Scientific programming (in C++)

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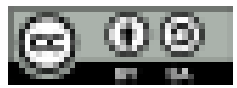
INFN-CNAF

School on Open Science Cloud
Perugia, June 2017

https://baltig.infn.it/giaco/201706_perugia_cpp



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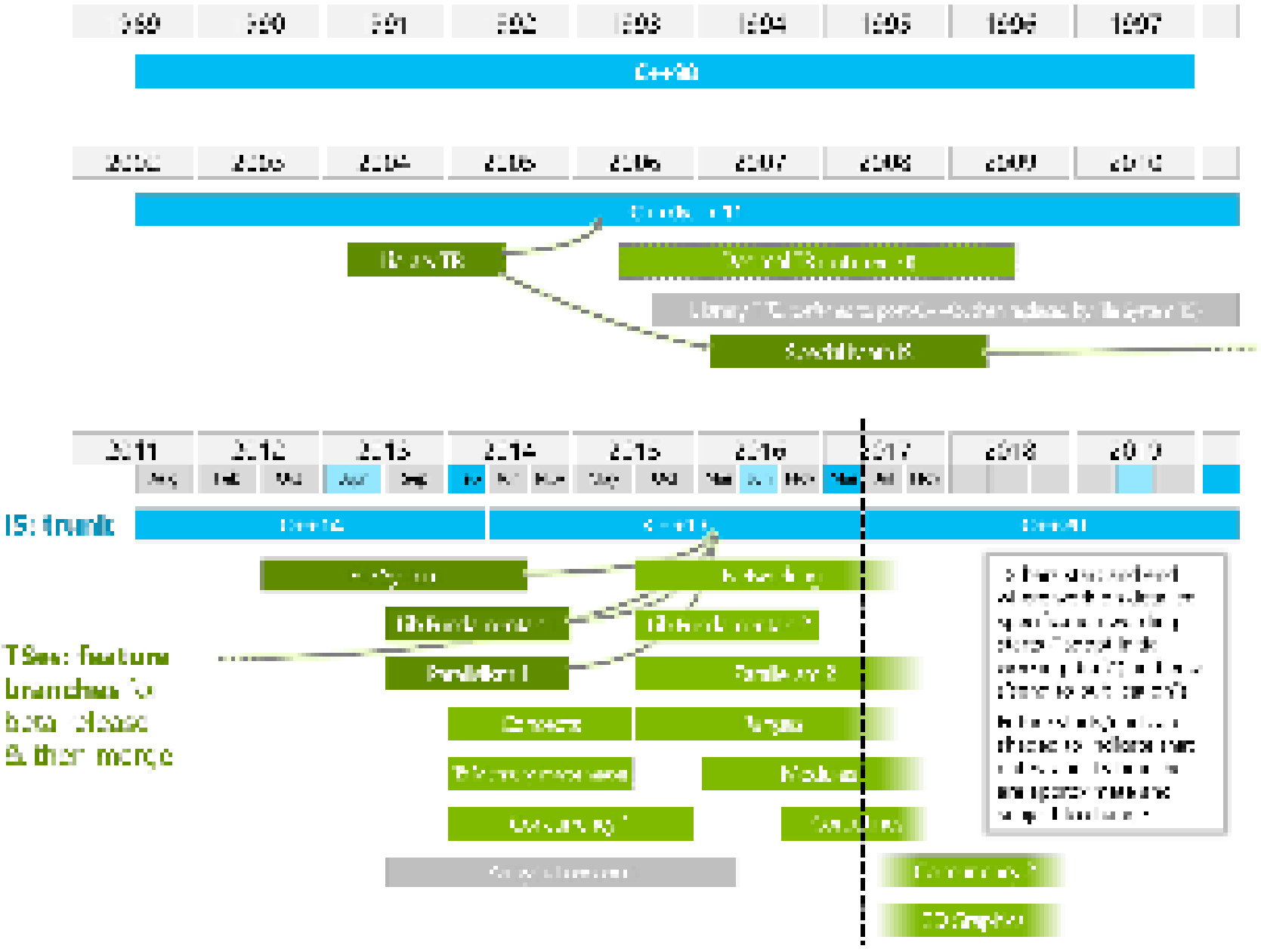
- multi-paradigm
- efficient (*"you don't pay for what you don't use"*)
- standard

C++ timeline



Online resources

- http://www.isocpp.org/
- http://en.cppreference.com/
- http://gcc.godbolt.org/
- http://coliru.stacked-crooked.com/

Standards

Working drafts, almost the same as the final published document

- C++03 `http://wg21.link/n1905`
- C++11 `http://wg21.link/n3242`
- C++14 `http://wg21.link/n4296`
- C++17 `http://wg21.link/n4659`

For the LaTeX sources see https://github.com/cplusplus/draft

The C++ standard library

- The standard library contains components of general use
  - containers (data structures)
  - algorithms
  - strings
  - input/output
  - random numbers
  - regular expressions
  - concurrency and parallelism
  - filesystem
  - ...

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- But templates are everywhere

“C” Arrays

Contiguous sequence of homogeneous objects in memory

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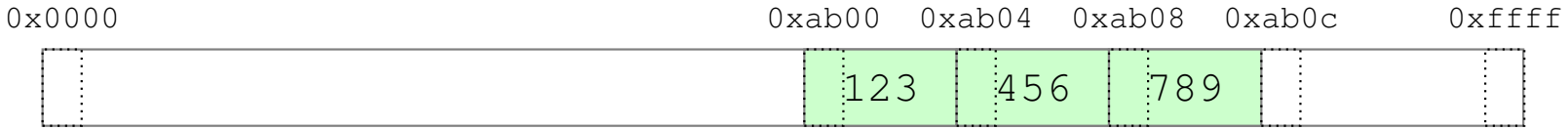

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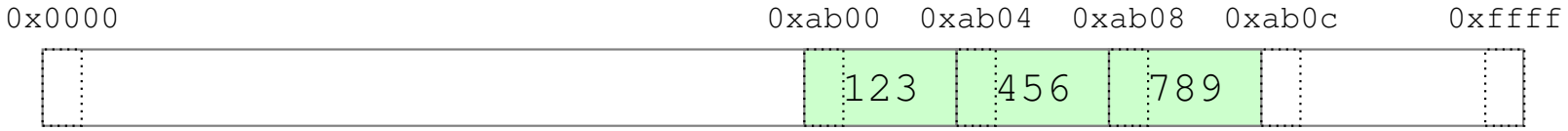


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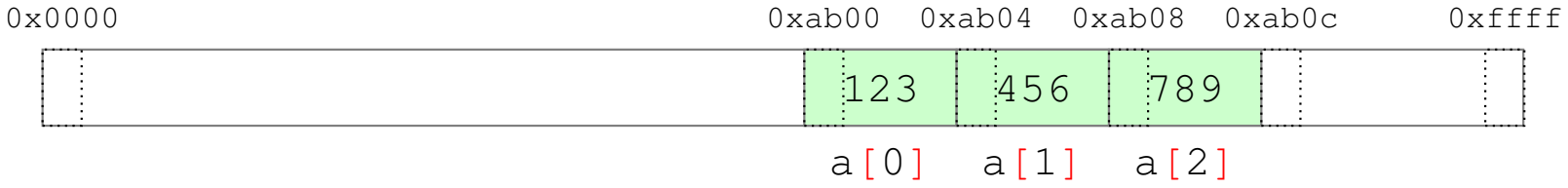


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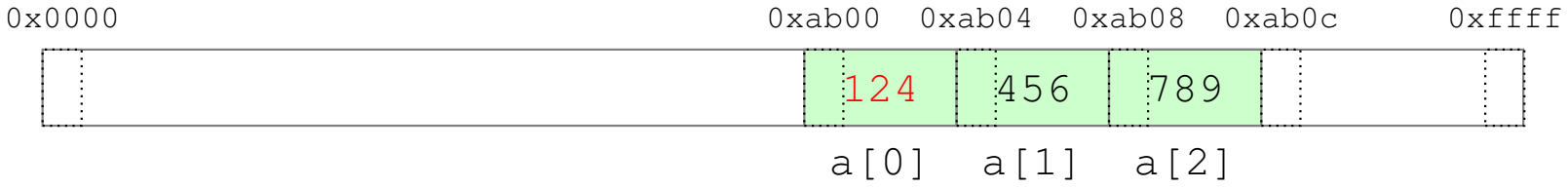


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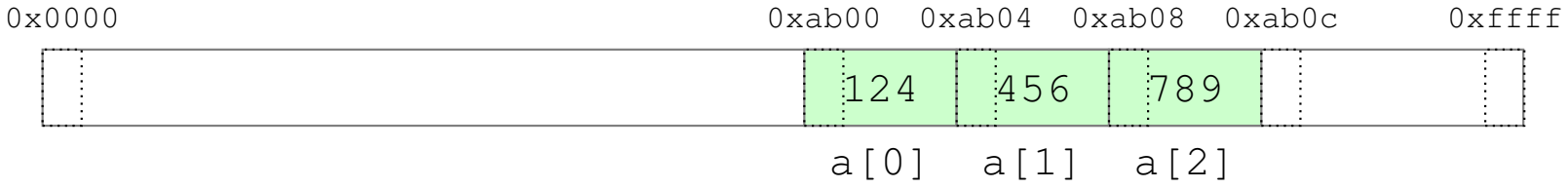


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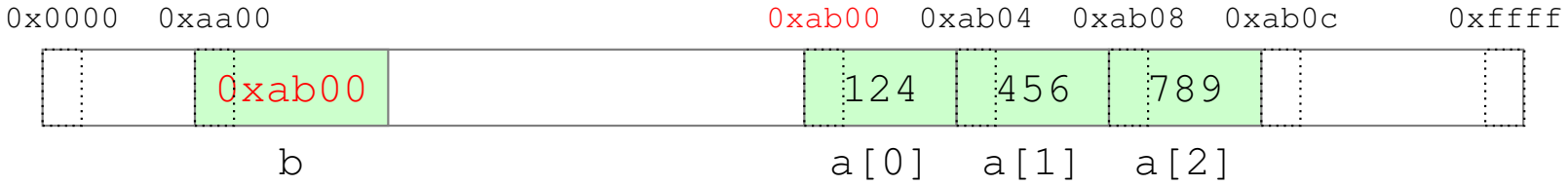


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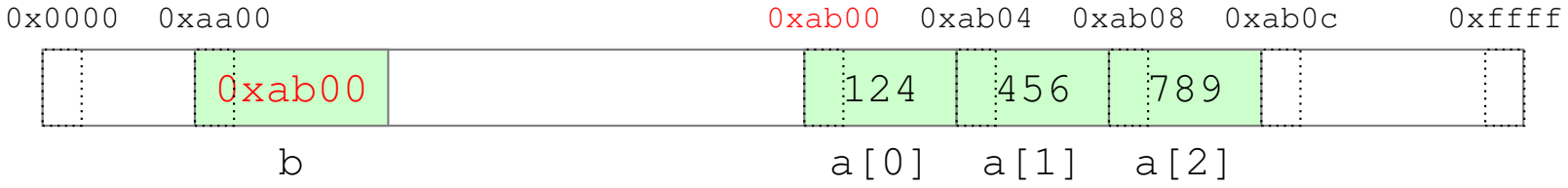


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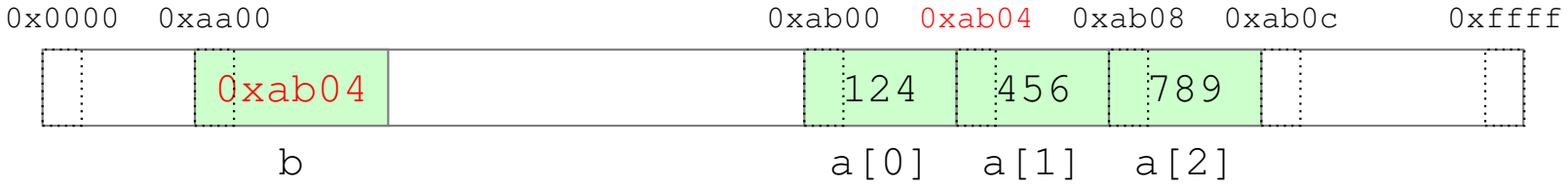


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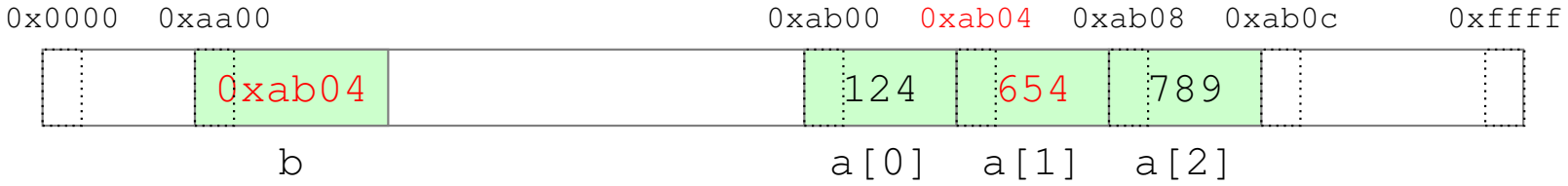


