odeint

Solving ordinary differential equations in C++

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Outline

The interface problem in C/C++

- Many frameworks exist to do numerical computations.
- Data has to be stored in containers or collections.
- GSL: `gsl_vector`, `gsl_matrix`
- NR: pointers with Fortran-style indexing
- Blitz++, MTL4, boost::ublas
- QT: `QVector`, wxWidgets: `wxArray`, MFC: `CArray`

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Theoretical solution of the interface mess

GoF Design Pattern: Adaptor, also known as Wrapper

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Alternative

Generic, container independent algorithms

Example

```
void CrankNicolsonEvolution::prepareVector(gsl_vector_complex* phi) {
  gsl_vector_complex* phi_temp = gsl_vector_complex_alloc(dim);
  //we need a copy of phi for this
  gsl_vector_complex_memcpy(phi_temp, phi);
  for( int i=1; i<dim-1; i++ ) {
    //phi_n = phi_n - i*dt/2 * (phi_n-1 + phi_n+1 + pot[n]*phi_n)
    gsl_vector_complex_set(phi, i, gsl_complex_add(
                gsl_vector_complex_get(phi_temp, i),
                gsl_complex_mul_imag(
                   gsl_complex_add(
                      gsl_complex_add( gsl_vector_complex_get(phi_temp, i-1),
                                    gsl_vector_complex_get(phi_temp, i+1)),
                      gsl_complex_mul_real( gsl_vector_complex_get(phi_temp, i),
                                         potential[i] )),
                   -dt/2.0)));
  }
  if( periodic ) {
    //periodic boundaries: i=0
    gsl_vector_complex_set(phi, 0, gsl_complex_add(
                gsl_vector_complex_get(phi_temp, 0),
                gsl_complex_mul_imag(
                   gsl_complex_add(
                      gsl_complex_add( gsl_vector_complex_get(phi_temp, dim-1),
                                       gsl_vector_complex_get(phi_temp, 1)),
                      gsl_complex_mul_real( gsl_vector_complex_get(phi_temp, 0),
                                         potential[0] )),
                   -dt/2.0)));
    //periodic boundaries: i=dim-1
    gsl_vector_complex_set(phi, dim-1, gsl_complex_add(
                gsl_vector_complex_get(phi_temp, dim-1),
                gsl_complex_mul_imag(
                   gsl_complex_add(
                      gsl_complex_add( gsl_vector_complex_get(phi_temp, dim-2),
                                       gsl_vector_complex_get(phi_temp, 0)),
                      gsl_complex_mul_real( gsl_vector_complex_get(phi_temp, dim-1),
                                         potential[dim-1] )),
                   -dt/2.0)));
  } else {
```

Portability of your algorithm

How to run your algorithm?

- Single machine, single CPU
- Single machine, multiple CPU's (OpenMP, threads, ...)
- Multiple machines (MPI)
- GPU (Cuda, Thrust, OpenCL)

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Which data types are used by your algorithm?

- Build-in data types – `double`, `complex<double>`
- Arbitrary precision types – GMP, MPFR
- Vectorial data types `float2d`, `float3d`

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- Vectorial data types `float2d`, `float3d`

Theoretical solution

GoF Design Pattern: Strategy, also known as Policy

Gamma, Holm, Johnson, Vlissides: *Design Patterns, Elements of Reuseable Object-Oriented Software*, 1998.

