odeint

Solving ordinary differential equations in C++

Karsten Ahnert[1,2] and Mario Mulansky[2]

[1] Ambrosys GmbH, Potsdam
[2] Institut für Physik und Astronomie, Universität Potsdam

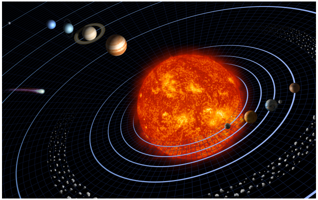
May 14, 2012

Outline

1. Introduction
2. Tutorial
3. Technical details
4. Conclusion and Discussion

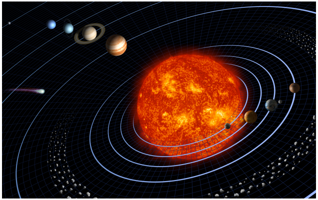
What is an ODE? – Examples

Newtons equations



What is an ODE? – Examples

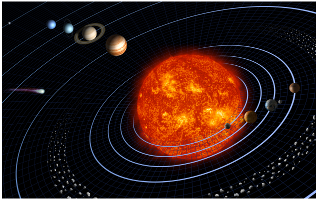
Newtons equations



Reaction and relaxation equations (i.e. blood alcohol content, chemical reaction rates)

What is an ODE? – Examples

Newtons equations

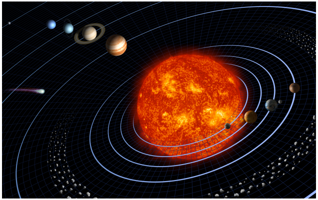


Granular systems

Reaction and relaxation equations (i.e. blood alcohol content, chemical reaction rates)

What is an ODE? – Examples

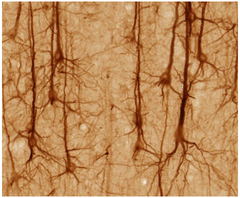
Newtons equations



Reaction and relaxation equations (i.e. blood alcohol content, chemical reaction rates)

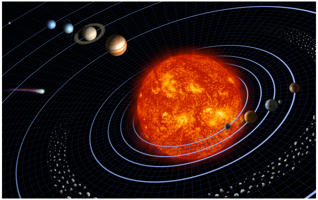
Granular systems

Interacting neurons



What is an ODE? – Examples

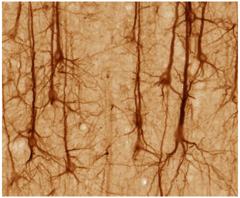
Newtons equations



Reaction and relaxation equations (i.e. blood alcohol content, chemical reaction rates)

Granular systems

Interacting neurons



- Many examples in physics, biology, chemistry, social sciences
- Fundamental in mathematical modelling

What is an ODE?

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

- $x(t)$ – dependent variable
- 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 and its IVP

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

Example: Explicit Euler

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

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

Solving ordinary differential equations in C++

Open source

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

odeint

Solving ordinary differential equations in C++

Open source

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

Download

- **`www.odeint.com`**

odeint

Solving ordinary differential equations in C++

Open source

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

Download

- **`www.odeint.com`**

Modern C++

- Generic programming, functional programming, template-meta programming
- Fast, easy-to-use and extendable.
- Container independent
- Portable

Motivation

We want to solve ODEs $\dot{x} = f(x, t)$

- using `double`, `std::vector`, `std::array`, ... as state types.
- with complex numbers,
- on one, two, three-dimensional lattices, and or on graphs.
- on graphic cards.
- with arbitrary precision types.

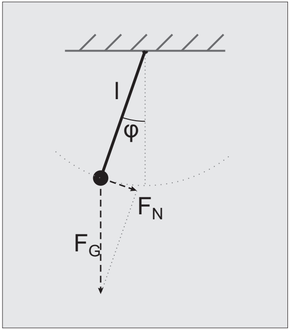
Existing libraries support only one state type!

Container independent and **portable** algorithms are needed!

Let's step into odeint

1. Introduction
2. Tutorial
3. Technical details
4. Conclusion and Discussion

Example – Pendulum



Newtons law: $ma = F$

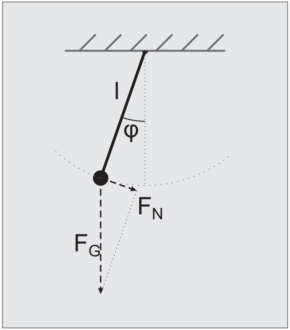
Acceleration: $a = l\ddot{\varphi} = \frac{d^2\varphi}{dt^2}$

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

$\Longrightarrow$ **ODE for** φ

$$\ddot{\varphi} = -g/l\sin\varphi = -\omega_0^2\sin\varphi$$

Example – Pendulum



$$\ddot{\varphi} = -\omega_0^2 \sin \varphi$$

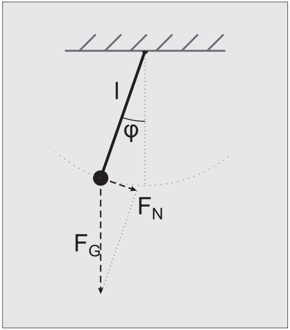
Small angle: $\sin \varphi \approx \varphi$