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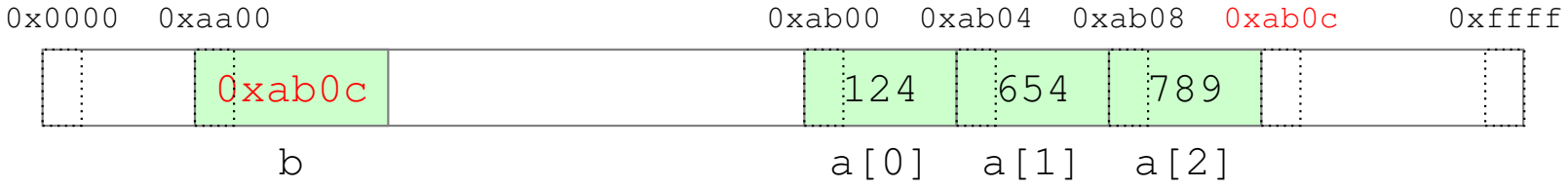


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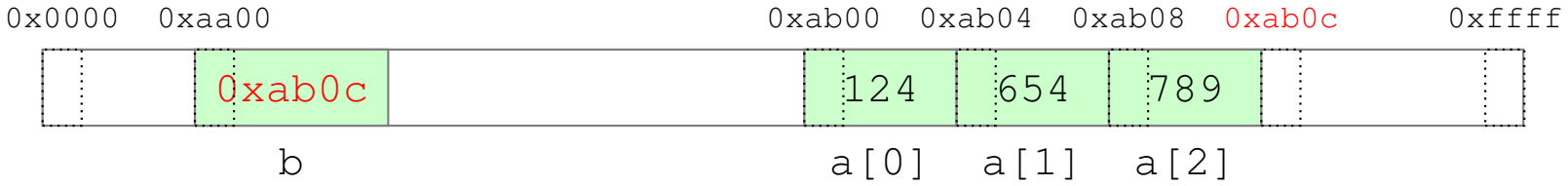


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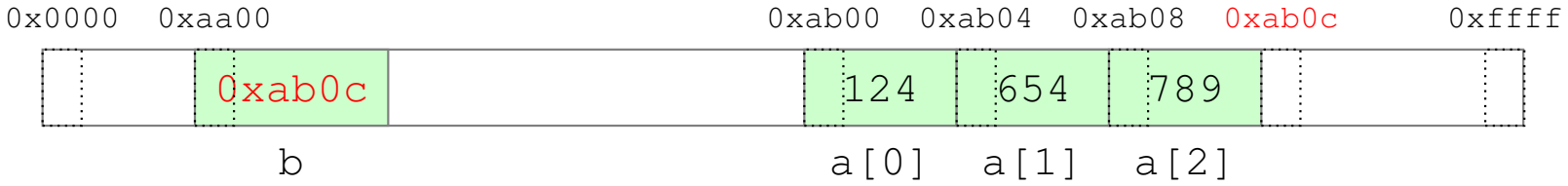


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*b;                         // undefined behavior
if (b == a + 3) { ... }     // ok, but not more than this
```

Containers

- Objects that contain and own other objects
- Different characteristics and operations, some common traits
- Implemented as class templates

Sequence The client decides where an element gets inserted

- `array`, `vector`, `list`, `forward_list`, `deque`

Associative The container decides where an element gets inserted

Ordered The elements are sorted

- `map`, `multimap`, `set`, `multiset`

Unordered The elements are hashed

- `unordered_*`

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Type-safe, no-runtime overhead alternative to a native array

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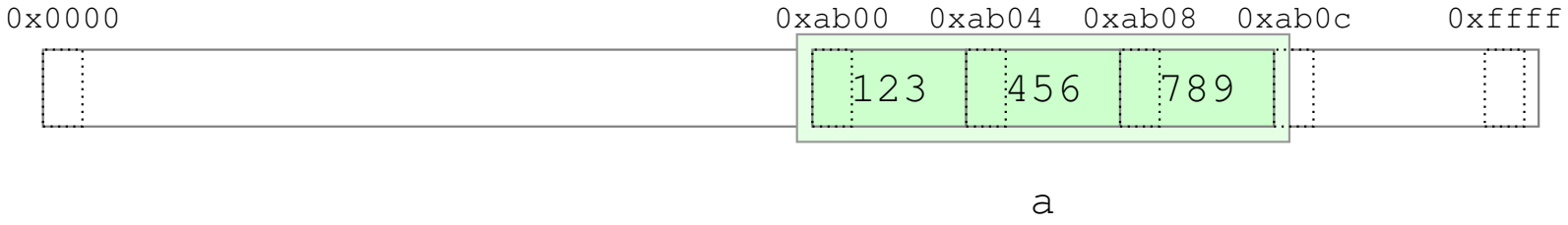


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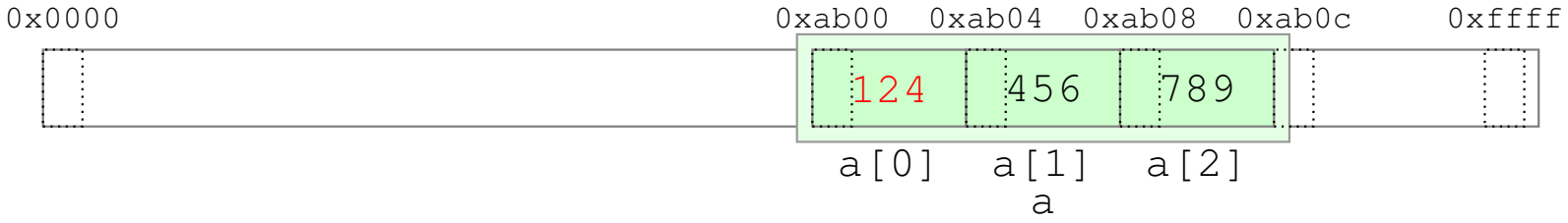


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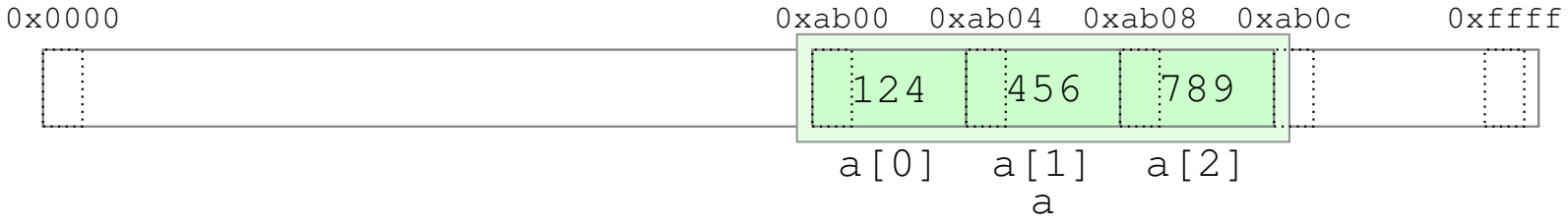


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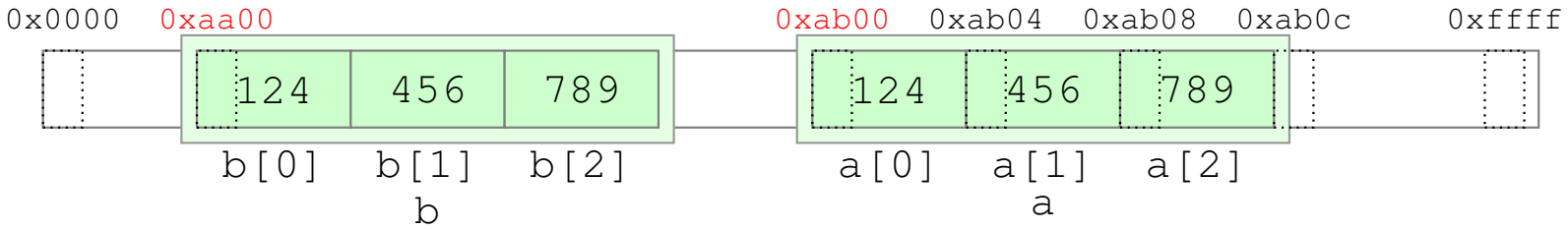


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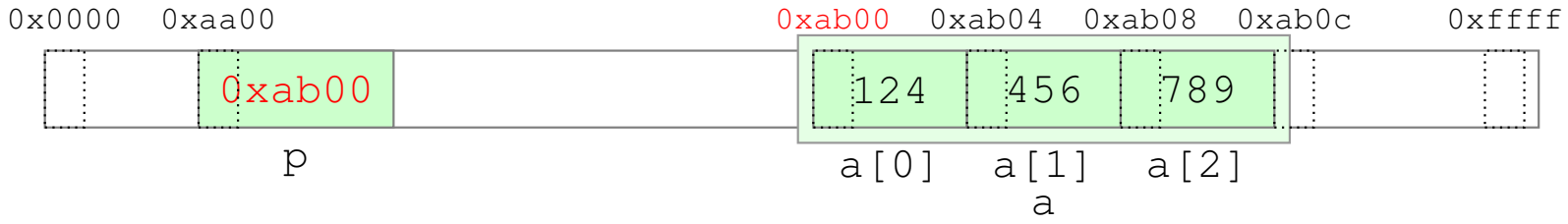


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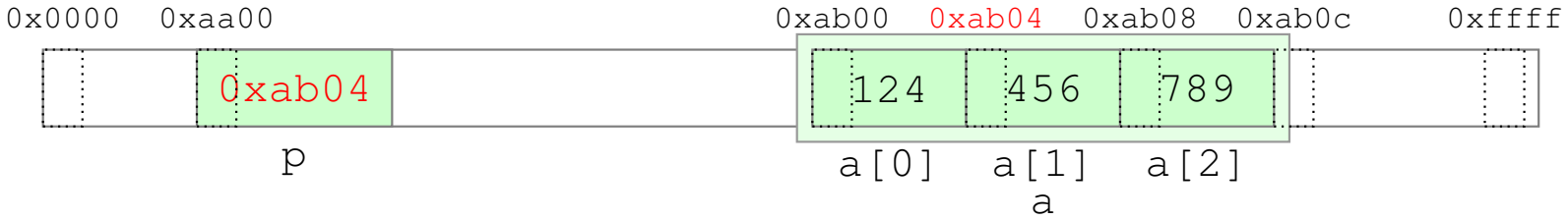


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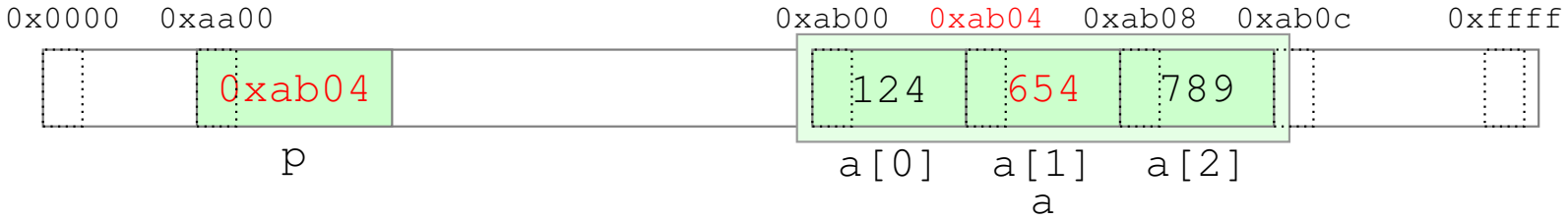


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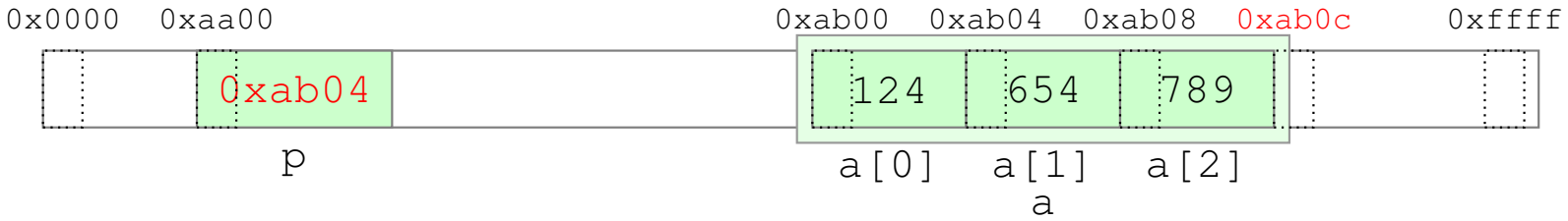


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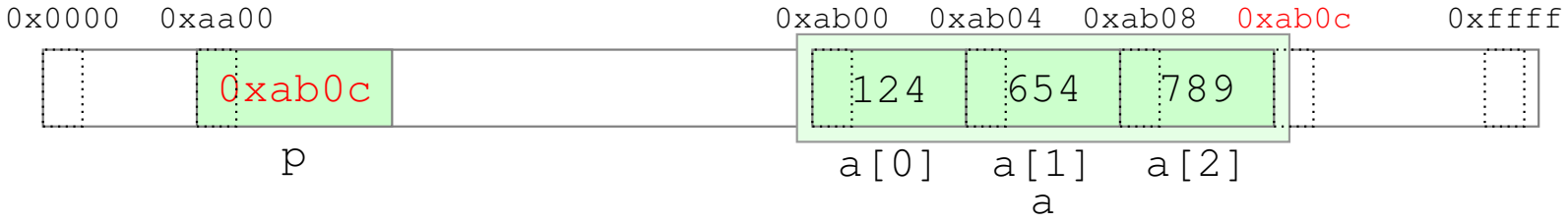


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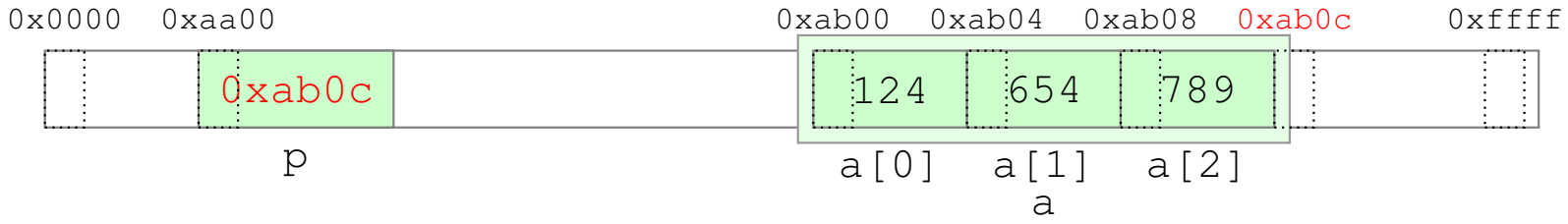


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if (p == a.data() + a.size()) { ... } // ok
```