Numerical integration of ODEs

Find a numerical solution of an ODE an its initial value problem

$$\dot{x} = f(x,t)\ , \qquad x(t=0) = x_0$$

Example: Explicit Euler

$$x(t+\Delta t) = x(t) + \Delta t\ f(x(t),t) + \mathcal{O}(\Delta t^2)$$

General scheme of order s

$$x(t)\ \mapsto\ x(t+\Delta t) \qquad \text{, or}$$

$$x(t+\Delta t) = \mathcal{F}_t x(t) + \mathcal{O}(\Delta t^{s+1})$$

odeint

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Open source

- Boost license – do whatever you want do to with it

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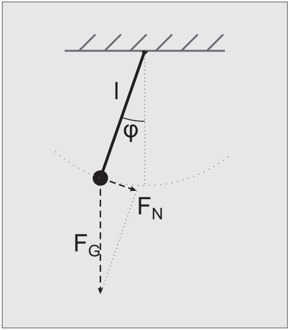
Modern C++

- Generic programming, functional programming
- Heavy use of the C++ template system
- Fast, easy-to-use and extendable.
- Container independent
- Portable

Example – Pendulum



Pendulum – Newtons law

$ma = F$

Acceleration

$a = l\ddot{\varphi}$

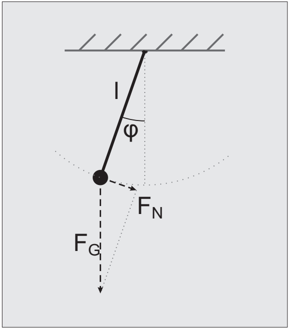
Force

$F = F_N = -mg \sin \varphi$

Result in an ode for the angle

$\ddot{\varphi} = -g/l \sin \varphi$

Example – Pendulum



$\ddot{\varphi} = -g/l \sin\varphi$

Small angle $\sin\varphi \approx \phi$

Harmonic oscillator

$\ddot{\varphi} = -g/l\varphi$

An analytic solution is known

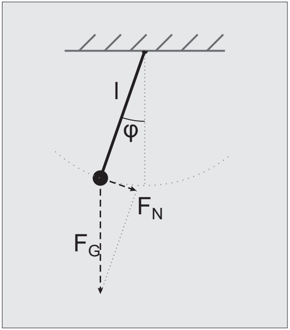
$\varphi = A\cos\omega t + B\sin\omega t$

Amplitude A and B must be determined from initial conditions:

$\varphi(t=0) = \varphi_0$, $\dot{\varphi}(t=0) = \dot{\varphi}_0$

$B = \varphi_0$, $A = \dot{\varphi}_0/\omega$

Example – Pendulum



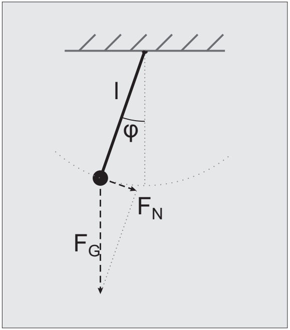
Full equation $\ddot{\varphi} = g/l \sin\varphi$ has also analytic solution Jacobi elliptic function

Lets enhance the ODE, add friction and external driving

$\ddot{\varphi} = g/l \sin\varphi - \mu\dot{\varphi} + \varepsilon \sin\omega t$

No analytic solution is known. We need to solve this equation numerically.

Example – Pendulum



$\ddot{\varphi} = g/l \sin\varphi - \mu\dot{\varphi} + \varepsilon \sin\omega t$

Create a first order ODE

$x_1 = \varphi$, $x_2 = \dot{\varphi}$

$\dot{x}_1 = x_2$, $\dot{x}_2 = -g/l \sin x_1 - \mu x_2 + \varepsilon \sin\omega t$

x_1 and x_2 are the state space variables.

Let’s solve the pendulum example numerically

$\dot{x}_1 = x_2$, $\dot{x}_2 = -g/l \sin x_1 - \mu x_2 + \varepsilon \sin \omega t$

```
#include <boost/numeric/odeint.hpp>

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

```
typedef std::array< double , 2 > state_type;
```

```
struct pendulum
{
  double m_mu , m_omega , m_epsilon;

  pendulum( double mu , double omega , double epsilon )
  : m_mu( mu ) , m_omega( omega ) , m_epsilon( epsilon ) { }

  void operator()( const state_type &x , state_type &dxdt , double t ) const
  {
    dxdt[0] = x[1];
    dxdt[1] = - sin( x[0] ) - m_mu * x[1] + m_epsilon * sin( m_omega * t );
  }
};
```

Let's solve the pendulum example numerically

$\varphi(0) = 1$, $\dot{\varphi}(0) = 0$

