Solving ordinary differential equations in C++

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Outline

- Introduction
- 2 Tutorial
- Technical details
- 4 Discussion

What is an ODE?

Examples

- Newtons equations (Bild Sonnensystem)
- Reaction and relaxation equations (Alkoholabbau im Blut)
- Granular systems (Bild)
- Interacting neurons (Bild)

Fundamental in mathematical modelling

What is an ODE?

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

achtung die gleichung hinter auch klein machen

- x dependent variable, function under consideration
- *t* indenpendent variable (time)
- f(x, t) defines the ODE

Initial Value Problem (IVP):

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

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

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

Solving ordinary differential equations in C++

Open source

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www.odeint.com

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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

Who uses odeint

Used as backend to solve ODEs in

```
netevo (logo einfuegen)
ompl (Open Motion planning library) (logo einfuegen)
```

. . .

Motivation: 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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Theoretical solution of the interface mess

GoF Design Pattern: Adaptor, also known as Wrapper

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 memcpv(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, θ),
                                           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

Portability of your algorithm

How to run your algorithm?

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Which data types are used by your algorithm?

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Theoretical solution

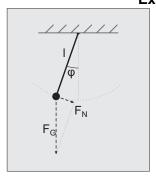
GoF Design Pattern: Strategy, also known as Policy

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

Lets step into odeint

- Introduction
- 2 Tutorial
- Technical details
- 4 Discussion

Example – Pendulum



Pendulum - Newtons law ma = F

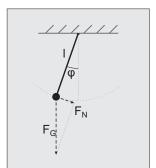
Acceleration
$$a = I\ddot{\varphi}$$

Force

 $F = F_N = -mg \sin \varphi$ Result in an ode for the angle

Result in an ode for the angle
$$\ddot{\varphi} = -g/l \sin \varphi$$

Example - Pendulum

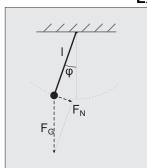


$$\ddot{\varphi} = -g/l \sin \varphi$$
Small angle $\sin \varphi \approx \phi$
Harmonic oscillator
 $\ddot{\varphi} = -g/l \varphi$

An analytic solution is known $\varphi = A\cos\omega t + B\sin\omega t$ Amplitude A and B must be de-

termined 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

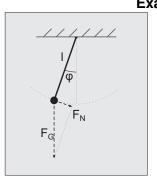


Full equation $\ddot{\varphi}=g/I\sin\varphi$ has also analytic solution Jacobi elliptic function Lets enhance the ODE, add friction and external driving

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

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

Example – Pendulum



 $\ddot{\varphi} = g/I \sin \varphi - \mu \dot{\varphi} + \varepsilon \sin \omega t$ Create a first order ODE $x_1 = \varphi, x_2 = \dot{\varphi}$ $\dot{x_1} = x_2, \dot{x_2} = -g/I \sin x_1 - \mu x_2 + \mu x_3 + \mu x_4 + \mu x_5 + \mu x_5$

 $x_1 - x_2$, $x_2 - g/r\sin x_1 - \mu x_2 + \varepsilon \sin \omega t$ x_1 and x_2 are the state space variables.

Let's solve the pendulum example numerically

```
#include <boost/numeric/odeint.hpp>
namespace odeint = boost::numeric::odeint;
```

$$\dot{x_1} = x_2, \, \dot{x_2} = -g/I\sin x_1 - \mu x_2 + \varepsilon\sin\omega t$$

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

Let's solve the pendulum example numerically $\dot{x_1} = x_2, \dot{x_2} = -g/l\sin x_1 - \mu x_2 + \varepsilon \sin \omega t$

```
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";
```

Simulation

$$\mu = 0, \, \omega_E = 0, \, \varepsilon = 0$$
 $\mu = 0.1, \, \omega_F = 0, \, \varepsilon = 0$