std::array

```
template<class T, unsigned N> class array {
  T elems[N]; // no space overhead wrt to native array
public:
  size_t size() const { return N; }
  T* data() { return elems; }
  T const* data() const { return elems; }
  T& operator[](unsigned n) { return elems[n]; } // no checks!
  T const& operator[](unsigned n) const { return elems[n]; }
  ...
};

template<class T, unsigned N>
bool operator==(array<T, N> const& l, array<T, N> const& r) {
  return std::equal(l.data(), l.data() + N, r.data());
}

template<class T, unsigned N>
bool operator<(array<T, N> const& l, array<T, N> const& r) {
  return std::lexicographical_compare(
      l.data(), l.data() + N
    , r.data(), r.data() + N
  );
}
...
```

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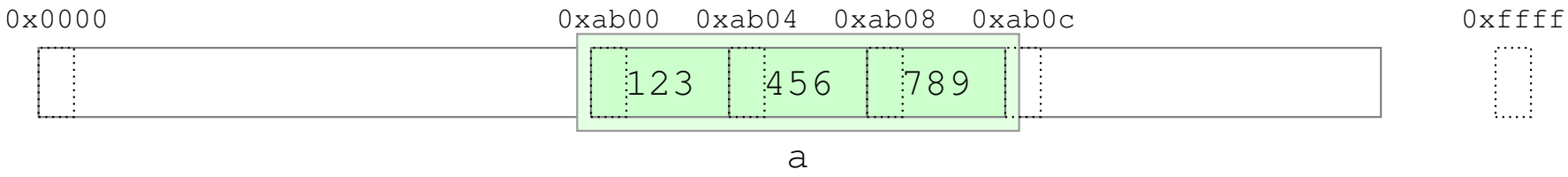
Set	`set_union set_intersection set_difference ...`
Min/Max	`min max minmax lexicographical_compare clamp ...`
Numeric	`iota accumulate inner_product partial_sum adjacent_difference ...`

Range

- A range is defined by a pair of iterators [*first*, *last*), with *last* referring to one past the last element in the range
  - the range is *half-open*
  - *first* == *last* means the range is empty
  - *last* can be used to return failure
- An iterator is a generalization of a pointer
  - it supports the same operations, possibly through overloaded operators
  - certainly `*` `++` `->` `==` `!=`, maybe `--` `+` `-` `+=` `-=` `<`
- Ranges are typically obtained from containers calling specific methods

Range (cont.)

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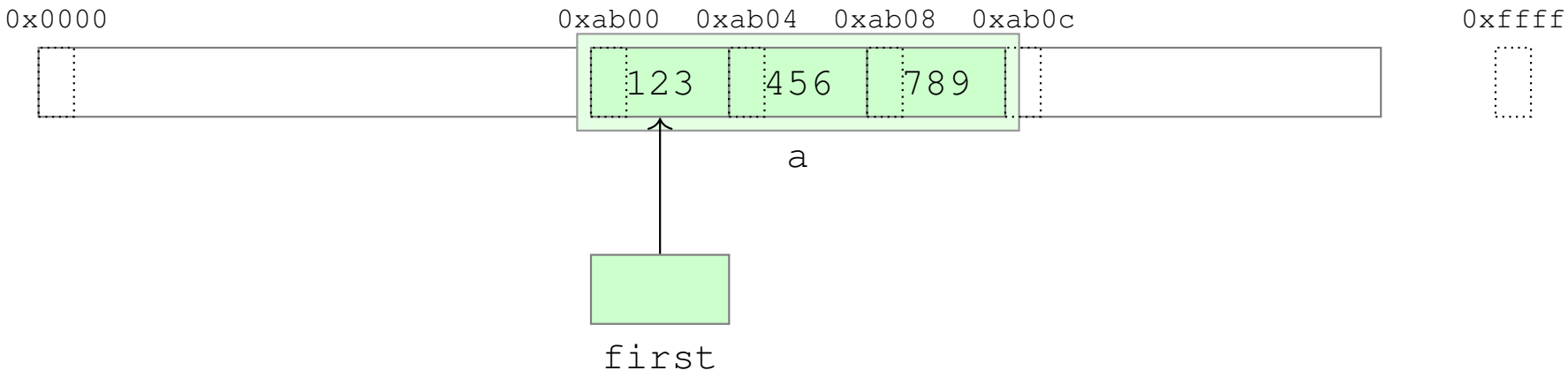


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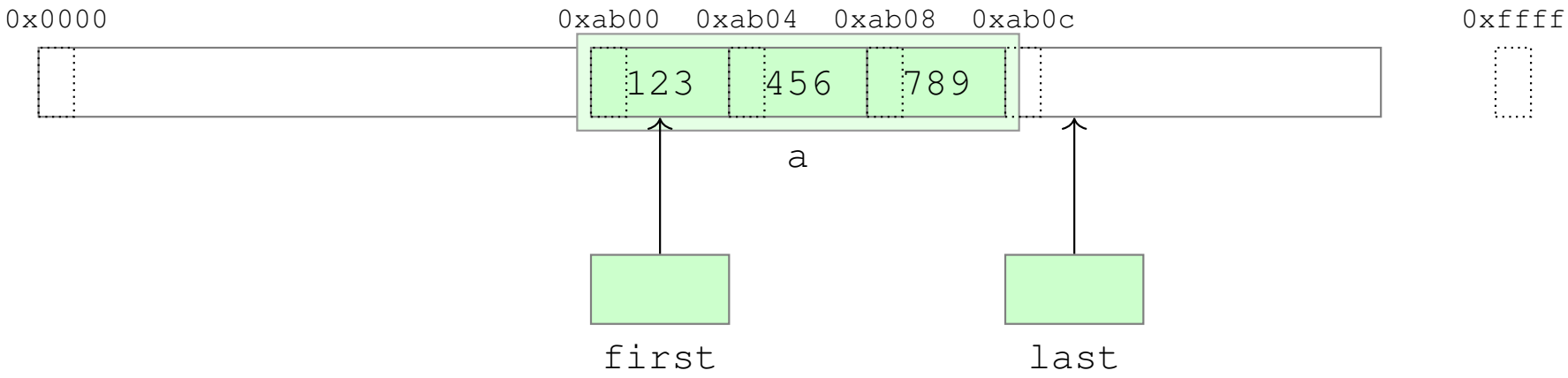


```
std::array<int,3> a = {123, 456, 789};
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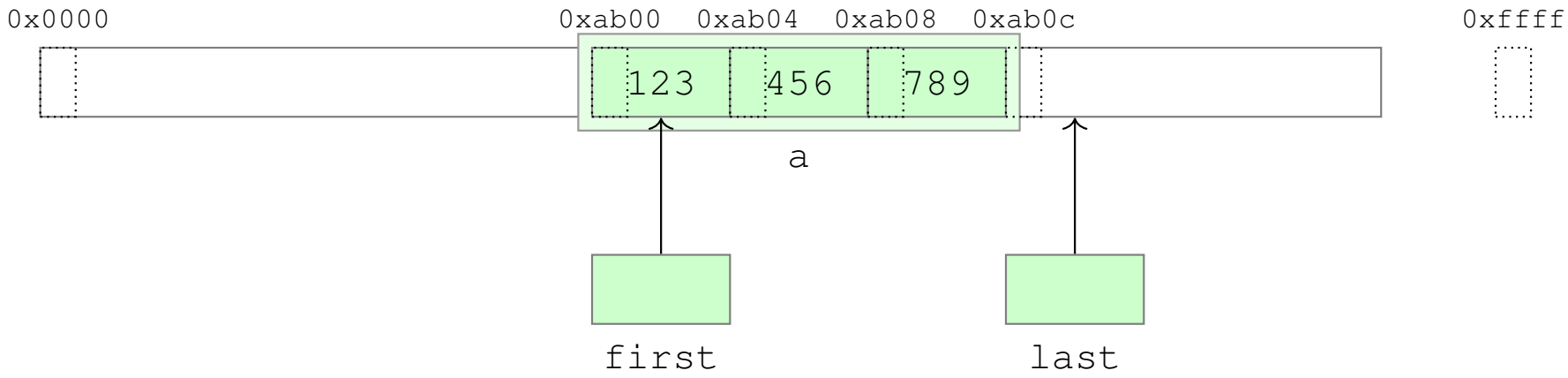
auto last = a.end();             // or std::end(a)
```

Range (cont.)

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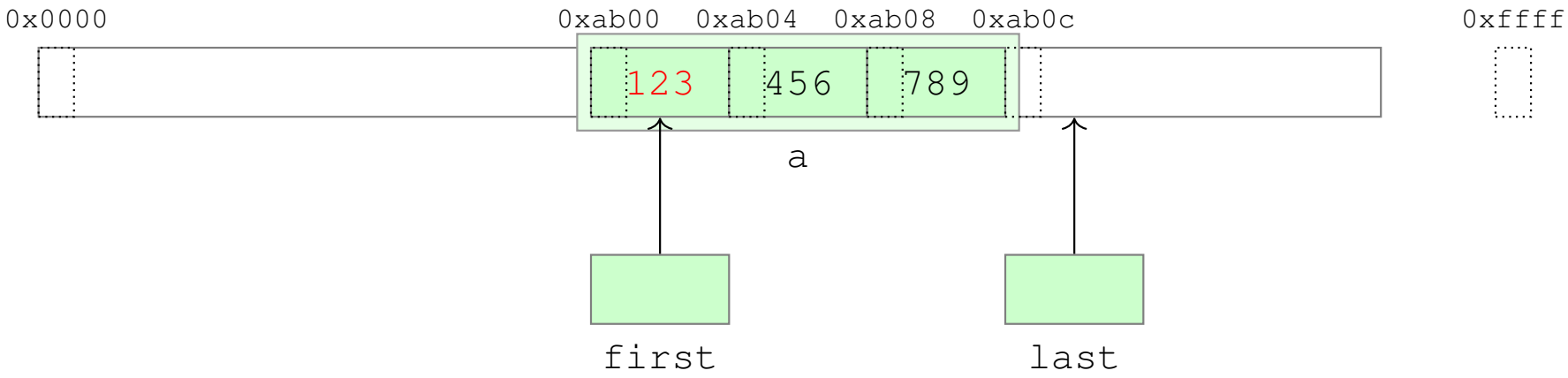


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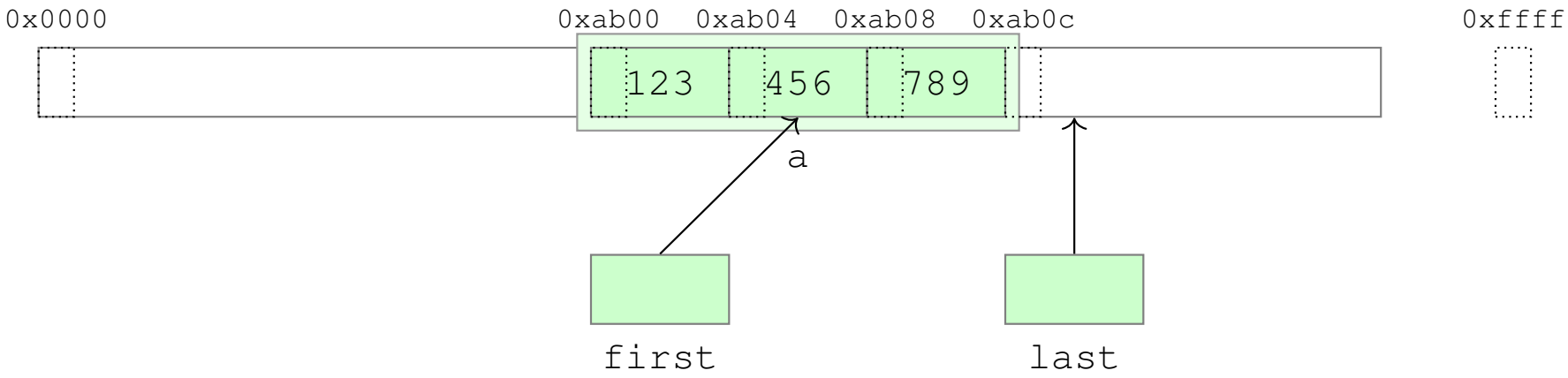