Harmonic oscillator $\ddot{\varphi} = -\omega_0^2 \varphi$

Analytic solution:
$\varphi = A \cos \omega_0 t + B \sin \omega_0 t$

Determine A and B from initial condition

Example – Pendulum



Full equation: $\ddot{\varphi} = -\omega_0^2 \sin \varphi$

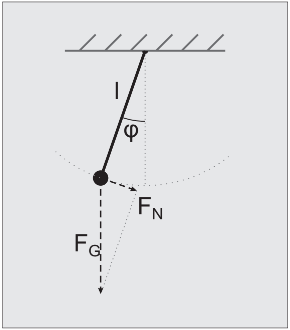
Pendulum with friction and external driving:

$$\ddot{\varphi} = -\omega_0^2 \sin \varphi - \mu \dot{\varphi} + \varepsilon \sin \omega_E t$$

No analytic solution is known

$\Longrightarrow$ **Solve this equation numerically.**

Example – Pendulum



$$\ddot{\varphi} = -\omega_0^2 \sin\varphi - \mu\dot{\varphi} + \varepsilon \sin\omega_E t$$

Create a first order ODE

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

$$\dot{x}_1 = x_2$$
$$\dot{x}_2 = -\omega_0 \sin x_1 - \mu x_2 + \varepsilon \sin\omega_E t$$

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;
```

$$\dot{x}_1 = x_2 \ , \quad \dot{x}_2 = -\omega_0 \sin x_1 - \mu x_2 + \varepsilon \sin \omega_E t$$

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

Let's solve the pendulum example numerically

$\dot{x}_1 = x_2$, $\dot{x}_2 = -\omega_0^2 \sin x_1 - \mu x_2 + \varepsilon \sin \omega_E t$ $\qquad \omega_0^2 = 1$

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

  pendulum(double mu,double omega,double eps)
  : m_mu(mu),m_omega(omega),m_eps(eps) { }

  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_eps * sin(m_omega*t);
  }
};
```

Let's solve the pendulum example numerically

$$\varphi(0) = x_1(0) = 1 \;, \quad \dot{\varphi}(0) = x_2(0) = 0$$

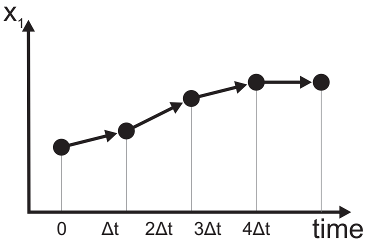
```
odeint::runge_kutta4< state_type > rk4;
pendulum p( 0.1 , 1.05 , 1.5 );

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;
```

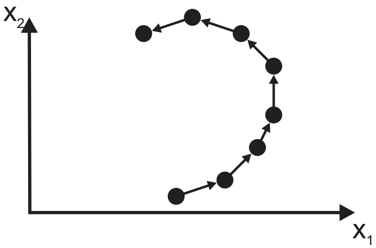
$$x(0) \mapsto x(\Delta t)$$

Let's solve the pendulum example numerically

```
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";
}
```

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





Simulation

Oscillator

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

Damped oscillator:

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

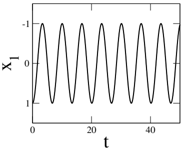
Damped, driven oscillator:

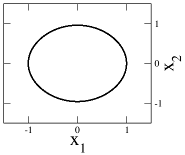
$\mu = 0.1\,,\ \omega_E = 1.05\,,\ \varepsilon = 1.5$

Simulation

Oscillator

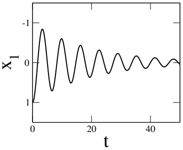
$\mu = 0\,,\ \omega_E = 0\,,\ \varepsilon = 0$

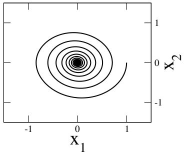




Damped oscillator:

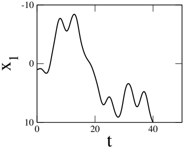
$\mu = 0.1\,,\ \omega_E = 0\,,\ \varepsilon = 0$

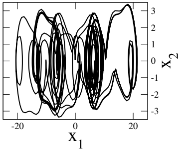




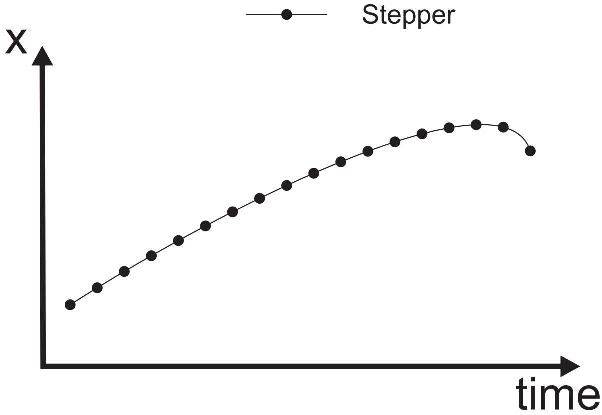
Damped, driven oscillator:

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

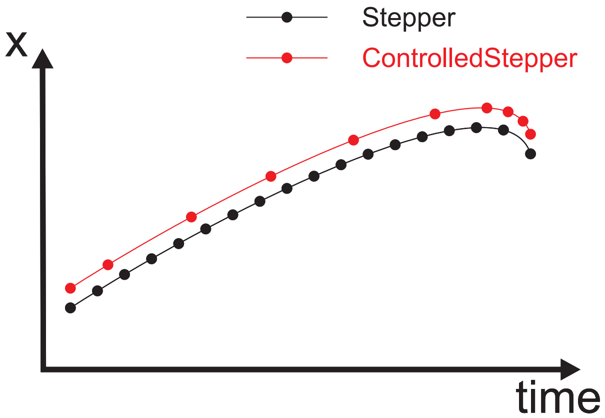




Controlled steppers – Step size control



Controlled steppers – Step size control



Controlled steppers

```
auto s = make_controlled( 1.0e-6 , 1.0e6,
  runge_kutta_fehlberg78<state_type>() );

controlled_step_result res =
  s.try_step(ode,x,t,dt);
```

Tries to perform the step and updates *x*, *t*, and *dt*!

It works because Runge-Kutta-Fehlberg has error estimation:

```
runge_kutta_fehlberg78<state_type> s;
s.do_step(ode,x,t,dt,xerr);
```

Controlled steppers

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

Non-trivial time-stepping logic

Use integrate functions!

```
integrate_adaptive(s,ode,x,t_start,t_end,dt);
integrate_adaptive(s,ode,x,t_start,t_end,dt,
    observer);
```

Observer: Callable object `obs(x,t)`

Example (using Boost.Phoenix):

```
integrate_adaptive(s,ode,x,t_start,t_end,dt,
  cout << arg1[0] << " " << arg1[1] << "\n" );
```

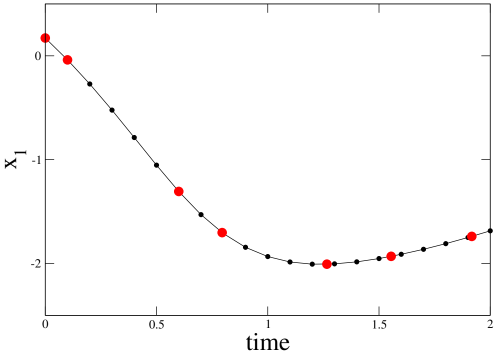
More integrate versions:

`integrate_const`, `integrate_times`, ...

Adaptive step size vs. constant step size

```
integrate_const(s,ode,x,t,dt,obs);
```

```
integrate_adaptive(s,ode,x,t,dt,obs);
```

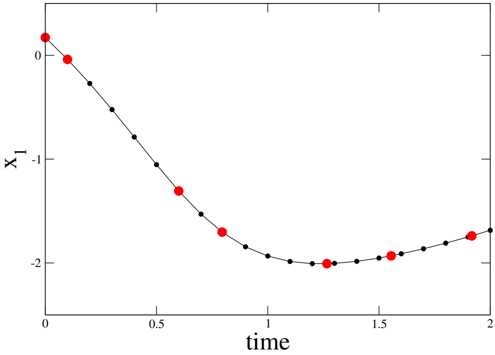


Problem: Equidistant observation with adaptive step size integration?

Dense output stepper

```
auto s = make_dense_output( 1.0e-6 , 1.0e-6 ,
    runge_kutta_dopri5< state_type >() );
integrate_const( s , p , x , t , dt );
```

Interpolation within integration interval with the same precision as the stepper!



More steppers

Stepper Concepts: Stepper, ErrorStepper, ControlledStepper, DenseOutputStepper

Stepper types:

- Implicit – `implicit_euler`, `rosenbrock4`
- Symplectic – `symplectic_rkn_sb3a_mclachlan`
- Predictor-Corrector – `adams_bashforth_moulton`
- Extrapolation – `bulirsch_stoer`
- Multistep methods – `adams_bashforth_moulton`

Some of them have step-size control and dense-output!

For details see the odeint documentation!

Small summary

- Very easy example – nonlinear driven pendulum
- Basic features of odeint
- Different steppers – steppers, error steppers, controlled steppers, dense output steppers
- Integrate functions

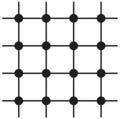
Small summary

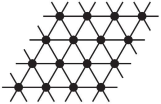
- Very easy example – nonlinear driven pendulum
- Basic features of odeint
- Different steppers – steppers, error steppers, controlled steppers, dense output steppers
- Integrate functions

Now, let's look at some advanced features!

