Iterators and Ranges for numerical problems

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Outline

1. Introduction
2. Iterators and ranges for dynamical systems
3. Iterators for GPUs
4. Conclusion

Introduction

Iterators

Unique way to traverse containers
Unique way to apply iterative IO
Unique way of expressing algorithms

Example – basic use

```
for( auto iter = values.begin() ;
     iter != values.end() ;
     ++iter )
{
    cout << *iter << endl;
}
```

Example – basic use

```
for( auto iter = values.begin() ;
     iter != values.end() ;
     ++iter )
{
    cout << *iter << endl;
}
```

C++11 - use range based for

```
for( auto v : values )
{
    cout << v << endl;
}
```

Example – Container traversal

```
list< double > values;
list< double > values2( values.size() );
```

Can be used in

```
transform( values.begin() , values.end() ,
           values2.begin() ,
           []( double x ) {
               return x * 2.0; } );
```

Example – Container traversal

```
vector< double > values;
vector< double > values2( values.size() );
```

Can be used in

```
transform( values.begin() , values.end() ,
           values2.begin() ,
           []( double x ) {
               return x * 2.0; } );
```

Examples – IO

Input

```
vector< double > values;
copy_if( istream_iterator< double >( cout ) ,
         istream_iterator< double >() ,
         back_inserter( values ) ,
         []( double x ) { return x > 0.0; } );
```

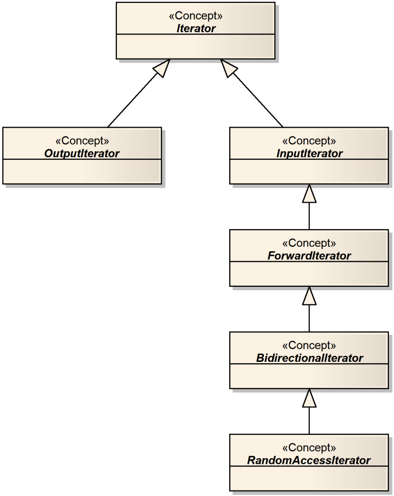
Output

```
vector< double > values;
// fill values
copy_if( values.begin() , values.end() ,
         ostream_iterator< double >( std::cout , "\n" ) ,
         []( double x ) { return x > 0.0; } );
```

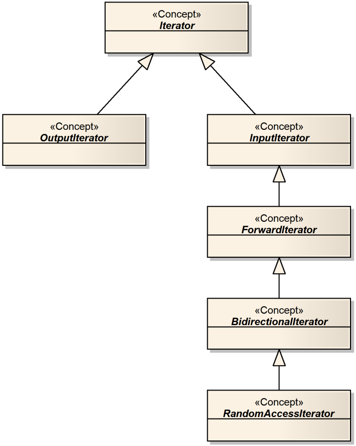
Examples – Combine algorithms

Find a nice real life example.

Iterator types – Concepts



Iterator types – Concepts

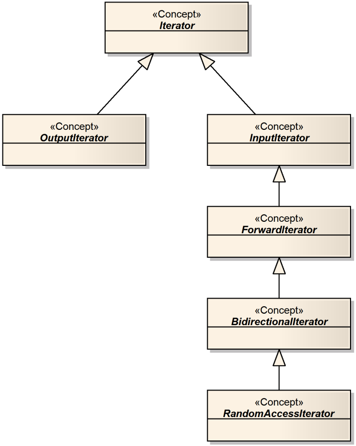


OutputIterator

```
*i = o;
*i++ = o;
i++;
++i;
```

Are special, `back_inserter`, `ostream_iterator`, ...

Iterator types – Concepts



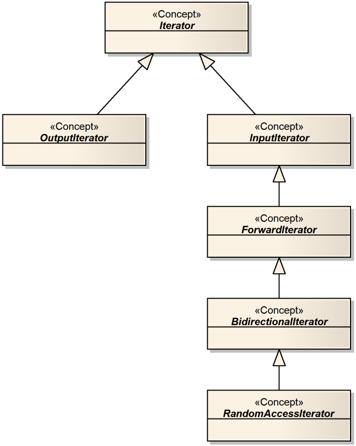
InputIterator a.k.a. Single-Pass Iterator

```
bool r = i != j;
val x = *i;
iterator j = ++i;
i++;
val x = *i++;
```