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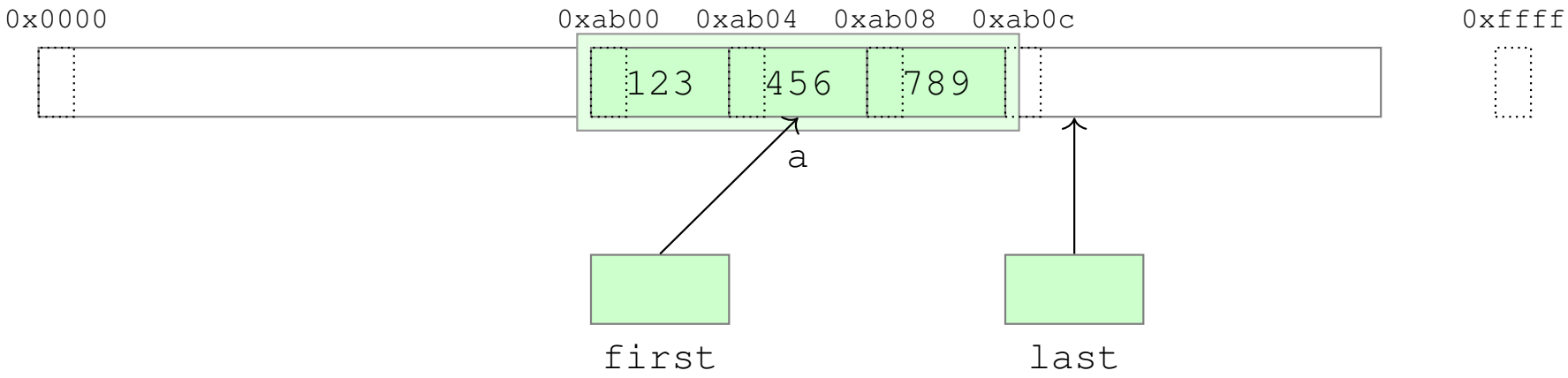


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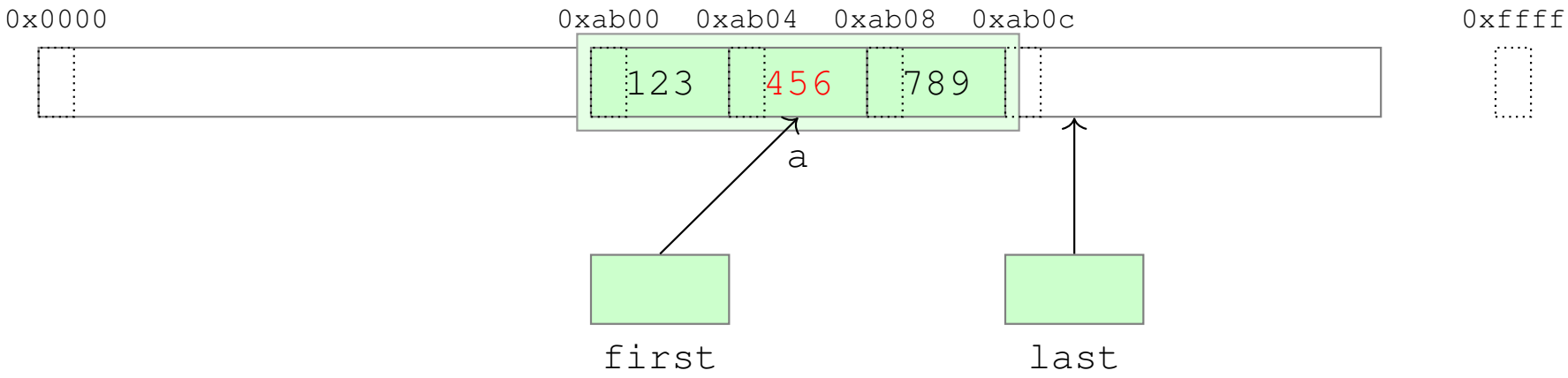


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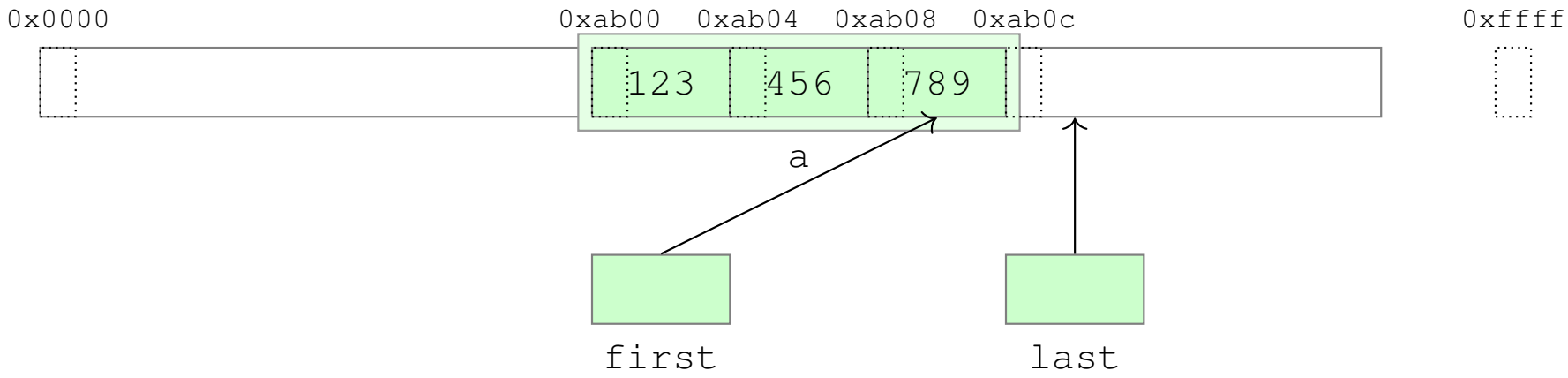


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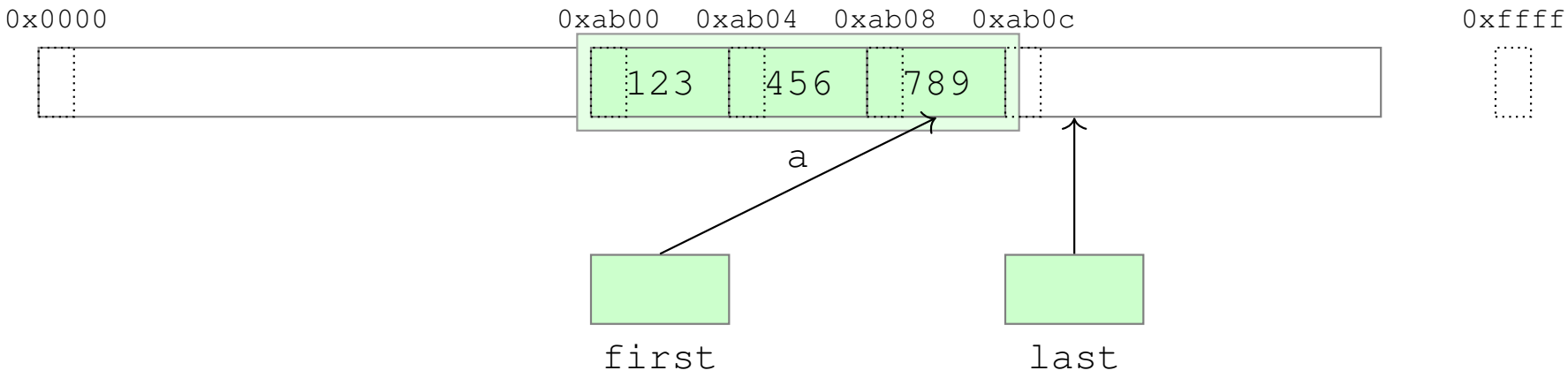


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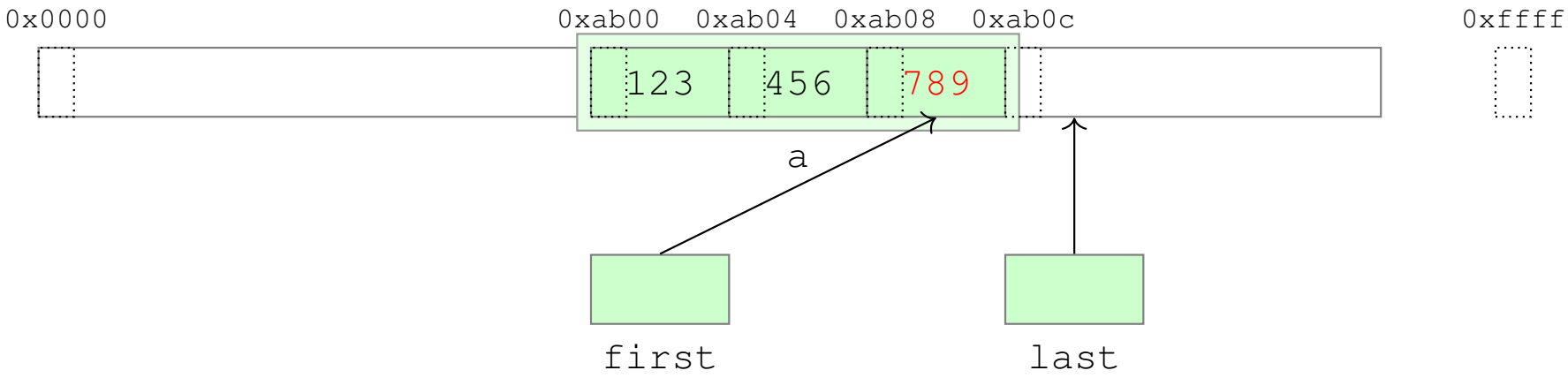


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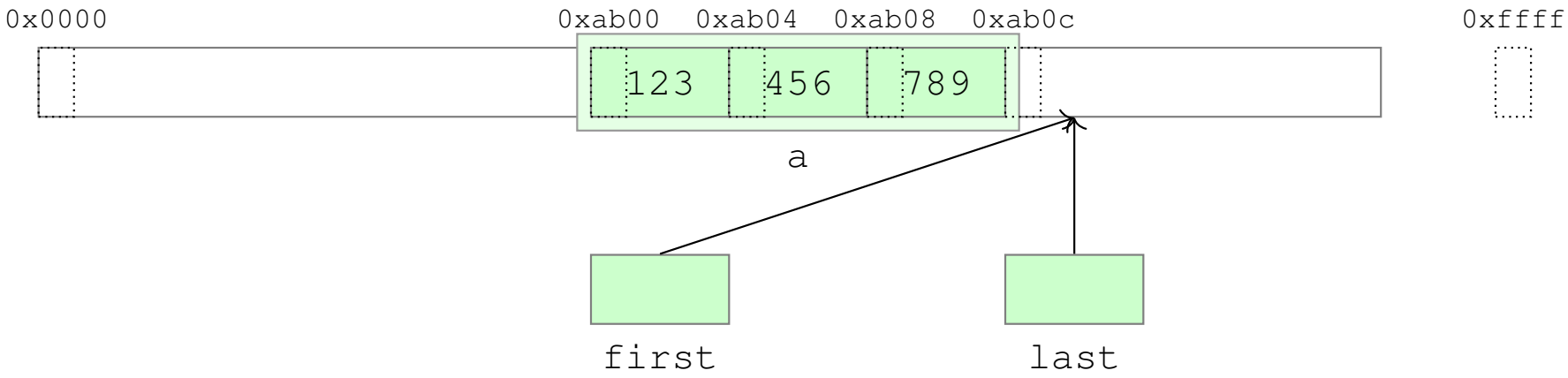


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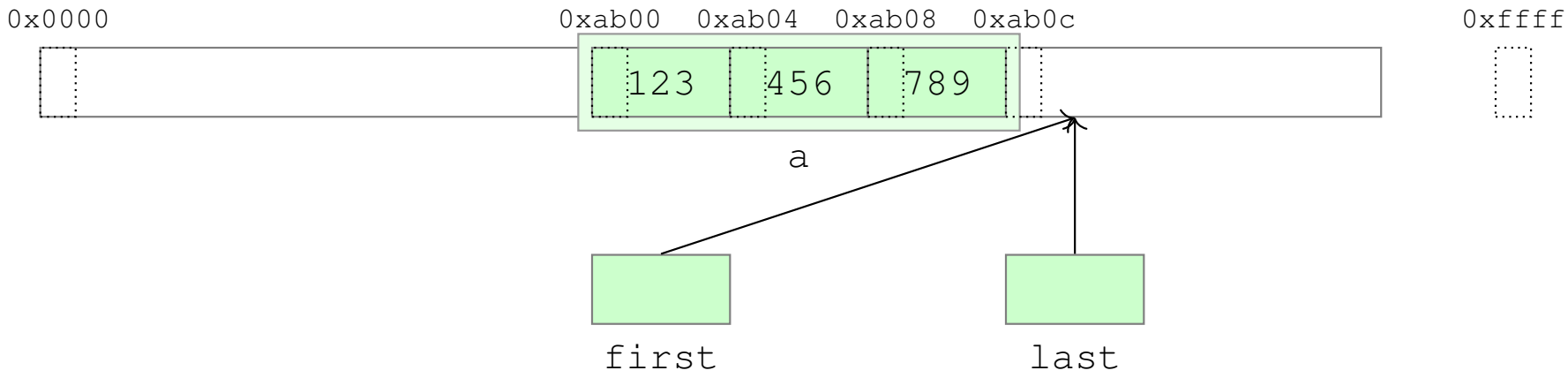


