput. Theoret. Chem., 993(2012)13-19.
- W. Ozimiński, P. Garnuszek, E. Bednarek, J.Cz. Dobrowolski. The Platinum Complexes with Histamine: Pt(II)(Hist)Cl2, Pt(II)(Iodo-Hist)Cl2 and Pt(IV)(Hist)2Cl2. Inorg Chim Acta 360: 1902-1914 (2007).

Relevant previous projects or activities

- COST Action TD1004 "Theragnostics Imaging and Therapy: An Action to Develop Novel Nanosized Systems for Imaging-Guided Drug Delivery"
- COST Action CM1105 "Functional Metal Complexes that Bind to Biomolecules".
- NCN Project No. UMO-2011/03/B/ST5/02734 In vitro and in vivo investigations of the radiometals influence on the ability of CCK2R receptors imaging by the radiolabelled gastrin analogs (30.08.2012 – 29.08.2015)
- CROSSGRID, "Development of Grid Environment for Interactive Applications"

Relevant infrastructure to the proposed work

- Świerk Computing Centre (CIŚ) is situated at National Centre for Nuclear Research (NCBJ) in Świerk near Warsaw and is a High Performance Computing centre which provides computational resources and expertise in parallel computing and big data processing for activities performed at NCBJ especially IT support for Polish nuclear energy and related fields of science and technology such as computational fluid dynamics, nuclear physics, high energy physics, astrophysics, medical imaging, complex systems and big data analyses. CIŚ also hosts an EGI certified GRID computing site and is a Tier2 site for CMS (Compact Muon Solenoid) and LHCb experiments. Computational resources currently available at CIŚ consist of 13760 cores, 83456 GB RAM and disk space of more than 3PB. Cluster is equipped with the QDR+FDR Infiniband and 10Gbps interconnect. For the needs of the LHC experiments, we provide 320 computing cores, 1280 GB RAM and more than 300 TB of storage space. The theoretical performance of CIŚ cluster is 285 TFLOPS.
- Research Nuclear Reactor MARIA

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