 $\mu = 0.1, \, \omega_F = 1.05, \, \varepsilon = 1.5$

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 , p , x , t_start ,

```
integrate_const( stepper , p , x , t , dt ,
  observer );
```

problem with controlled stepper

More steppers implicit, symplectic, predictor-corrector, multistep-methods

maybe small table

small summary (kann vielleicht auch wieder weg)

- Very easy example harmonic oscillator
- Basic features of odeint
- Different stepperControlled steppers
- Dense output steppers
- integrate functions

Now, advanced features

Lattice systems

- Lattice systems
- Discretizations of PDEs

- Lattice systems
- Discretizations of PDEs
- ODEs on Graphs

- Lattice systems
- Discretizations of PDEs
- ODEs on Graphs
- granular systems

Phase oscillator lattices

Any oscillator can be described by one variable, its phase. (Bild aus phd Talk)

Trivial dynamics: $\dot{\varphi} = \omega \varphi$

Vielleicht zusammenfuehren mit der naechsten Folie

Phase oscillator lattices

Coupled phase oscillators

Neurosciences

Heart dynamics

Synchronization

Any weakly perturbed oscillator system

$$\dot{\varphi}_{k} = \omega_{k}\varphi_{k} + q(\varphi_{k+1}, \varphi_{k}) + q(\varphi_{k}, \varphi_{k-1})$$

Phase compacton lattices

 $\dot{\varphi}_k = \cos \varphi_{k+1} - \cos \varphi_{k-1}$ state space contains *N* variables

typedef std::vector<double> state_type;

Animation with compactons and chaos space-time plot for visualization of compactons and chaos

Ensemble of phase oscillators

$$\dot{\varphi}_k = \omega_k + \sum_l \sin(\varphi_l - \varphi_k)$$

Synchronization, all oscillator oscillates with the same frequency

Synchronized state $\varphi_k = \omega_S t + \varphi_{0,k}$

Classical implementation

```
typedef std::vector<double> state_type;
struct phase_ensemble
    state type m omega;
    double m epsilon;
    phase ensemble (size t n, double q=1.0, double
        epsilon=1.0)
    : m omega(n,0.0), m epsilon(epsilon)
        create frequencies (q);
    void create_frequencies(double g) { ... }
    void operator()(const state_type &x,
       state_type &dxdt, double t) const
```

Solving ODEs with CUDA using thrust What is Thrust

Thrust is a parallel algorithms library which resembles the C++ Standard Template Library (STL). Thrust's high-level interface greatly enhances developer productivity while enabling performance portability between GPUs and multicore CPUs. Interoperability with established technologies (such as CUDA, TBB and OpenMP) facilitates integration with existing software. Develop high-performance applications rapidly with Thrust!



Solving ODEs with CUDA using thrust

- Large systems, discretizations of ODE, lattice systems, granular systems, etc.
- Parameter studies, integrate many ODEs in parallel with different parameters
- Initial value studies, integrate the same ODE with many different initial conditions in parallel

Lorenz system - Parameter study

$$\dot{x} = \sigma(y - x)$$
 $\dot{y} = Rx - y - xz$ $\dot{z} = -bz + xy$ (1)

Standard parameters $\sigma=$ 10, R= 28, b= 8/3 deterministic chaos, butterfly effect picture of Lorenz system

Lorenz system – Parameter study

Lyapunov exponents, perturbations of the original system

chaotic?

Vary R from 0 to 50, for which parameters the system is

Algebras and operations

$$x_i(t+\Delta t)=x_i(t)+\Delta t*f_i(x)$$

Algebras perform the iteration over *i* and operation the elementary addition.