```
odeint::rk4< state_type > rk4;
pendulum p( 0.1 , 1.05 , 1.5 );

state_type x = {{ 1.0 , 0.0 }};
double t = 0.0;

const double dt = 0.01;
rk4.do_step( p , x , t , dt );
t += dt;
```

$x(0) \mapsto x(\Delta t)$

```
std::cout << t << " " << x[0] << " " << x[1] << "\n";
for( size_t i=0 ; i<10 ; ++i )
{
  rk4.do_step( p , x , t , dt );
  t += dt;
  std::cout << t << " " << x[0] << " " << x[1] << "\n";
}
```

$x(0) \mapsto x(\Delta t) \mapsto x(2\Delta t) \mapsto x(3\Delta) \mapsto \ldots$

Simulation
$\mu = 0$, $\omega_E = 0$, $\varepsilon = 0$
$\mu = 0.1$, $\omega_E = 0$, $\varepsilon = 0$
$\mu = 0.1$, $\omega_E = 1.05$, $\varepsilon = 1.5$

Steppers

```
odeint::runge_kutta_fehlberg78< state_type > stepper;
```

```
odeint::runge_kutta_dopri5< state_type > stepper;
```

but controlled steppers are much better

Controlled steppers

insert graphic

```
auto stepper = make_controlled( 1.0e-6 , 1.0e6 ,  odeint::
      runge_kutta_fehlberg78< state_type >() );
odeint::controlled_step_result res = stepper.try_step( p , x , t , dt );
```

tries to perform the step and updates *x*, *t*, and *dt*

it works because runge kutta fehlberg has error estimation

Controlled steppers

```
auto stepper = make_controlled( 1.0e-6 , 1.0e6 ,  odeint::
     runge_kutta_fehlberg78< state_type >() );
while( t < t_end )
{
  odeint::controlled_step_result res = stepper.try_step( p , x , t , dt );
  while( res != odeint::success )
  {
    res = stepper.try_step( p , x , t , dt );
  }
}
```

Use integrate functions

```
integrate_adaptive( stepper , x , p , t_start , t_end , dt );
integrate_adaptive( stepper , x , p , t_start , t_end , dt , observer );
```

```
integrate_adaptive( stepper , p , x , t_start , t_end , dt ,
  std::cout << arg2 << "\t" << arg1[0] << "\t" << arg1[1] << "\n" );
```

integrate_const, integrate_times, . . .

controlled steppers

dense output stepper

integrate functions

Old Stuff

First example – Lorenz system

```
#include <iostream>
#include <boost/array.hpp>
#include <boost/numeric/odeint.hpp>

using namespace std;
using namespace boost::numeric::odeint;

const double sigma = 10.0;
const double R = 28.0;
const double b = 8.0 / 3.0;

typedef boost::array< double , 3 > state_type;

void lorenz( const state_type &x , state_type &dxdt , double t )
{
    dxdt[0] = sigma * ( x[1] - x[0] );
    dxdt[1] = R * x[0] - x[1] - x[0] * x[2];
    dxdt[2] = -b * x[2] + x[0] * x[1];
}

void write_lorenz( const state_type &x , const double t )
{
    cout << t << '\t' << x[0] << '\t' << x[1] << '\t' << x[2] << endl;
}
```

- The r.h.s. of the ODE is a simple function
- Observer

Lorenz system continued

Different steppers:

```
runge_kutta4< state_type > stepper;
```

Lorenz system continued

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```
controlled_runge_kutta< runge_kutta_cash_karp54< state_type > > stepper;
```

Lorenz system continued

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controlled_runge_kutta< runge_kutta_cash_karp54< state_type > > stepper;
```