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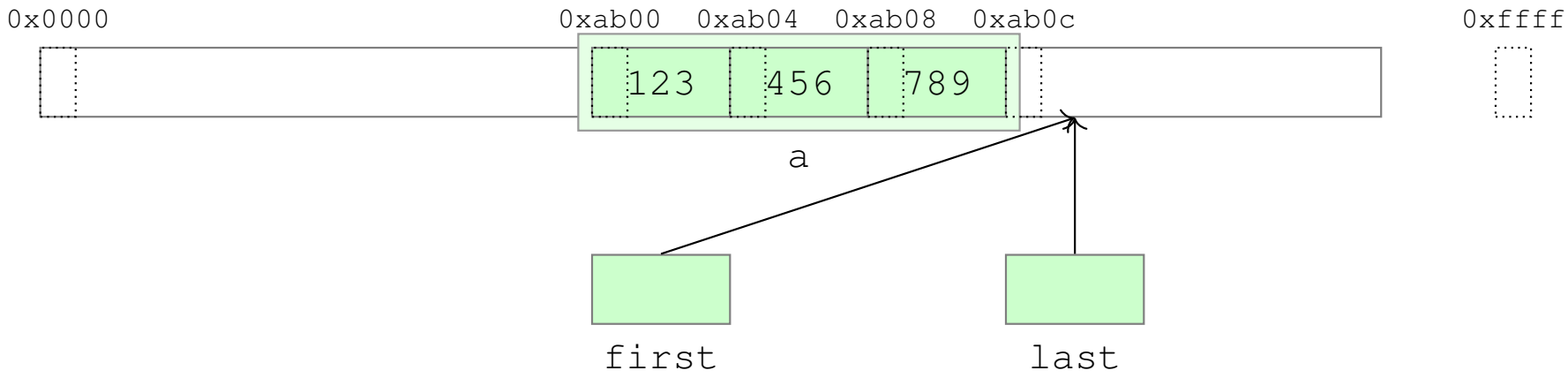
- `std::array<T>::iterator` models the *RandomAccessIterator* concept

Range (cont.)




```
std::array<int,3> a = {123, 456, 789};
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Generic programming

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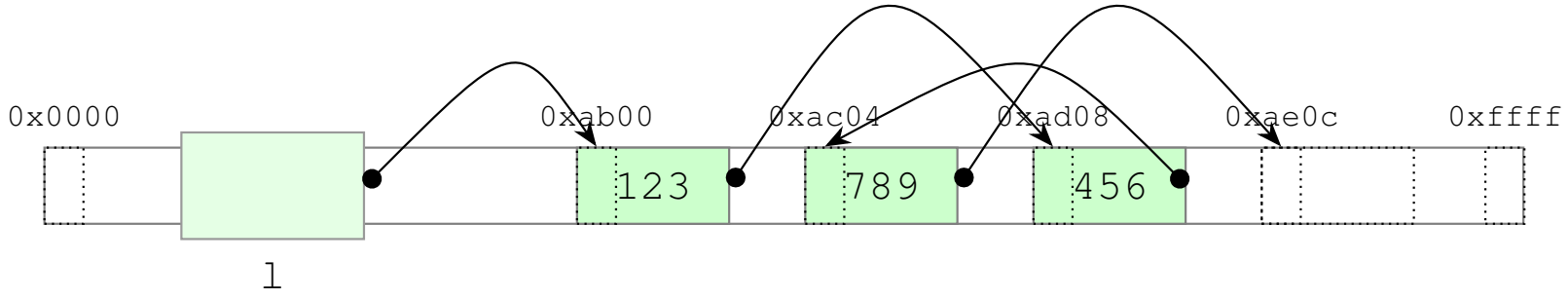
```
template <class Iterator, class T>
Iterator
find(Iterator first, Iterator last, const T& value)
{
  for (; first != last; ++first)
    if (*first == value)
      break;
  return first;
}
```

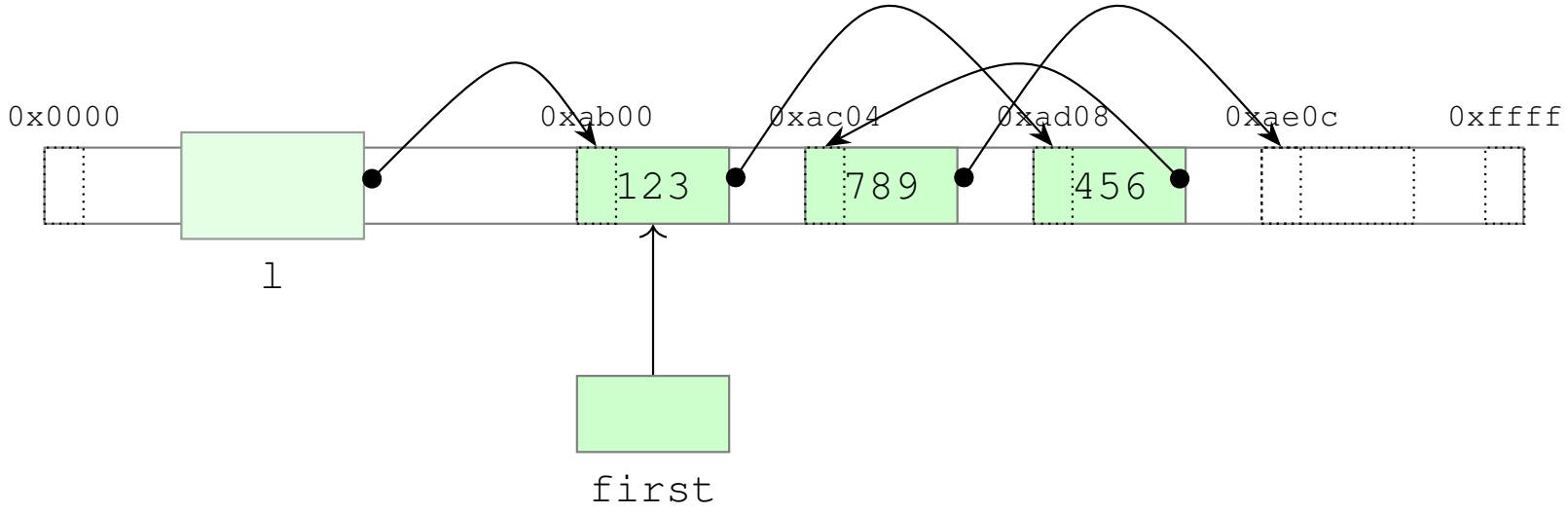
Range (cont.)




