

odeint

Solving ordinary differential equations in C++

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Outline

- 1 Introduction
- 2 Tutorial
- 3 odeint details
- 4 Outlook and conclusion

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`

But: All books on C++ recommend the use of the STL containers `std::vector`, `std::list`, ...

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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 and its initial value problem

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

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

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

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

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

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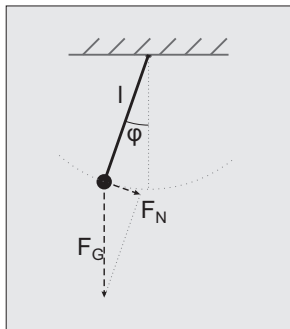
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Modern C++

- 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

$$a = l\ddot{\varphi}$$

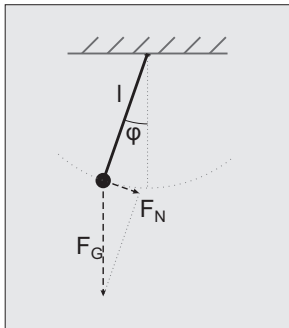
Force

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

Result in an ode for the angle

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

Example – Pendulum



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

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

Harmonic oscillator

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

An analytic solution is known

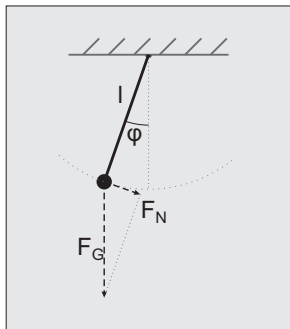
$$\varphi = A \cos \omega t + B \sin \omega t$$

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 fric-
tion 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.

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;
```

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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;
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```
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_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

$$\dot{q}_k = p_k$$

$$\dot{p}_k = -q_k^2 + \Delta q_k + \beta \{ (q_{k+1} - q_k)^3 - (q_k - q_{k-1})^3 \}$$

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

Second example – Fermi-Pasta-Ulam lattice

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

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

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 );
```


Second example – Fermi-Pasta-Ulam lattice

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```

Hamiltonian system \implies 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;
}
```

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Structure of odeint

Stepper Classes

- + *Stepper*
- + *ErrorStepper*
- + *ControlledStepper*
- + *DenseOutputStepper*

Integrate Functions

- + `integrate()`
- + `integrate_adaptive()`
- + `integrate_const()`
- + `integrate_n_steps`
- + `integrate_times`

Utils

- + `state_wrapper`
- + `resize()`
- + ...

Operations

- + `default_operations`
- + `mkl_operations`
- + `thrust_operations`

Algebra

- + `range_algebra`
- + `fusion_algebra`
- + `thrust_algebra`
- + `vector_space_algebra`
- + ...

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 $t, \Delta t$

Internals – Example Euler's method

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```
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
- ...

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```

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

$$y_i = f_i(x(t))$$
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```
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...”

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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

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- `integrate_const`
- `integrate_adaptive`
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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

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;
}
```

- 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.

- 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 );
```

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