`istream_iterator`, `istreambuf_iterator`

But, if `i == j` then `++i != ++j`

Iterator types – Concepts

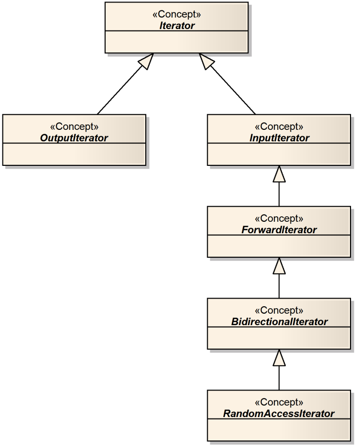


ForwardIterator

```
iterator j = i++;
```

But, if `i == j` then `++i == ++j`

Iterator types – Concepts

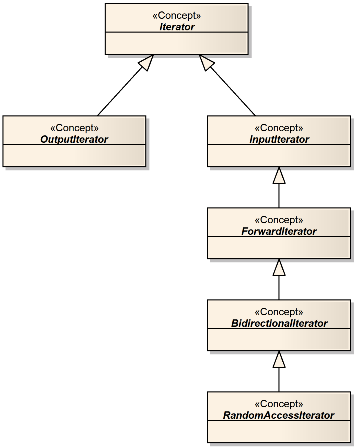


BidirectionalIterator

```
iterator j = --i;
iterator j = i--;
val x = *i--;
```

`map< K , V >::iterator,`
`list< T >::iterator`

Iterator types – Concepts



RandomAccessIterator

```
i += n;
i -= n;
val x = i[n];
long dist = i - j;
bool b = i < j;
```

`vector< T >::iterator`

Algorithms

```
I all_of
I any_of
I none_of
I for_each
I count
I count_if
I mismatch
I equal
I find
I find_if
I find_if_not
F find_end
I,F find_first_if
F adjacent_find
F search
F search_n
I,O copy
I,O copy_if
I,O copy_n
B,O copy_backward
I,O move
B,O move_backward
F fill
F fill_n
I,O transform
F generate
I generate_n
```

```
F remove
F remove_if
I,O remove_copy
I,O
remove_copy_if
F replace
F replace_if
I,O replace_copy
I,O
replace_copy_if
F swap_ranges
F iter_swap
B reverse
B,O reverse_copy
F rotate
F,O rotate_copy
R random_shuffle
R shuffle
F unique
I,O unique_copy
```

```
I is_partitioned
F,B partition
I,O partition_copy
B stable_partition
F partition_point
F is_sorted
F is_sorted_until
R sort
R partial_sort
I,R partial_sort_copy
R stable_sort
R nth_element
F lower_bound
F upper_bound
F binary_search
F equal_range
I,O merge
B inplace_merge
I includes
I,O set_difference
I,O set_intersection
I,O
set_symmetric_difference
I,O set_unition
```

```
R is_heap
R is_heap_until
R make_heap
R push_heap
R pop_heap
R sort_heap
F max_element
F min_element
F minmax_element
I lexicographical_compare
F is_permutation
B next_permutation
B prev_permutation
F iota
I accumulate
I inner_product
I,O adjacent_difference
I,O partial_sum
```

Ranges

Simplifying iterators
Generalization of iterators
First defined in Boost
Soon in the standard library?

```
vector< double > values;
boost::for_each( values , []( double x ) { cout
     << x << endl; } );
```

Ranges – more examples from boost

Filters
complicated algorithms

Ranges in Boost

Ranges are pairs of iterators.
Memory overhead
Filters grow exponential in size

Ranges for the native C++

Introduces new concepts:
Iterable, Container, Sentinel
The range is the main abstraction not the iterator
It holds all informations
Concepts, asymmetric algorithms, sentinels have their own type.