```
dense_output_runge_kutta< controlled_runge_kutta<
    runge_kutta_dopri5< state_type > > > stepper;
```

Lorenz system continued

Different steppers:

```
runge_kutta4< state_type > stepper;
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```

```
dense_output_runge_kutta< controlled_runge_kutta<
    runge_kutta_dopri5< state_type > > > stepper;
```

```
runge_kutta_dopri5< state_type > stepper;
make_dense_output( 1.0e-6 , 1.0e-6 , stepper );    // incomplete
```

Lorenz system continued

Different steppers:

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runge_kutta4< state_type > stepper;
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```

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dense_output_runge_kutta< controlled_runge_kutta<
    runge_kutta_dopri5< state_type > > > stepper;
```

```
runge_kutta_dopri5< state_type > stepper;
make_dense_output( 1.0e-6 , 1.0e-6 , stepper );     // incomplete
```

All together:

```
int main( int argc , char **argv )
{
    state_type x = {{ 10.0 , 1.0 , 1.0 }};
    runge_kutta_dopri5< state_type > stepper;
    integrate_const( make_dense_output( 1.0e-6 , 1.0e-6 , stepper )
                     lorenz , x , 0.0 , 10.0 , 0.01 , write_lorenz );
    return 0;
}
```

Second example – Fermi-Pasta-Ulam lattice

$$
\begin{aligned}
\dot{q}_k &= p_k \\
\dot{p}_k &= -q_k^2 + \Delta q_k + \beta\{(q_{k+1} - q_k)^3 - (q_k - q_{k-1})^3\}
\end{aligned}
$$

$$\Delta q_k = q_{k+1} - 2q_k + q_{k-1}$$

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$$\Delta q_k = q_{k+1} - 2q_k + q_{k-1}$$

State type consists of coordinates q and momentas p

```
typedef std::vector<double> vector_type;
vector_type q( 256 ) , p( 256 );
// initialize q,p
std::pair< state_type , state_type > state = std::make_pair( q , p );
```

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```

Hamiltonian system $\Longrightarrow$ Symplectic solvers needed

```
symplectic_rkn_sb3a_mclachlan< vector_type > stepper;
```

Fermi-Pasta-Ulam lattice continued

Trivial first component $\dot{q}_k = p_k$

```
struct fpu {
    double m_beta;
    fpu(double beta) : m_beta(beta) { }

    void operator()(const vector_type &q, vector_type &dpdt) const {
        // ...
    }
};
```

Fermi-Pasta-Ulam lattice continued

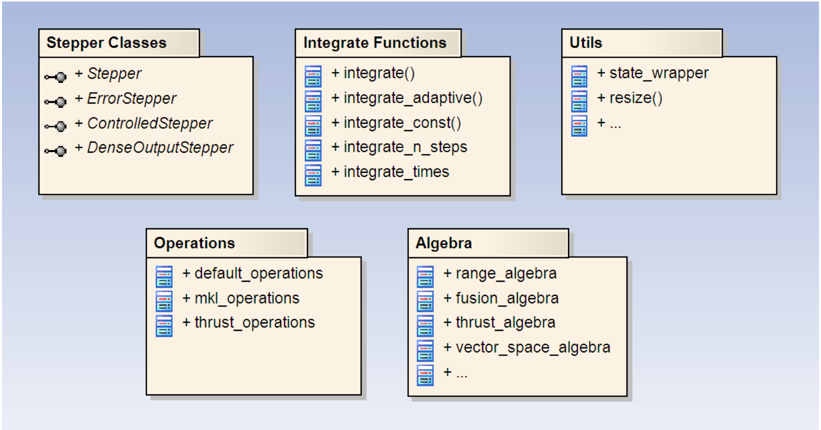
Trivial first component $\dot{q}_k = p_k$

```
struct fpu {
    double m_beta;
    fpu(double beta) : m_beta(beta) { }

    void operator()(const vector_type &q, vector_type &dpdt) const {
        // ...
    }
};
```

All together