```
std::forward_list<int> l = {123, 456, 789};
```

- `std::forward_list<T>::iterators` models the *ForwardIterator* concept

Range (cont.)

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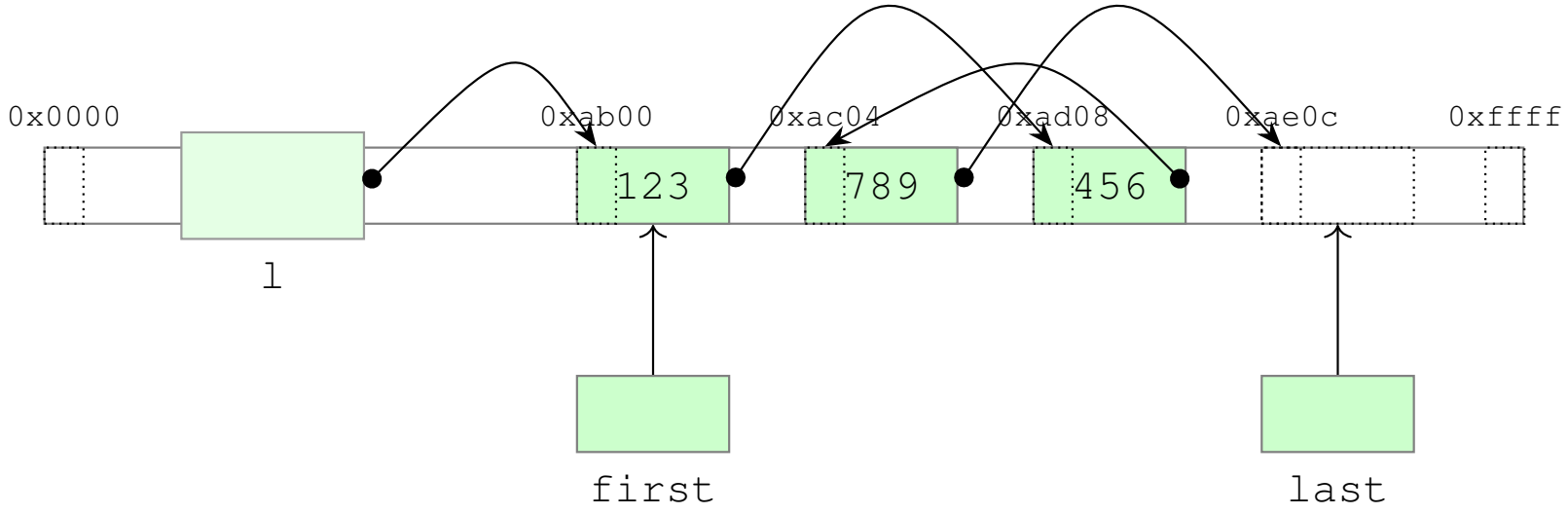


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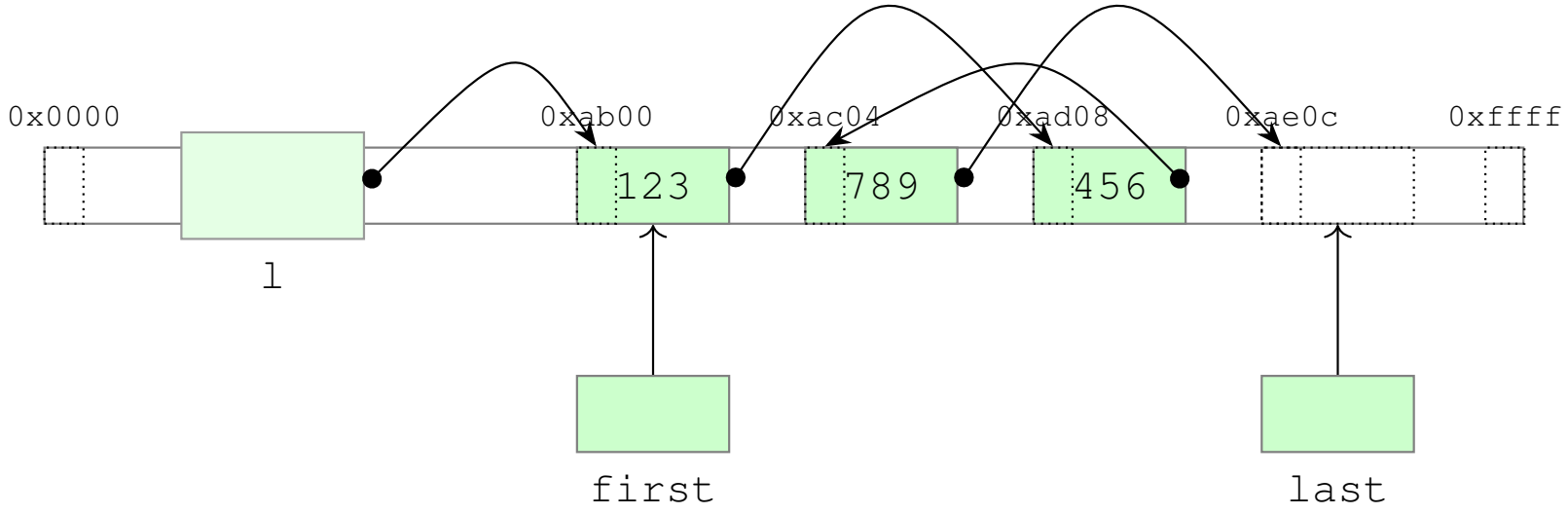


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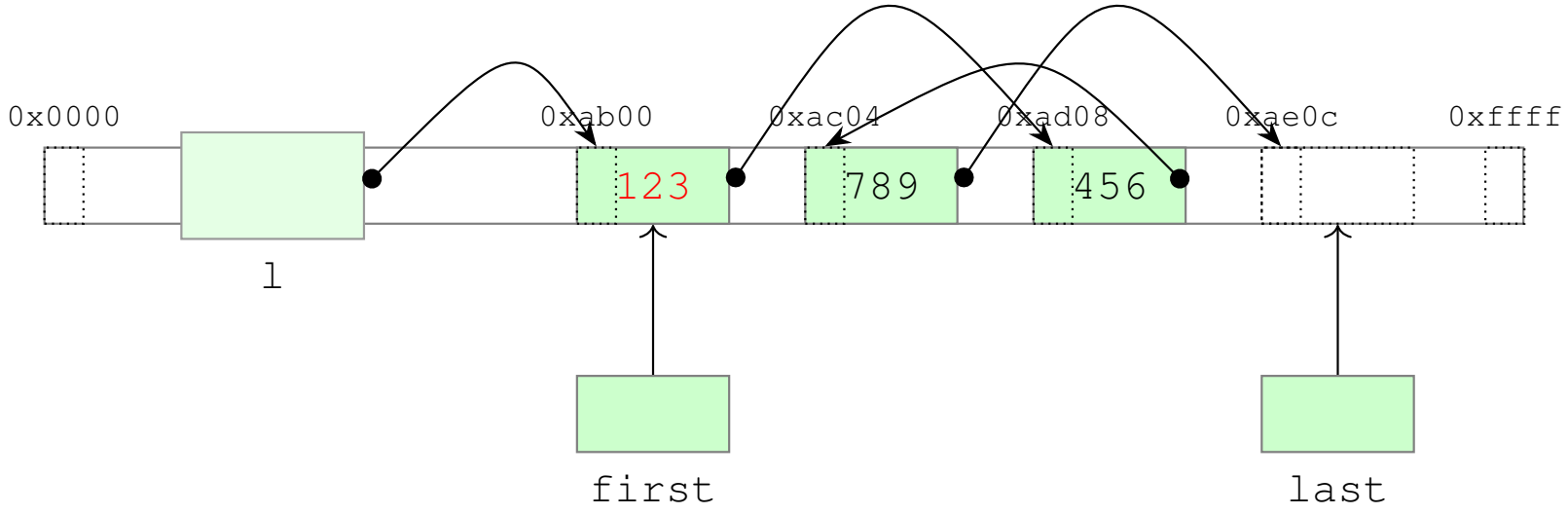


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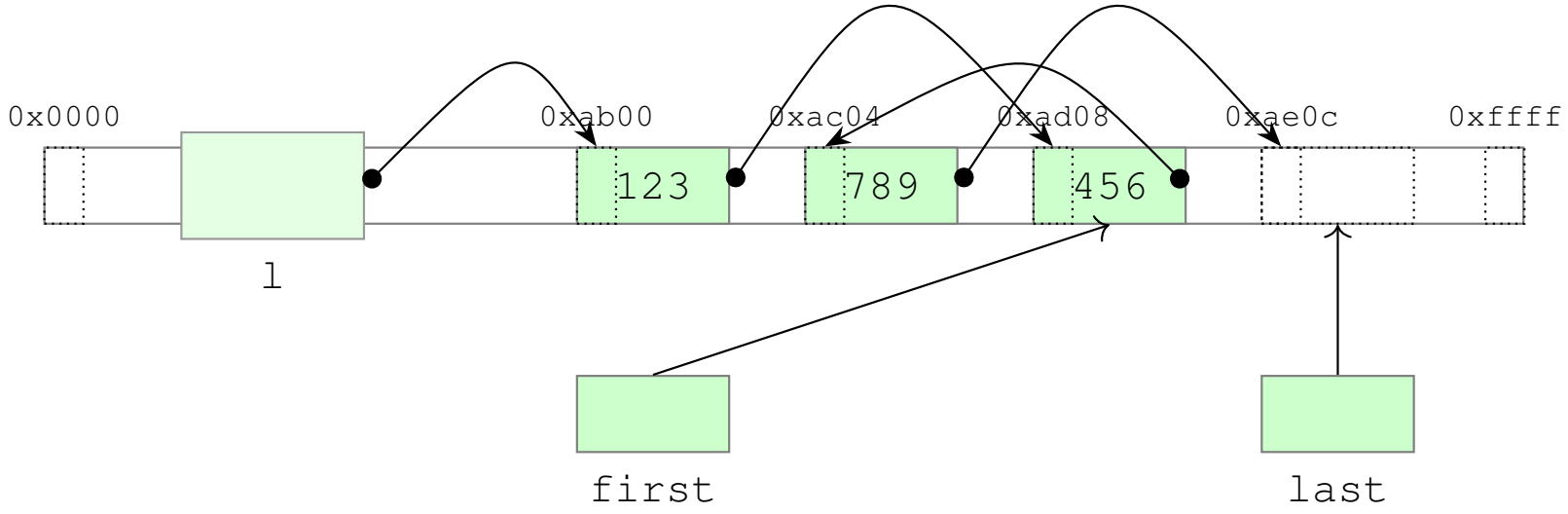


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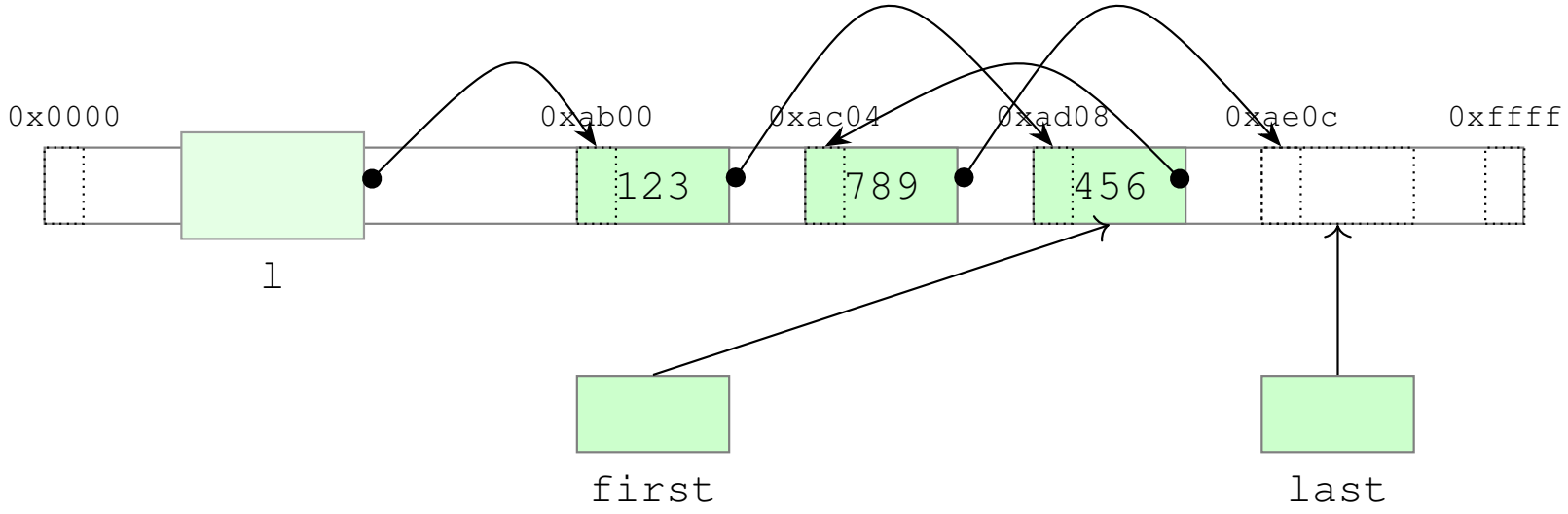


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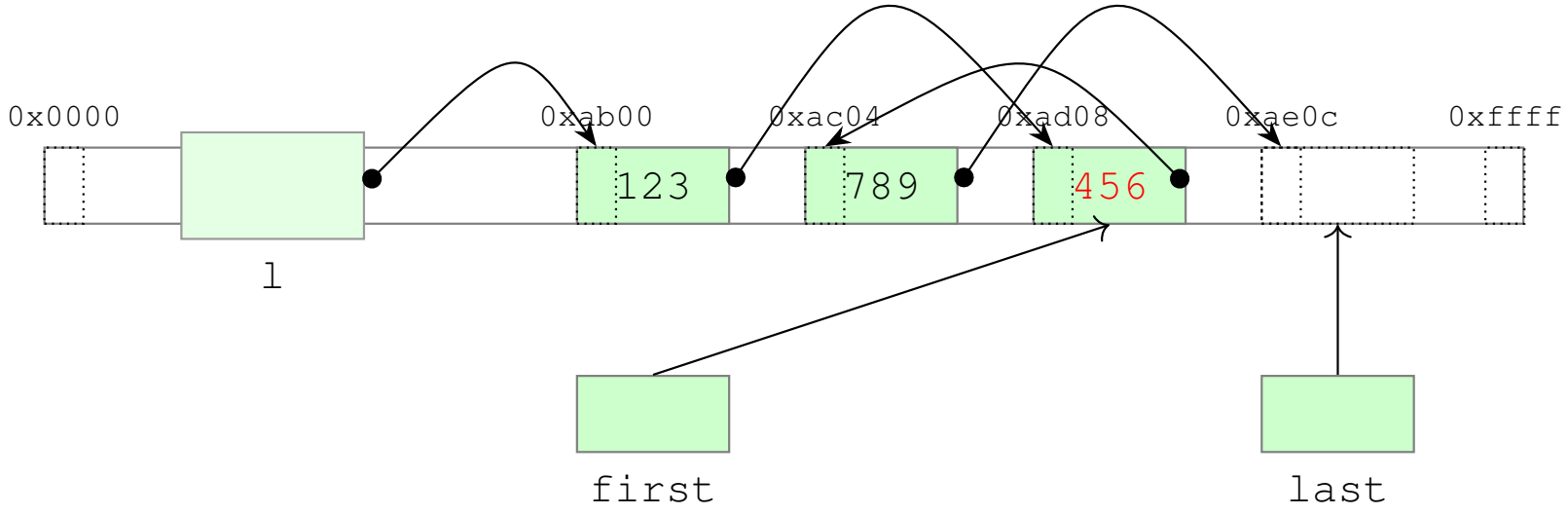


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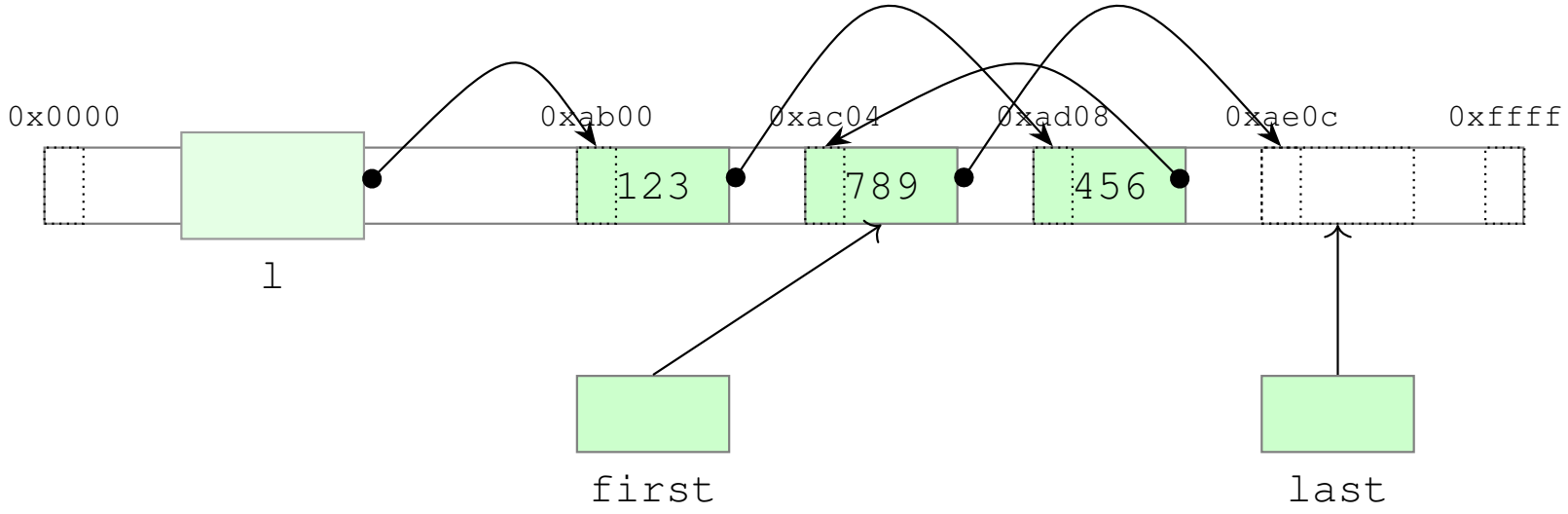


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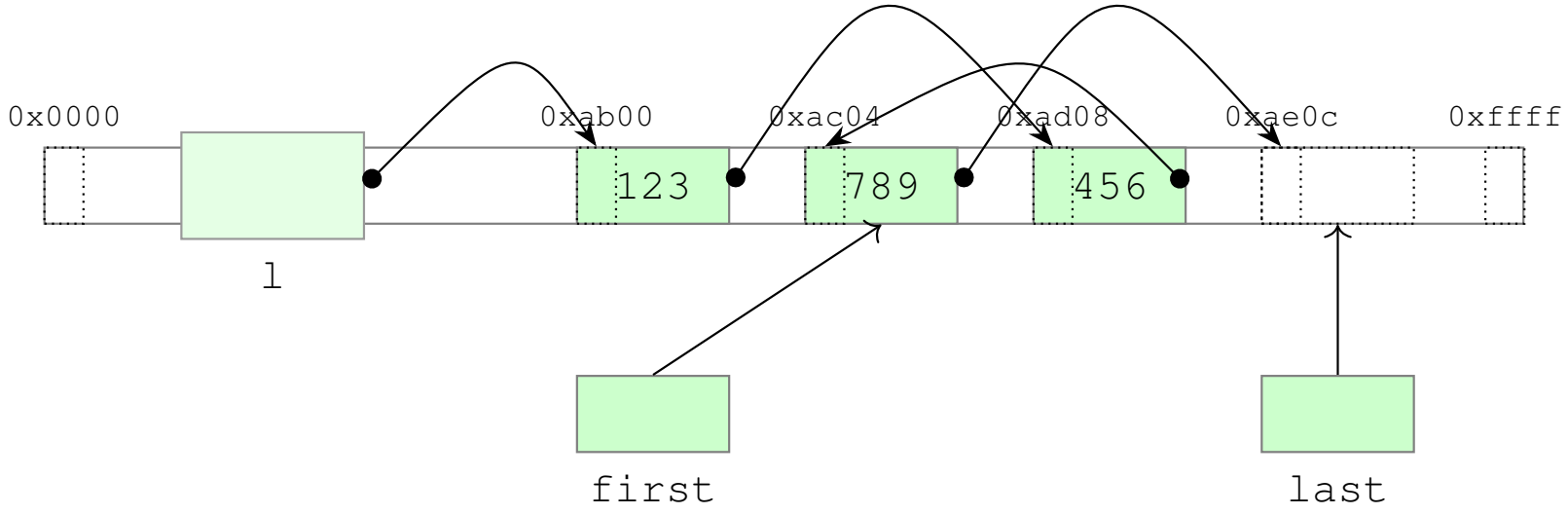


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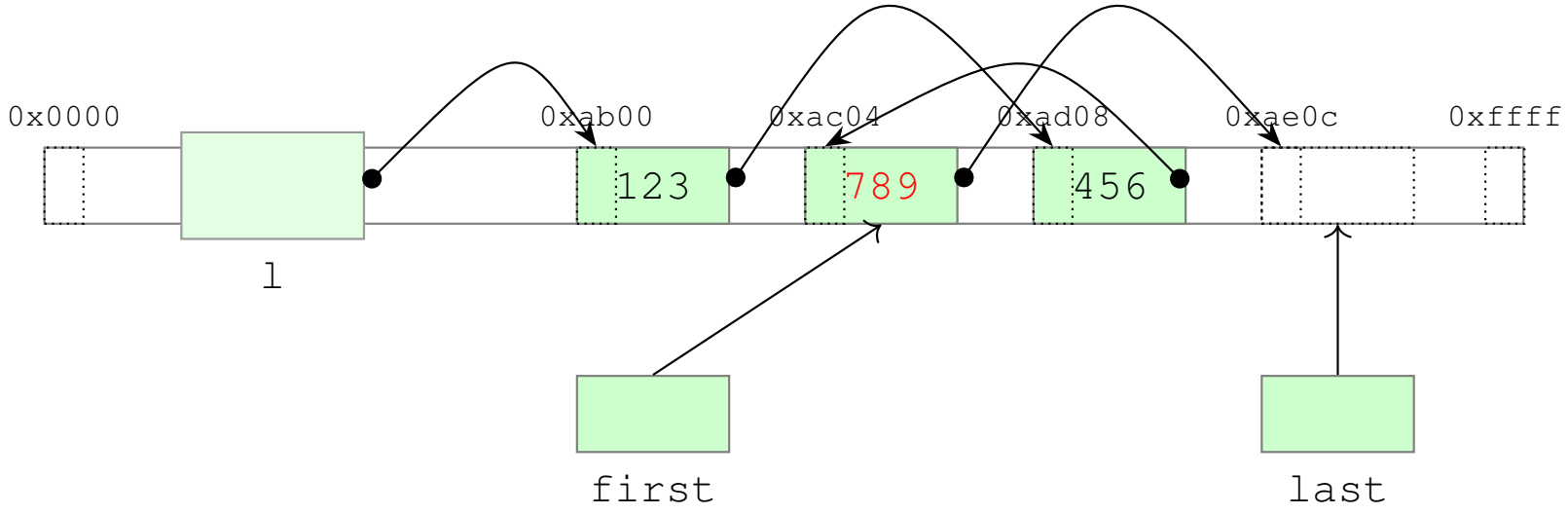


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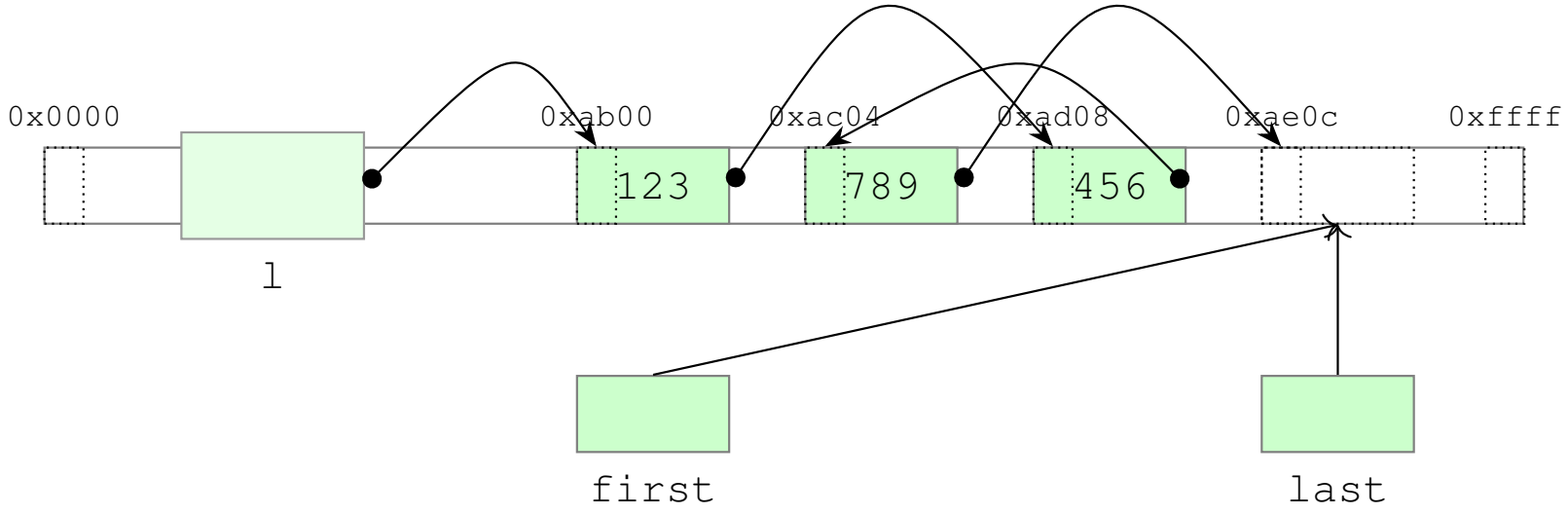


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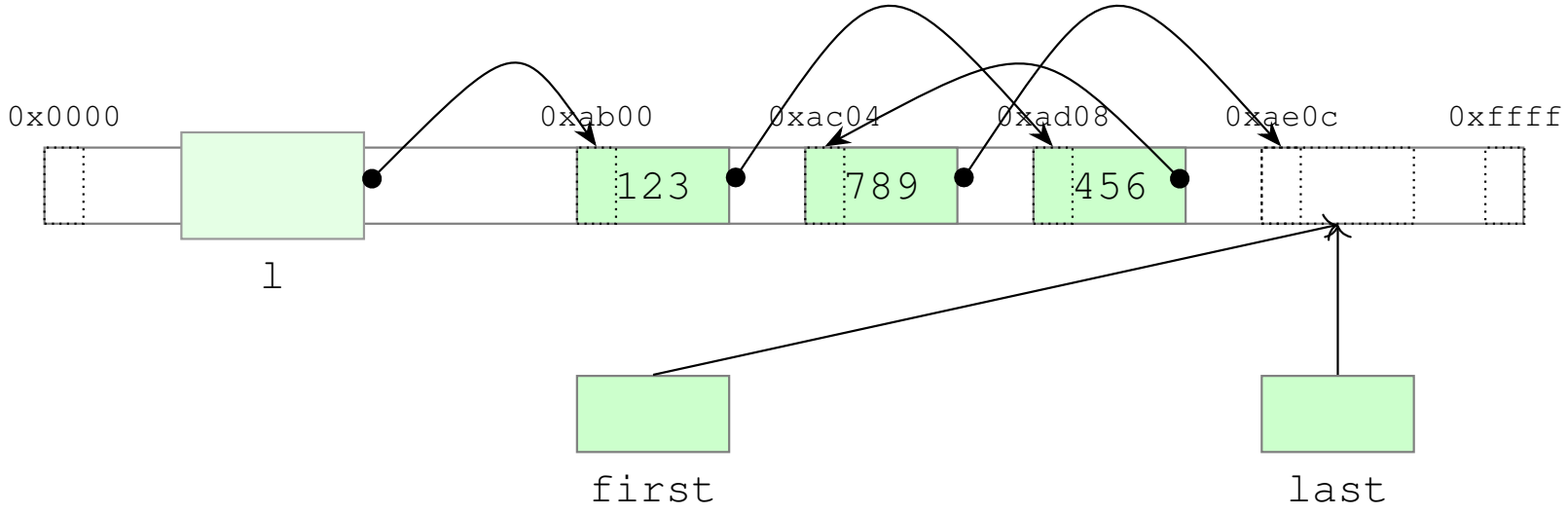


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Using the standard library