Large systems

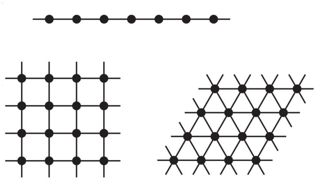
Lattice systems





Large systems

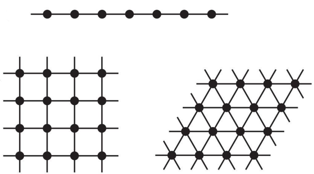
Lattice systems



Discretiztations of PDEs

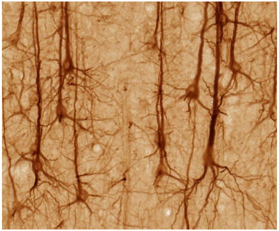
Large systems

Lattice systems



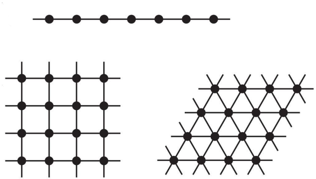
Discretiztations of PDEs

ODEs on graphs



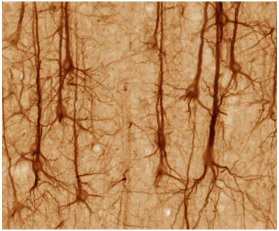
Large systems

Lattice systems

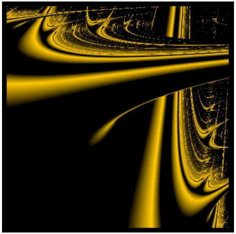


Discretiztations of PDEs

ODEs on graphs



Parameter studies



Phase compacton lattice

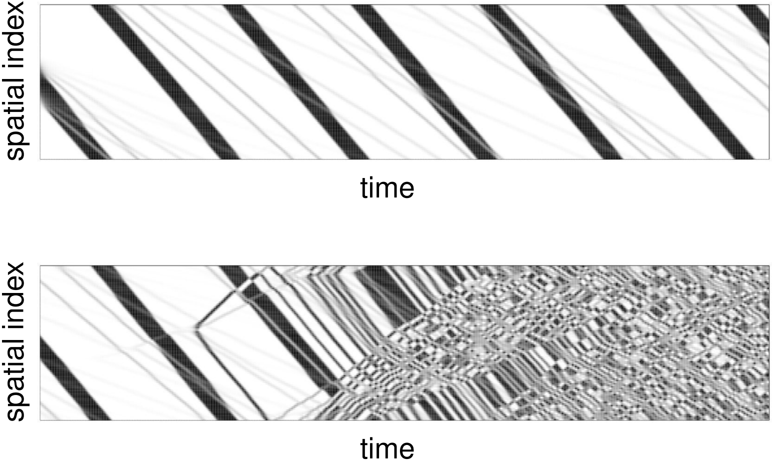
$$\dot{\varphi}_k = \cos \varphi_{k+1} - \cos \varphi_{k-1}$$

State space contains N variables

```
typedef std::vector<double> state_type;
```

Simulation

Phase compacton lattice – Space-time plots



Solving ODEs with CUDA using 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

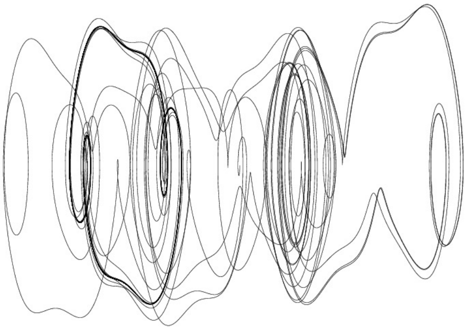
Applications and use cases for GPUs:

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

Nonlinear pendulum – Deterministic chaos

$$\dot{x} = y \qquad \dot{y} = -\sin(x) - \mu y + \varepsilon \sin \omega_E t$$

Perturbations grow exponentially fast – Butterfly effect



Nonlinear pendulum – Parameter study

$$\dot{x} = y \qquad \dot{y} = -\sin(x) - \mu y + \varepsilon \sin \omega_E t$$

Does one observe chaos over the whole parameter range?

Lyapunov exponents:

- Measure of chaos
- Growth rate of perturbations

Vary ε from 0 to 5.0 and ω_E from 0.5 to 1.5 and calculate the Lyapunov exponents!

Use CUDA and Thrust!

Intermezzo: Algebras and operations

Euler method

$$\text{for all i :} \qquad x_i(t+\Delta t) = x_i(t) + \Delta t \cdot f_i(x)$$

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

- Algebras perform the iteration over *i*.
- Operations perform the elementary addition.