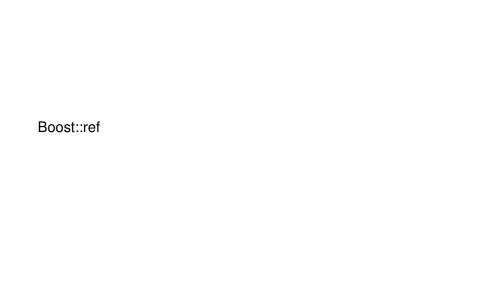
Algebras and operations enter the stepper as template parameters

```
typedef runge_kutta4<state_type, value_type,
    deriv_type, time_type,
    algebra, operations, resize_policy> stepper;
```

- default_operations
- range_algebra Boost.Ranges
- vector_space_algebra Passes the state directly to the operations
- fusion_algebra For compile time sequences, like std :: tuple < double, double >
- thrust_algebra and thrust_algebra for thrust

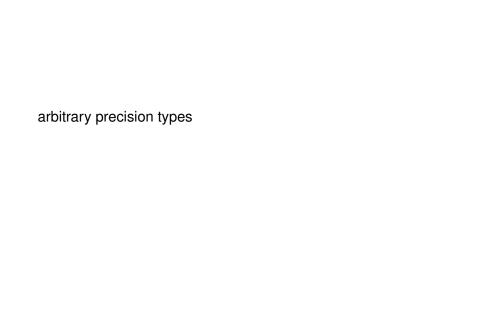
Thrust example for Lorenz system,
Implementation of the system function

More advanced features, die themen können auch auf mehreren folien zusammengefasst werden

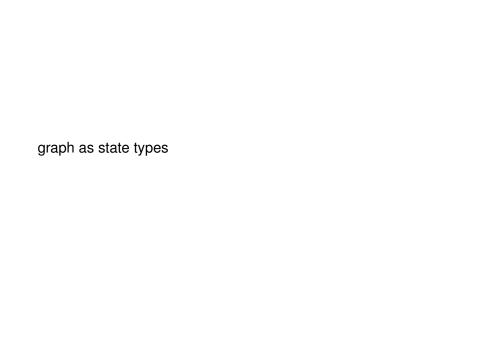


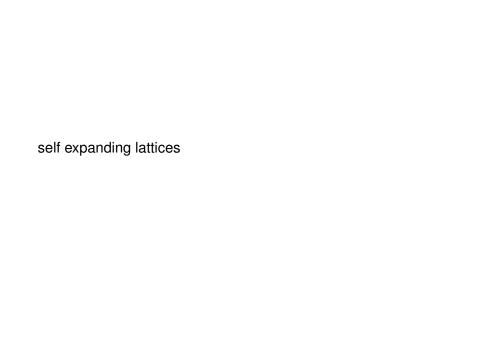
boost::range

complex state types, vielleicht auch nicht









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Discussion

Introduction

2 Tutorial

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Discussion



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];
```

Different steppers:

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

Different steppers:

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

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

Different steppers:

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

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

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

Different steppers:

```
runge_kutta4< state_type > stepper;

controlled runge kutta runge kutta cash karp54
```

< state_type > > stepper;

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

Different steppers:

```
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 10 }};
```

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

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

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

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

$$\dot{q}_{k} = p_{k}
\dot{p}_{k} = -q_{k}^{2} + \Delta q_{k} + \beta \{ (q_{k+1} - q_{k})^{3} - (q_{k} - q_{k-1})^{3} \}
\Delta q_{k} = q_{k+1} - 2q_{k} + q_{k-1}$$

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 );
```

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

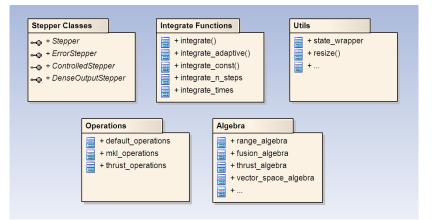
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Structure of odeint



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 Euler Runge-Kutta 4 Runge-Kutta Cash-Karp Runge-Kutta Fehlberg Runge-Kutta Dormand-Prince	Class name euler runge_kutta4 runge_kutta_cash_karp54 runge_kutta_runge_fehlberg78 runge_kutta_dopri5	Concept SD S SE SE 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 Bulirsch-Stoer	adams_bashforth_moulton bulirsch_stoer	S 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 10⁶ 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;
```

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