```
struct statistics_observer {
    void operator()( const state_type &x , double t ) const {
    // write the statistics
    }
};

int main(int argc, char **argv)
{
    vector_type q( 256 ) , p( 256 );
    // initialize q,p
    integrate_const( symplectic_rkn_sb3a_mclachlan< state_type >(), fpu(1.0),
        make_pair( q , p ), 0.0, 10.0, 0.01, statistics_observer() );
    return 0;
}
```

Structure of odeint



Internals – Example Euler's method

User provides

$$y_i = f_i(x(t), t)$$

odeint provides

$$x_i(t + \Delta t) = x_i(t) + \Delta t \cdot y_i$$

(In general vector operations like $z_i = a_1 x_{1,i} + a_2 x_{2,i} + \dots$)

Instantiation

```
euler<state_type, value_type, deriv_type,
    time_type, algebra, operations > stepper;
```

All elements for container independence and portability are already included in this line!

Internals – Example Euler's method

$$y_i = f_i(x(t))$$
$$x_i(t + \Delta t) = x_i(t) + \Delta t \cdot y_i$$

```
euler<state_type, value_type, deriv_type,
    time_type, algebra, operations > stepper;
```

Data types

- `state_type` – the type of x
- `value_type` – the basic numeric type, e.g. `double`
- `deriv_type` – the type of y
- `time_type` – the type of t, Δt

Internals – Example Euler's method

$$y_i = f_i(x(t))$$
$$x_i(t + \Delta t) = x_i(t) + \Delta t \cdot y_i$$

```
euler<state_type, value_type, deriv_type,
    time_type, algebra, operations > stepper;
```

Algebra policies, perform the iteration

Algebra must be a class with public methods

- `for_each1(x,op)` – Performs $op(x_i)$ for all i
- `for_each2(x1,x2,op)` – Performs $op(x1_i, x2_i)$ for all i
- ...

Internals – Example Euler's method

$$y_i = f_i(x(t))$$
$$x_i(t + \Delta t) = x_i(t) + \Delta t \cdot y_i$$

```
euler<state_type, value_type, deriv_type,
    time_type, algebra, operations > stepper;
```

Operations do the basic computation

Operations must be a class with the public classes (functors)

- `scale_sum1` – Calculates $x = a1 \cdot y1$
- `scale_sum2` – Calculates $x = a1 \cdot y1 + a2 \cdot y2$
- ...

Internals – Example Euler's method

$$y_i = f_i(x(t))$$
$$x_i(t + \Delta t) = x_i(t) + \Delta t \cdot y_i$$

```
euler<state_type, value_type, deriv_type,
    time_type, algebra, operations > stepper;
```

All together

```
m_algebra.for_each3(xnew ,xold, y ,
   operations_type::scale_sum2<value_type,time_type>(1.0,dt));
```

Stepper concepts

Concepts

“... In generic programming, a concept is a description of supported operations on a type...”

Stepper concepts

Concepts

"... In generic programming, a concept is a description of supported operations on a type..."

odeint provides

- Stepper concept
  `stepper.do_step(sys,x,t,dt);`
- ErrorStepper concept
  `stepper.do_step(sys,x,t,dt,xerr);`
- ControlledStepper concept
  `stepper.try_step(sys,x,t,dt);`
- DenseOutputStepper concept
  `stepper.do_step(sys);`
  `stepper.calc_state(t,x);`

Supported methods

Method	Class name	Concept
Euler	`euler`	SD
Runge-Kutta 4	`runge_kutta4`	S
Runge-Kutta Cash-Karp	`runge_kutta_cash_karp54`	SE
Runge-Kutta Fehlberg	`runge_kutta_runge_fehlberg78`	SE
Runge-Kutta Dormand-Prince	`runge_kutta_dopri5`	SED
Runge-Kutta controller	`controlled_runge_kutta`	C
Runge-Kutta dense output	`dense_output_runge_kutta`	D
Symplectic Euler	`symplectic_euler`	S
Symplectic RKN	`symplectic_rkn_sb3a_mclachlan`	S
Rosenbrock 4	`rosenbrock4`	ECD
Implicit Euler	`implicit_euler`	S
Adams-Bashforth-Moulton	`adams_bashforth_moulton`	S
Bulirsch-Stoer	`bulirsch_stoer`	CD

S – fulfills stepper concept
E – fulfills error stepper concept
C – fulfills controlled stepper concept
D – fulfills dense output stepper concept

Integrate functions

- `integrate_const`
- `integrate_adaptive`
- `integrate_times`
- `integrate_n_steps`

Perform many steps, use all features of the underlying method

Integrate functions

- `integrate_const`
- `integrate_adaptive`
- `integrate_times`
- `integrate_n_steps`

Perform many steps, use all features of the underlying method

An additional observer can be called