Intermezzo: Algebras and operations

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

Default template parameters:

- `range_algebra` – Boost.Ranges
- `default_operations`

For Thrust:

- `thrust_algebra`
- `thrust_operations`
- `thrust::device_vector`

Calculate an ensemble of pendulums

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

state_type x( 2*N );
// initialize x
integrate_const( stepper() , pendulum_ensemble() ,
   x , 0.0 , 1000.0 , dt );
```

Memory layout:

x_1	x_2		...			x_N	y_1	y_2		...			y_N

Everything seems easy!

But how does `pendulum_ensemble` look like?

Ensemble of nonlinear pendulums

```
struct pendulum_ensemble {
  size_t N;
  state_type eps , omega;

  template< class State , class Deriv >
  void operator()(
    const State &x , Deriv &dxdt , value_type t ) const {

    thrust::for_each(
      thrust::make_zip_iterator( thrust::make_tuple(
        x.begin() , x.begin()+N ,
        eps.begin() , omega.begin() ,
        dxdt.begin(), dxdt.begin()+N
      ) ) ,
      thrust::make_zip_iterator( thrust::make_tuple(
        x.begin()+N , x.begin()+2*N
        eps.end() , omega.end() ,
        dxdt.begin()+N,dxdt.begin()+2*N
      ) ) ,
      pendulum_functor(t) );
  }

  // ...
};
```

Ensemble of nonlinear pendulums

```
struct pendulum_ensemble
{
  // ...

  struct pendulum_functor
  {
    double time;
    pendulum_functor( double _time ) : time(_time) { }

    template< class T > __host__ __device__
    void operator()( T t ) const
    {
      value_type x = thrust::get< 0 >( t );
      value_type y = thrust::get< 1 >( t );
      value_type eps = thrust::get< 2 >( t );
      value_type omega = thrust::get< 3 >( t );
      thrust::get< 4 >( t ) = x
      thrust::get< 5 >( t ) = -x - mu*y
            + eps * sin( omega * time );
    }
  };
};
```

Advanced features - continued

Reference wrapper `std::ref`, `boost::ref`

The ODE and the observers are always passed by value

```
integrate_const(s,ode,x,0.0,1.0,dt,obs);
s.do_step(ode,x,t,dt);
```

Reference wrapper `std::ref`, `boost::ref`

The ODE and the observers are always passed by value

```
integrate_const{s,ode,x,0.0,1.0,dt,obs);
s.do_step(ode,x,t,dt);
```

Use `std::ref` or `boost::ref` to pass by reference

```
integrate_const{s,std::ref(ode),x,0.0,1.0,dt,
  std::ref(obs));
```

Using Boost.Range

Use Boost.Range to integrate separate parts of the overall state

Example: Lyapunov exponents for the Lorenz system

Complete ODE = Lorenz system + Perturbation

- Calculate transients by solving only the Lorenz system (initialize x, y, z)
- Solve whole system (state + perturbations)

```
std::vector<double> x(6,0.0);
integrate(s,lorenz,
  make_pair(x.begin(),x.begin()+3),
  0.0,10.0,dt);
integrate(s,lorenz_pert,x,10.0,1000.0,dt);
```

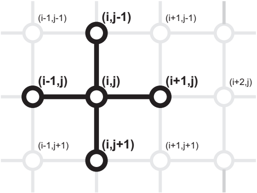
ODEs with complex numbers

Discrete Nonlinear Schrödinger equation

$$\mathrm{i}\dot{\Psi}_k = \varepsilon_k \Psi_k + V(\Psi_{k+1} + \Psi_{k-1}) - \gamma |\Psi_k|^2 \Psi_k \quad , \quad \Psi_k \in \mathbb{C}$$

```
typedef std::vector<std::complex<double> > state_type;

struct dnls
{
  std::vector<double> eps;
  void operator()(const state_type &x, state_type &dxdt,
    double t) const
  {
    // ...
  }
};

runge_kutta_fehlberg78< state_type > stepper;
```

Matrices as state types



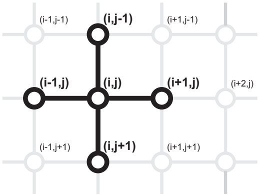
Example:

Two-dimensional phase lattice

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

```
typedef ublas::matrix<double> state_type1;
typedef mtl::dense2D<double> state_type2;

runge_kutta_fehlberg78< state_type1 , double ,
  state_type1 , double , vector_space_algebra > stepper1;
```

Matrices as state types



Example:

Two-dimensional phase lattice

$$\begin{aligned}\dot{\varphi}_{i,j} =& q(\varphi_{i+1,j},\varphi_{i,j}) + q(\varphi_{i-1,j},\varphi_{i,j}) \\ &+ q(\varphi_{i,j+1},\varphi_{i,j}) + q(\varphi_{i,j-1},\varphi_{i,j})\end{aligned}$$

```
typedef ublas::matrix<double> state_type1;
typedef mtl::dense2D<double> state_type2;

runge_kutta_fehlberg78< state_type1 , double ,
  state_type1 , double , vector_space_algebra > stepper1;
```

Compile-time sequences and Boost.Units

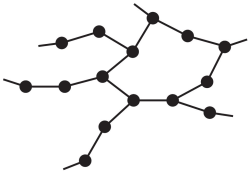
$$\begin{pmatrix} \dot{x} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} v \\ f(x, v) \end{pmatrix}$$

- x – length, dimension m
- v – velocity, dimension ms^{-1}
- a – acceleration, dimension ms^{-2}