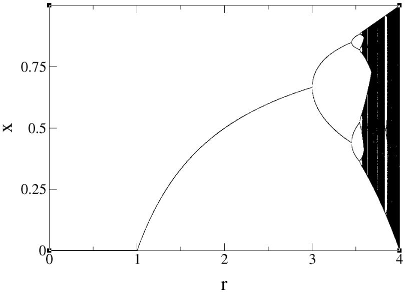
Iterators and ranges for dynamical systems

Dynamical systems – Maps

$$x_{n+1} = f(x_n)$$

Example: Logistic map

$$x_{n+1} = r\, x_n(1 - x_n)$$

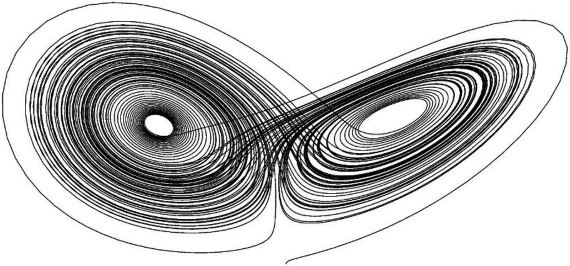


Dynamical systems – ODEs

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x, t)$$

Example: Lorenz attractor

$$\dot{x} = \sigma(y - x) \quad , \quad \dot{y} = x(\rho - z) - y \quad , \quad \dot{z} = xy - \beta z$$



Numerical solution:

$$x(t + \Delta t) = F(x(t))$$

Newton method

Find the root

$$0 = f(x)$$

Newtons method

- Choose x_0
- Iterate $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

Map range

Abstraction for $x_{n+1} = f(x_n)$

Two versions:

1. `map_range` - stop predicate
2. `counted_map_range` - iterates *n*-times

Models the SinglePassRange concept

Map range – implementation

```
template< typename T1 , ... > class map_range
{
    struct iterator { ... };
 public:
    // ...
    iterator begin() { return iterator( this ); }
    iterator end() { return iterator( nullptr ); }
    // ...
};
```

Range algorithms redirect to iterator algorithms:

```
template< typename R , typename F >
void for_each( R const& r , F f ) {
    std::for_each( r.begin() , e.end() , f );
}
```

Map range

```
template< typename T , typename F , typename C >
class map_range
{
    struct iterator { ... };

  public:
    map_range( T value , F func , C condition )
    : m_value { std::move( value ) }
    , m_func { std::move( func ) }
    , m_condition( condition )
    {}

    iterator begin() const { return iterator( this ); }
    iterator end() const { return iterator( nullptr ); }

private:
    mutable T m_value;
    mutable F m_func;
    C m_condition;
};
```

Map range

```
struct iterator {
    iterator( map_range const* _r ) : r( _r ) {}

    iterator& operator++() {
        r->m_value = r->m_func( r->m_value );
        if( r->m_condition( r->m_value ) ) {
            r = nullptr;
        }
        return *this;
    }

    T& operator*() const {
        return r->m_value; }
    bool operator==( iterator const& o ) const {
        return ( r == o.r ); }
    bool operator!=( iterator const& o ) const {
        return ! ( *this == o );
    }

    map_range const* r;
};
```

Counted map range

```
template< typename T , typename F >
class counted_map_range
{
    struct iterator { ... };

public:
    counted_map_range( T value , F func , size_t
        max_iterations )
    : m_current_iteration { 0 }
    , m_max_iterations { max_iterations }
    , m_value { std::move( value ) }
    , m_func { std::move( func ) }
    {}

    iterator begin() const { return iterator( this ); }
    iterator end( void ) { return iterator( nullptr ); }

private:
    mutable size_t m_current_iteration = 0;
    const size_t m_max_iterations;
    mutable T m_value;
    mutable F m_func;
};
```

Factory functions

```
template< typename T , typename F , typename C >
auto make_map_range( T t , F f , C condition )
{
    return map_range< T , F , C >(
        std::move( t ) ,
        std::move( f ) ,
        std::move( condition ) );
}
```

```
template< typename T , typename F >
auto make_counted_map_range( T t , F f , size_t
    max_iterations )
{
    return counted_map_range< T , F >(
        std::move( t ) ,
        std::move( f ) ,
        max_iterations );
}
```

Examples – generalized iota

Generalized Iota:

```
size_t n = 10;
auto iota = make_counted_map_range( 1 , []( auto x ) {
    return x * 2; } , 10 );

std::vector< int > values;
boost::copy( iota_range , std::back_inserter( values ) );
for( auto i : values ) { cout << i << endl; }
```

Examples – generalized iota

Problem: We can not easily generate a square iota:
$1, 4, 9, 16, 25, 36, ...$

Examples – generalized iota

Problem: We can not easily generate a square iota:
$1, 4, 9, 16, 25, 36, ...$
Introduce a projected map range.

```
auto iota_range = make_projected_counted_map_range(
    1
    , []( auto x ) { return x+1 ; }
    , 11
    , []( auto x ) { return x*x; }
    );
for( auto i : iota_range ) { std::cout << i << std::endl; }
```