```
#include <array>      // note the angular brackets
                      // for standard headers


std::array<int,5> a;
```

Using the standard library

```
#include <array>      // note the angular brackets
#include <random>     // for standard headers


std::array<int,5> a;
std::default_random_engine e;
std::uniform_int_distribution<int> dist(1, 6);
```

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#include <algorithm>

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std::sort(a.begin(), a.end());
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std::sort(a.begin(), a.end());
    std::find(a.begin(), a.end(), 123)
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std::generate_n(a.begin(), a.size(), [&](){ return dist(e); });
std::sort(a.begin(), a.end());
if (std::find(a.begin(), a.end(), 123) == a.end()) {
  // 123 not found in a
}
```

std::vector

- The *default* container
- Similar to an array, but adjusts its size dynamically

```
std::vector<int> v; // size is 0
v.push_back(123);   // size is 1
...
v[42];
```

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std::array<int,5> a;
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std::generate_n(v.begin(), v.size(), [&](){ return dist(e); });
std::sort(v.begin(), v.end());
if (std::find(v.begin(), v.end(), 123) == v.end()) {
  // 123 not found in v
}
```

std::list

- Bi-directional list
- Node-based, scattered in memory

```
std::list<int> l;
v.push_back(123);
v.push_front(456);
...
*std::next(l.begin(), 42);
```

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std::generate_n(l.begin(), l.size(), [&](){ return dist(e); });
std::sort(l.begin(), l.end());
if (std::find(l.begin(), l.end(), 123) == l.end()) {
  // 123 not found in l
}
```

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std::default_random_engine e;
std::uniform_int_distribution<int> dist(1, 6);
std::generate_n(l.begin(), l.size(), [&](){ return dist(e); });
std::sort(l.begin(), l.end()); // error
if (std::find(l.begin(), l.end(), 123) == l.end()) {
  // 123 not found in l
}
```

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```

Function objects

A mechanism to define *something-callable-like-a-function*

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```
auto cat(
  string const& s, int i
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  return s + '-' + to_string(i);
}


auto s = cat("XY", 5); // XY-5
```

Function objects

A mechanism to define *something-callable-like-a-function*

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auto cat(
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}



auto s = cat("XY", 5); // XY-5

vector<int> v{2,3,5};
auto s = accumulate(
    begin(v), end(v),
    string{"XY"}, cat
); // XY-2-3-5
```

Function objects

A mechanism to define *something-callable-like-a-function*

- A class with an `operator()`

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vector<int> v{2,3,5};
auto s = accumulate(
    begin(v), end(v),
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); // XY-2-3-5
```

```
struct Cat {
 auto operator() (
  string const& s, int i
 ) const {
  return s + '-' + to_string(i);
 }
};
```

Function objects

A mechanism to define *something-callable-like-a-function*

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auto cat(
  string const& s, int i
) {
  return s + '-' + to_string(i);
}



auto s = cat("XY", 5); // XY-5

vector<int> v{2,3,5};
auto s = accumulate(
    begin(v), end(v),
    string{"XY"}, cat
); // XY-2-3-5
```

```
struct Cat {
 auto operator() (
  string const& s, int i
 ) const {
  return s + '-' + to_string(i);
 }
};

Cat cat{};
```

Function objects

A mechanism to define *something-callable-like-a-function*

- A class with an `operator()`

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auto cat(
  string const& s, int i
) {
  return s + '-' + to_string(i);
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Cat cat;
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```

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); // XY-2-3-5
```

```
struct Cat {
 auto operator() (
  string const& s, int i
 ) const {
  return s + '-' + to_string(i);
 }
};

Cat cat;
auto s = cat("XY", 5); // XY-5

vector<int> v{2,3,5};
auto s = accumulate(
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); // XY-2-3-5
```