```
typedef units::quantity< si::time , double > time_type;
typedef units::quantity< si::length , double > length_type;
typedef units::quantity< si::velocity , double > velocity_type;
typedef units::quantity< si::acceleration , double > acceleration_type;

typedef fusion::vector< length_type , velocity_type > state_type;
typedef fusion::vector< velocity_type , acceleration_type > deriv_type;

typedef runge_kutta_dopri5< state_type , double , deriv_type , time_type ,
      fusion_algebra > stepper_type;
```

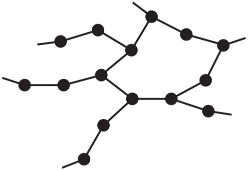
What else

- ODEs on graphs

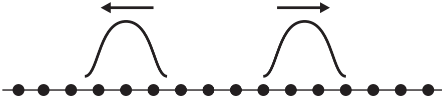


What else

- ODEs on graphs



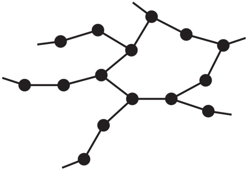
- Automatic memory management



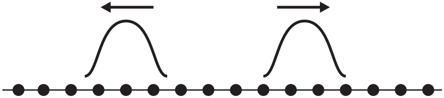
Enlarge the lattice when waves hit the boundaries

What else

- ODEs on graphs



- Automatic memory management



Enlarge the lattice when waves hit the boundaries

- Arbitrary precision types, GMPXX

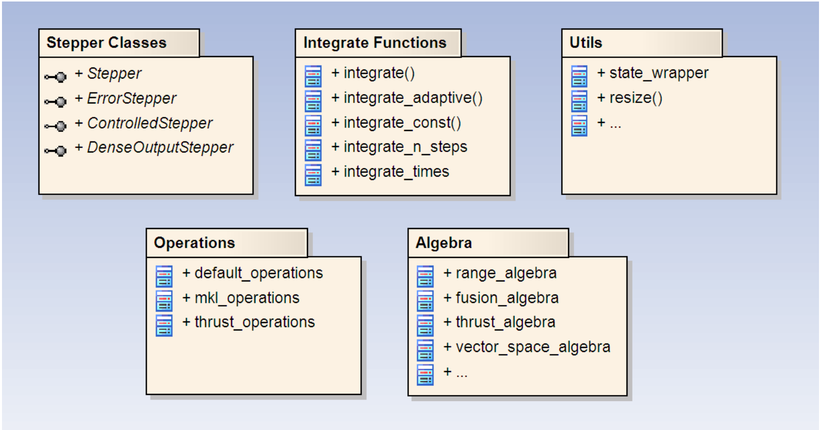
1 Introduction

2 Tutorial

3 Technical details

4 Conclusion and Discussion

Structure of odeint



Independent Algorithms

Goal

Container- and computation-independent implementation of the numerical algorithms.

Benefit

High flexibility and applicability, odeint can be used for virtually any formulation of an ODE.

Approach

Detach the algorithm from memory management and computation details and make each part interchangeable.

Mathematical Algorithm

Typical mathematical computation performed to calculate the solution of an ODE ($\dot{\vec{x}} = \vec{f}(\vec{x}, t)$):

$$
\begin{aligned}
\vec{F}_1 &= \vec{f}(\vec{x}_0, t_0) \\
\vec{x}' &= \vec{x}_0 + a_{21} \cdot \Delta t \cdot \vec{F}_1 \\[1em]
\vec{F}_2 &= \vec{f}(\vec{x}', t_0 + c_1 \cdot \Delta t) \\
\vec{x}' &= \vec{x}_0 + a_{31} \cdot \Delta t \cdot \vec{F}_1 + a_{32} \cdot \Delta t \cdot \vec{F}_2 \\
&\vdots \\
\vec{x}_1 &= \vec{x}_0 + b_1 \cdot \Delta t \cdot \vec{F}_1 + \cdots + b_s \cdot \Delta t \cdot \vec{F}_s
\end{aligned}
$$

Strucutural Requirements

$$\vec{F}_1 = \vec{f}(\vec{x}_0, t_0) \qquad\qquad \vec{x}' = \vec{x}_0 + a_{21} \cdot \Delta t \cdot \vec{F}_1$$

Types:

- vector type, mostly, but not neccessarily, some container like `vector<double>` (actually we have `state_type` and `deriv_type`)
- time type, usually `double`
- value type, fundamental arithmetic type

Strucutural Requirements

$$\vec{F}_1 = \vec{f}(\vec{x}_0, t_0) \qquad \vec{x}' = \vec{x}_0 + a_{21} \cdot \Delta t \cdot \vec{F}_1$$

Types:

- vector type, mostly, but not neccessarily, some container like `vector<double>` (actually we have `state_type` and `deriv_type`)
- time type, usually `double`
- value type, fundamental arithmetic type

Function Call:

```
void rhs( const vector_type &x , vector_type &
    dxdt , const time_type t )
{ /* user defined */ }

rhs( x0 , F1 , t ); //memory allocation for F1?
```

- Memory allocation for temporary results (`F1`, `x'`)

Computational Requirements

$$\vec{x}_1 = \vec{x}_0 + b_1 \cdot \Delta t \cdot \vec{F}_1 + \cdots + b_s \cdot \Delta t \cdot \vec{F}_s$$

- vector-vector addition
- scalar-scalar multiplication
- scalar-vector multiplication

$\longrightarrow$ vector space

Type Declarations

Tell odeint which types your are working with:

```
/* define your types */
typedef vector<double> state_type;
typedef vector<double> deriv_type;
typedef double value_type;
typedef double time_type;

/* define your stepper algorithm */
typedef runge_kutta4< state_type , value_type ,
    deriv_type , time_type > stepper_type;
```

Reasonable standard values for the template parameters allows for:

```
typedef runge_kutta4<state_type> stepper_type;
```

Memory Allocation / Resizing

Two possible situations: dynamic size / fixed size `vector_type`

dynamic size - memory allocation required

- e.g. `vector<double>`
- declare type as resizeable
- specialize resize template
- use `initially_resizer`, `always_resizer`, or `never_resizer` in stepper

fixed size - memory allocation not required

- e.g. `array<double,N>`
- declare type as not resizeable
- that's it

Declare Resizeability

```
/* by default any type is not resizable */
template< class Container >
struct is_resizeable
{
    typedef boost::false_type type;
    const static bool value = type::value;
};

/* specialization for std::vector */
template< class T, class A >
struct is_resizeable< std::vector< T , A  > >
{
    typedef boost::true_type type;
    const static bool value = type::value;
};
```

To use a new dynamic sized type, this has to be specialized by the user.

Tell odeint how to resize

Again: only required if `is_resizeable<state_type>::type == boost::true_type`.

Class Template responsible for resizing:

```
template< class StateOut , class StateIn >
struct resize_impl
{
    /* standard implementation */
    static void resize( StateOut &x1 , const
        StateIn &x2 )
    {
        x1.resize( boost::size( x2 ) );
    }
};
```

For anything that does not support `boost::size` and/or `resize` the user must provide a specialization.

Tell odeint when to resize

```
typedef initially_resizer resizer; // default
```

Resizing only at first step (memory allocation)

```
typedef always_resizer resizer;
```

Resizing at every step (expanding lattice)

```
typedef never_resizer resizer;
```

Resizing manually by the user (`stepper.adjust_size`)

```
typedef runge_kutta4< state_type , value_type ,
    deriv_type , time_type , algebra ,
    operations , resizer > stepper_type;
```

Vector Computations

$$\vec{x}_1 = \vec{x}_0 + b_1 \cdot \Delta t \cdot \vec{F}_1 + \cdots + b_s \cdot \Delta t \cdot \vec{F}_s$$

Split into two parts:

1. Algebra: responsible for iteration over vector elements
2. Operations: does the mathematical computation on the elements

Similar to `std::for_each`

```
Algebra algebra;

algebra.for_each3( x1 , x0 , F1 ,
    Operations::scale_sum2( 1.0, b1*dt );
```

Vector Computations

$$\vec{x}_1 = \vec{x}_0 + b_1 \cdot \Delta t \cdot \vec{F}_1 + \cdots + b_s \cdot \Delta t \cdot \vec{F}_s$$

Split into two parts:

1. Algebra: responsible for iteration over vector elements
2. Operations: does the mathematical computation on the elements

Similar to `std::for_each`

```
Algebra algebra;

algebra.for_each3( x1 , x0 , F1 ,
    Operations::scale_sum2( 1.0, b1*dt );
```

The types `Algebra` and `Operations` are template parameters of the steppers, hence exchangeable.

Vector Computations

```
state_type x1, x2, ...
algebra_type algebra;
```

Algebra has to have defined the following member functions:

- `algebra.for_each1( x1 , unary_operation );`
- `algebra.for_each2( x1, x2, binary_operation );`
- `algebra.for_each3( ... );`

⋮

- `algebra.for_each15( .. , fifteen_ary_op );`

Vector Computations

```
state_type x1, x2, ...
algebra_type algebra;
```

Algebra has to have defined the following member functions:

- `algebra.for_each1( x1 , unary_operation );`
- `algebra.for_each2( x1, x2, binary_operation );`
- `algebra.for_each3( ... );`

⋮

- `algebra.for_each15( .. , fifteen_ary_op );`

odeint takes the operations from the class `Operations`.

Operations

`Operations` is a class with the following member classes:

- `scale`
- `scale_sum1`
- `scale_sum2`

$\vdots$

- `scale_sum14`

These classes need a constructor and `()`-operator that works together with the algebra:

```
value_type b1, b2;
time_type dt;
algebra.for_each3( x1 , x0 , F1 ,
   Operations::scale_sum2( 1.0, b1*dt );
```

This computes: $\vec{x}_1 = 1.0 \cdot \vec{x}_0 + b_1 \Delta t \cdot \vec{F}_1$.

Example Implementation: `range_algebra`

```
struct range_algebra {
...
 template< class S1 , class S2 , class S3 , class Op >
 static void for_each3( S1 &s1, S2 &s2, S3 &s3, Op op )
 {
   detail::for_each3( boost::begin(s1), boost::end(s1),
                      boost::begin(s2), boost::begin(s3),
                      op );
 }
...
};

namespace detail {
...
 template< class Iter1, class Iter2, Iter3, class Op >
 void for_each3( Iter1 first1, Iter1 last1,
                 Iter2 first2, Iter3 first3, Op op )
 {
     for( ; first1 != last1 ; )
         op( *first1++ , *first2++ , *first3++ );
 }
...
};
```

Example Implementation: `default_operations`

```
template< class Fac1 , class Fac2 >
struct scale_sum2
{
  const Fac1 m_alpha1;
  const Fac2 m_alpha2;

  scale_sum2( Fac1 alpha1 , Fac2 alpha2 )
    : m_alpha1( alpha1 ) , m_alpha2( alpha2 )
  { }

  template< class T1 , class T2 , class T3 >
  void operator()( T1 &t1 , const T2 &t2 ,
      const T3 &t3 )
  { t1 = m_alpha1 * t2 + m_alpha2 * t3; }

  typedef void result_type;
};
```

For example `vector< double >`:

```
typedef vector< double > state_type;
typedef vector< double > deriv_type;
typedef double value_type;
typedef double time_type;

typedef runge_kutta4< state_type , value_type ,
                      deriv_type , time_type ,
                      range_algebra ,
                      default_operations
                    > stepper_type
```

As these are also the default values, this can be shortened:

```
typedef runge_kutta4<state_type> stepper_type;
```

`range_algebra & default_operations` work also with

- `vector< complex<double> >`
- `list< double >`
- `array< double , N >`

range_algebra & default_operations work also with

- vector< complex<double> >
- list< double >
- array< double , N >

What about

- Ublas vector
- trivial state_type like double
- generally: state_type that support operators +, *

$\longrightarrow$ vector_space_algebra!

vector_space_algebra

```
struct vector_space_algebra {
...
 template< class S1 , class S2 , class S3 ,
     class Op >
 static void for_each3( S1 &s1 , S2 &s2 ,
                         S3 &s3 , Op op )
 {
   op( s1 , s2 , s3 );
 }
...
};
```

- delegates `state_type` directly to the operations
- no iteration
- works together with `default_operations` with any `state_type` that supports operators `+`, `*`

Other Examples

fusion_algebra: works with compile-time sequences like `fusion::vector` of Boost.Units

thrust_algebra & thrust_operations: Use thrust library to perform computation on CUDA graphic cards

mkl_operations: Use Intel's Math Kernel Library

See tutorial and documentation on `www.odeint.com` for more.

Other Examples

fusion_algebra: works with compile-time sequences like `fusion::vector` of Boost.Units

thrust_algebra & thrust_operations: Use thrust library to perform computation on CUDA graphic cards

mkl_operations: Use Intel's Math Kernel Library

See tutorial and documentation on `www.odeint.com` for more.

Important

Division into Algebra and Operations gives us great flexibility. However, state type, algebra and operations must coorporate to make odeint work!

More details

- State wrapper for construction/destruction of state types
- More requirements on Algebras when using controlled steppers (`algebra.reduce`)
- Implicit routines using Ublas
- Generation functions to create controlled / dense output steppers
- TMP Runge-Kutta implementation (see my talk on Thursday afternoon!)

1 Introduction

2 Tutorial

3 Technical details

4 Conclusion and Discussion

Conclusion

odeint is a modern C++ library for solving ODEs that is

- easy-to-use
- highly-flexible
  - data types (topology of the ODE, complex numbers, precision, ...)
  - computations (CPU, CUDA, OpenMP, ...)
- fast

Where can odeint be used?

- Science
- Game engine and physics engines
- Simulations
- Modelling
- Data analysis
- High performance computing

Who uses odeint

NetEvo – Simulation dynamical networks

OMPL – Open Motion Planning Library

icicle – cloud/precipitation model

Score – Commercial Smooth Particle Hydrodynamics Simulation

VLE – Virtual Environment Laboratory (planned to use odeint)

Several research groups

…

Roadmap

Near future:

- Current release – documentation, bug fixing
- Boost Review process
- Implicit steppers

Further plans

- Dormand-Prince 853 steppers
- More algebras: MPI, cublas, TBB, John Maddock's arbitrary precision library, Boost SIMD library

Perspective

- C++11 version
- sdeint – methods for stochastic differential equations
- ddeint – methods for delay differential equations