```
integrate_const(stepper, sys, x, t_start,
t_end, dt, obs);
```

More internals

- Header-only, no linking → powerful compiler optimization
- Memory allocation is managed internally
- No virtual inheritance, no virtual functions are called
- Different container types are supported, for example
    - STL containers (`vector`, `list`, `map`, `tr1::array`)
    - MTL4 matrix types, blitz++ arrays, Boost.Ublas matrix types
    - `thrust::device_vector`
    - Fancy types, like Boost.Units
    - ANY type you like
- Explicit Runge-Kutta-steppers are implemented with a new template-metaprogramming method
- Different operations and algebras are supported
    - MKL
    - Thrust
    - gsl

ODEs on GPUs

Graphical processing units (GPUs) are able to perform up to 10^6 operations at once in parallel

Frameworks

- CUDA from NVIDIA
- OpenCL
- Thrust a STL-like library for CUDA and OpenMP

Applications:

- Parameter studies
- Large systems, like ensembles or one- or two dimensional lattices
- Discretizations of PDEs

odeint supports CUDA, through Thrust

Example: Parameter study of the Lorenz system

```
typedef thrust::device_vector<double> state_type;
typedef runge_kutta4<state_type ,value_type ,state_type ,value_type ,
     thrust_algebra ,thrust_operations > stepper_type;

struct lorenz_system {

    lorenz_system(size_t N ,const state_type &beta)
    : m_N(N) , m_beta(beta) {}

    void operator()(  const state_type &x , state_type &dxdt , double t ){
        // ..
    }

    size_t m_N;
    const state_type &m_beta;
};

int main( int arc , char* argv[] )
{
    const size_t N = 1024;

    vector<value_type> beta_host(N);
    for( size_t i=0 ; i<N ; ++i )
        beta_host[i] = 56.0 + value_type( i ) * ( 56.0 ) / value_type( N - 1
             );
    state_type beta = beta_host;
    state_type x( 3 * N , 10.0 );
    integrate_const( stepper_type() , lorenz(N,beta) , x , 0.0 , 10.0 , 0.01
         );

    return 0;
}
```

Conclusion

- odeint provides a fast, flexible and easy-to-use C++ library for numerical integration of ODEs.
- Its container independence is a large advantage over existing libraries.
- Portable
- Generic programming is the main programming technique.

Outlook

- Submission to the boost libraries
- Dynamical system classes for easy implementation of interacting dynamical systems
- More methods: implicit methods and multistep methods.
- Implementation of the Taylor series method

```
taylor_fixed_order< 25 , 3 > taylor_type stepper;

stepper.do_step(
    fusion::make_vector
    (
        sigma * ( arg2 - arg1 ) ,
        R * arg1 - arg2 - arg1 * arg3 ,
        arg1 * arg2 - b * arg3
    ) , x , t , dt );
```

Resources

Download and documentation

`odeint.com`

An article about the used techniques exists at

`http://www.codeproject.com/KB/recipes/odeint-v2.aspx`

Development

`https://github.com/headmyshoulder/odeint-v2`

Contributions and feedback

are highly welcome