Example - logistic map

```
double r = 3.2;
auto l = [r]( auto x ) {return r * x * ( 1.0 - x ); };
auto range = make_counted_map_range( 0.5 , l , 1000 );
for( auto x : range ) { cout << x << endl; }
```

Example – Newton method

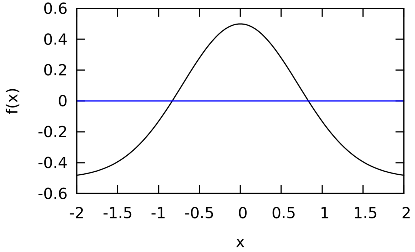
```
auto newton_range(
    auto x , auto f , auto df ,
    auto break_condition )
{
    return make_map_range(
        x ,
        [f,df]( auto x ) { return x - f( x ) / df( x ); } ,
        break_condition );
}
```

Example – Newton method

```
auto f = []( auto x ) { return exp(-x*x) - 0.5; };
auto df = []( auto x ) { return -2.0*x * exp(-x*x); };
auto cond  = [f]( auto x ) {
    return std::abs(f(x)) < 1.0e-12; };

auto range = newton_range( 1.0 , f , df , cond );

for( auto r : range )
    std::cout << r << " : " << f( r ) << std::endl;
```



Example – ODE solver

Solve $\dot{x} = f(x, t)$, Solver $F : x(t + \delta t) = F(x(t))$
Example Boost.Odeint:

```
namespace odeint = boost::numeric::odeint;

auto lorenz = []( auto const& x , auto& dxdt , auto t )
{
    dxdt[0] = 10.0 * ( x[1] - x[0] );
    dxdt[1] = 28.0 * x[0] - x[1] - x[0] * x[2];
    dxdt[2] = -8.0 / 3.0 * x[2] + x[0] * x[1];
};

using state_type = std::array< double , 3 >;
odeint::runge_kutta4< state_type > stepper;

state_type x {{ 10.0 , 10.0 , 10.0 }};
double t = 0.0 , dt = 0.01;
stepper.do_step( lorenz , x , t , dt );
t += dt;
```

Integrate functions:

```
auto obs = []( auto x , auto t ) { std::cout << t << " " << x[0] << "\n"; };
odeint::integrate_const( stepper , lorenz , x , 0.0 , 10.0 , dt , obs );
```

Example – ODE Solver

```
auto make_ode_range( auto sys , auto stepper , auto x ,
    auto t0 , auto dt , auto t1 )
{
    auto solve = [sys,stepper,dt]( auto x ) mutable {
        stepper.do_step( sys , x.first , x.second , dt );
        x.second += dt;
        return x; };
    auto cond = [t1]( auto const& x ) { return x.second > t1; };
    auto range = make_map_range( std::make_pair(x,t0) , solver , cond );
    return range;
}
```

Can be used as

```
state_type x {{ 10.0 , 10.0 , 10.0 }};
stepper_type stepper;
auto range = make_ode_range( lorenz , stepper , x , 0.0 , 0.1 , 100.0 );

for( auto r : range )
    std::cout << r.second << " " << r.first[0] << " " << r.first[1] << "\n";
```

ODE ranges

Superior to integrate functions:

- Break conditions are easy
- ODE-Ranges can be used in a natural C++ way, `find`, `transform` , etc.

But, the implementation has some drawbacks -> custom range implementations

- Better performance.
- Step size control – complicated iteration.
- Break condition can use the last two values.

Map range - applications

- Generalized iota
- Ordinary differential equations
- Maps (dynamical maps)
- Converging algorithms
- Functional random number generators

Iterators for GPUs algorithms

High-level libraries for GPUs

1. Thrust
2. VexCL
3. Boost.Compute
4. ViennaCL
5. Cuda-MTL

Thrust

STL-like library for Cuda
Design is based on iterators

Iterators in Thrust

`device_vector::iterator`
`host_vector::iterator`
special iterators
Algorithms

Implementation details of Thrust iterators

Special iterators for Thrust

zip iterator
transform iterator

Special problems - and solutions

Norm

Special problems - and solutions

Bucket sort

Solving an ensemble of low-dimensional ODEs

Lorenz example and ODEs

Conclusion

Outlook

References