Function objects

A mechanism to define *something-callable-like-a-function*

- A class with an `operator()`

```
auto cat(
  string const& s, int i
) {
  return s + '-' + to_string(i);
}



auto s = cat("XY", 5); // XY-5

vector<int> v{2,3,5};
auto s = accumulate(
    begin(v), end(v),
    string{"XY"}, cat
); // XY-2-3-5
```

```
struct Cat {
 auto operator() (
  string const& s, int i
 ) const {
  return s + '-' + to_string(i);
 }
};

Cat cat;
auto s = Cat{}("XY", 5); // XY-5

vector<int> v{2,3,5};
auto s = accumulate(
    begin(v), end(v),
    string{"XY"}, cat
); // XY-2-3-5
```

Function objects

A mechanism to define *something-callable-like-a-function*

- A class with an `operator()`

```
auto cat(
  string const& s, int i
) {
  return s + '-' + to_string(i);
}



auto s = cat("XY", 5); // XY-5

vector<int> v{2,3,5};
auto s = accumulate(
    begin(v), end(v),
    string{"XY"}, cat
); // XY-2-3-5
```

```
struct Cat {
 auto operator() (
  string const& s, int i
 ) const {
  return s + '-' + to_string(i);
 }
};

Cat cat;
auto s = Cat{}("XY", 5); // XY-5

vector<int> v{2,3,5};
auto s = accumulate(
    begin(v), end(v),
    string{"XY"}, Cat{}
); // XY-2-3-5
```

Function objects

A function object, being the instance of a class, can have state

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```
class CatWithState {
  char c_;
 public:
  explicit CatWithState(char c) : c_{c} {}
  auto operator()(string const& s, int i) const {
    return s + c_ + to_string(i);
  }
};
```

Function objects

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    return s + c_ + to_string(i);
  }
};

CatWithState cat1{'-'};
auto s1 = cat1("XY", 5); // XY-5
```

Function objects

A function object, being the instance of a class, can have state

```
class CatWithState {
  char c_;
 public:
  explicit CatWithState(char c) : c_{c} {}
  auto operator()(string const& s, int i) const {
    return s + c_ + to_string(i);
  }
};

CatWithState cat1{'-'};
auto s1 = cat1("XY", 5); // XY-5

CatWithState cat2{'+'};
auto s2 = cat2("XY", 5); // XY+5
```

Function objects

A function object, being the instance of a class, can have state

```
class CatWithState {
  char c_;
 public:
  explicit CatWithState(char c) : c_{c} {}
  auto operator()(string const& s, int i) const {
    return s + c_ + to_string(i);
  }
};

CatWithState cat1{'-'};
auto s1 = cat1("XY", 5); // XY-5

CatWithState cat2{'+'};
auto s2 = cat2("XY", 5); // XY+5

vector<int> v{2,3,5};
auto s3 = accumulate(..., cat1); // XY-2-3-5
auto s4 = accumulate(..., cat2); // XY+2+3+5
```

Function objects

A function object, being the instance of a class, can have state

```
class CatWithState {
  char c_;
 public:
  explicit CatWithState(char c) : c_{c} {}
  auto operator()(string const& s, int i) const {
    return s + c_ + to_string(i);
  }
};

CatWithState cat1{'-'};
auto s1 = CatWithState{'-'}("XY", 5); // XY-5

CatWithState cat2{'+'};
auto s2 = CatWithState{'+'}("XY", 5); // XY+5

vector<int> v{2,3,5};
auto s3 = accumulate(..., CatWithState{'-'}); // XY-2-3-5
auto s4 = accumulate(..., CatWithState{'+'}); // XY+2+3+5
```

Function objects (cont.)

An example from the standard library

```
#include <random>

// random bit generator (mersenne twister)
std::mt19937 gen;

// generate N 32-bit unsigned integer numbers
for (int n = 0; n != N; ++n) {
  std::cout << gen() << '\n';
}

// generate N floats distributed normally (mean: 0., stddev: 1.)
std::normal_distribution<float> dist;
for (int n = 0; n != N; ++n) {
  std::cout << dist(gen) << '\n';
}

// generate N ints distributed uniformly between 1 and 6 included
std::uniform_int_distribution<> roll_dice(1, 6);
for (int n = 0; n != N; ++n) {
  std::cout << roll_dice(gen) << '\n';
}
```

Lambda expression

- A concise way to create an unnamed function object
- Useful to pass actions/callbacks to algorithms, threads, frameworks, ...

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struct Cat {
 auto operator()(
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  return s + '-' + to_string(i);
 }
};

class CatWithState {
 char c_;
public:
 explicit CatWithState(char c)
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 auto operator()
 (string const& s, int i) const
 {return s + c_ + to_string(i);}
};
```

```
accumulate(..., Cat{});
```

```
accumulate(...,CatWithState{'-'});
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accumulate(...,
 [](string const& s, int i) {
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 }
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accumulate(...,CatWithState{'-'});
```

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struct Cat {
 auto operator()(
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};

class CatWithState {
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public:
 explicit CatWithState(char c)
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 auto operator()
 (string const& s, int i) const
 {return s + c_ + to_string(i);}
};
```

```
accumulate(..., Cat{});

accumulate(...,
 [](string const& s, int i) {
   return s + '-' + to_string(i);
 }
);

accumulate(...,CatWithState{'-'});

char c{'-'};
accumulate(...,
  [=](string const& s, int i) {
    return s + c + to_string(i);
  }
);
```

Lambda expression (cont.)

The evaluation of a lambda expression produces an unnamed function object (a *closure*)

- The `operator()` corresponds to the code of the body of the lambda expression
- The data members are the captured local variables

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```
auto l = []
```

```
class SomeUniqueName {

 public:
  explicit SomeUniqueName(      )
                {}
  auto operator()

};


auto l = SomeUniqueName{ };
```

Lambda expression (cont.)

The evaluation of a lambda expression produces an unnamed function object (a *closure*)

- The `operator()` corresponds to the code of the body of the lambda expression
- The data members are the captured local variables

```
auto l = [](int i)
{ return i + v; }
```

```
class SomeUniqueName {

 public:
  explicit SomeUniqueName(      )
                {}
  auto operator()(int i)
  { return i + v ; }
};


auto l = SomeUniqueName{ };
```

Lambda expression (cont.)

The evaluation of a lambda expression produces an unnamed function object (a *closure*)

- The `operator()` corresponds to the code of the body of the lambda expression
- The data members are the captured local variables

```
int v = 3;

auto l = [](int i)
{ return i + v; }
```

```
class SomeUniqueName {

 public:
  explicit SomeUniqueName(      )
                {}
  auto operator()(int i)
  { return i + v ; }
};

int v = 3;
auto l = SomeUniqueName{ };
```

Lambda expression (cont.)

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```
int v = 3;

auto l = [=](int i)
{ return i + v; }
```

```
class SomeUniqueName {
  int v_;
 public:
  explicit SomeUniqueName(int v)
    : v_{v} {}
  auto operator()(int i)
  { return i + v_; }
};

int v = 3;
auto l = SomeUniqueName{v};
```

Lambda expression (cont.)

The evaluation of a lambda expression produces an unnamed function object (a *closure*)

- The `operator()` corresponds to the code of the body of the lambda expression
- The data members are the captured local variables

```
int v = 3;

auto l = [=](int i)
{ return i + v; }

auto r = l(5); // 8
```

```
class SomeUniqueName {
  int v_;
 public:
  explicit SomeUniqueName(int v)
    : v_{v} {}
  auto operator()(int i)
  { return i + v_; }
};

int v = 3;
auto l = SomeUniqueName{v};
auto r = l(5); // 8
```

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- The `operator()` corresponds to the code of the body of the lambda expression
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```
auto l = [v = 3](int i)
{ return i + v; }

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```
class SomeUniqueName {
  int v_;
 public:
  explicit SomeUniqueName(int v)
    : v_{v} {}
  auto operator()(int i)
  { return i + v_; }
};

int v = 3;
auto l = SomeUniqueName{v};
auto r = l(5); // 8
```

Lambda expression (cont.)

The evaluation of a lambda expression produces an unnamed function object (a *closure*)

- The `operator()` corresponds to the code of the body of the lambda expression
- The data members are the captured local variables

```
auto l = [v = 3](int i) -> int
{ return i + v; }

auto r = l(5); // 8
```

```
class SomeUniqueName {
  int v_;
 public:
  explicit SomeUniqueName(int v)
    : v_{v} {}
  int  operator()(int i)
  { return i + v_; }
};

int v = 3;
auto l = SomeUniqueName{v};
auto r = l(5); // 8
```

Lambda: capturing

- Automatic variables used in the body need to be captured
  - `[]` capture nothing
  - `[=]` capture all by value
  - `[k]` capture `k` by value
  - `[&]` capture all by reference
  - `[&k]` capture `k` by reference
  - `[=, &k]` capture all by value but `k` by reference
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```
int v = 3;
auto l = [v] {};
```

```
class SomeUniqueName {
  int v_;
 public:
  explicit SomeUniqueName(int v)
    : v_v {}
  ...
};

auto l = SomeUniqueName{v};
```

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```
int v = 3;
auto l = [&v] {};
```

```
class SomeUniqueName {
  int& v_;
 public:
  explicit SomeUniqueName(int& v)
    : v_v {}
  ...
};

auto l = SomeUniqueName{v};
```

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```
int v = 3;
auto l = [&v] {};
```

```
class SomeUniqueName {
  int& v_;
 public:
  explicit SomeUniqueName(int& v)
    : v_v {}
  ...
};

auto l = SomeUniqueName{v};
```

- Global variables are available without being captured

Lambda: `const` and `mutable`

- By default the call to a lambda is `const`
  - Variable captured by value are not modifiable

```
[] {};
```

```
struct SomeUniqueName {
  auto operator()() const {}
};
```

Lambda: `const` and `mutable`

- By default the call to a lambda is `const`
  - Variable captured by value are not modifiable
- A lambda can be declared `mutable`

```
[]() mutable {};
```

```
struct SomeUniqueName {
  auto operator()() {}
};
```

Lambda: `const` and `mutable`

- By default the call to a lambda is `const`
  - Variable captured by value are not modifiable
- A lambda can be declared `mutable`

```
[]() mutable -> void {};
```

```
struct SomeUniqueName {
  void operator()() {}
};
```

Lambda: `const` and `mutable`

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  - Variable captured by value are not modifiable
- A lambda can be declared `mutable`

```
[]() mutable -> void {};
```

```
struct SomeUniqueName {
  void operator()() {}
};
```

- Variables captured by reference can be modified
  - There is no way to capture by `const&`

```
int v = 3;
[&v] { ++v; }();
assert(v == 4);
```

Lambda: dangling reference

Be careful not to have dangling references in a closure

- It's similar to a function returning a reference to a local variable

```
auto make_lambda()
{
  int v = 3;
  return [&] { return v; }; // return a closure
}

auto l = make_lambda();
auto d = l(); // the captured variable is dangling here
```

```
auto start_in_thread()
{
  int v = 3;
  return std::async([&] { return v; });
}
```

std::function

- Type-erased wrapper that can store and invoke any callable entity with a certain signature
  - function, function object, lambda, member function
- Some space and time overhead, so use only if a template parameter is not satisfactory

std::function

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```
#include <functional>

int sum_squares(int x, int y) { return x * x + y * y; }

int main() {
  std::vector<std::function<int(int, int)>> v {
    std::plus<>{},        // has a compatible operator()
    std::multiplies<>{}, // idem
    &sum_squares)
  };
  for (int k = 10; k <= 1000; k *= 10) {
    v.push_back([k](int x, int y) -> int { return k * x + y; });
  }

  for (auto const& f : v) { std::cout << f(4, 5) << '\n'; }
}
```

Smart pointers and custom deleters

- `unique_ptr` and `shared_ptr` can be used as general-purpose resource handlers
- The resource release is not necessarily done with `delete`
- `unique_ptr` and `shared_ptr` support a *custom deleter*

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```
FILE* f = std::fopen(...);
...
std::fclose(f);
```

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Usual problems:

- Who owns the resource?
- Forgetting to release
- Releasing twice
- Early return/throw

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```
auto s = std::shared_ptr<FILE>{
  std::fopen(...),
  std::fclose
};
```

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```
auto s = std::shared_ptr<FILE>{
  std::fopen(...),
  std::fclose
};

auto u = std::unique_ptr<
    FILE,
    int(*)(FILE*)
  >{
  std::fopen(...),
  &std::fclose
};
```

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```
auto s = std::shared_ptr<FILE>{
  std::fopen(...),
  std::fclose
};

auto u = std::unique_ptr<
    FILE,
    decltype(&std::fclose)
  >{
  std::fopen(...),
  &std::fclose
};
```

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  >{
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  std::fclose
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```

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auto s = std::shared_ptr<FILE>{
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    std::function<void(FILE*)>
  >{
  std::fopen(...),
  [](FILE* f){ std::fclose(f); }
};
```

Smart pointers and custom deleters

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```
FILE* f = std::fopen(...);
...
std::fclose(f);
```

Usual problems:

- Who owns the resource?
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```
auto s = std::shared_ptr<FILE>{
  std::fopen(...),
  std::fclose
};

auto u = std::unique_ptr<
    FILE,
    std::function<void(FILE*)>
  >{
  std::fopen(...),
  [](auto f){ std::fclose(f); }
};
```

Hands-on

Starting from `algo.cpp`, write code to

- sum all the elements of the vector
- multiply all the elements of the vector
- sort the vector in ascending and descending order
- move the even numbers to the beginning
- move the three central numbers to the beginning
- erase from the vector the elements that satisfy a predicate
- ...