Boost.odeint

Solving ordinary differential equations in C++

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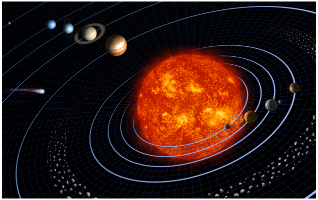
Outline

1. Introduction
2. Tutorial
3. Conclusion and Discussion

What is an ODE? – Examples

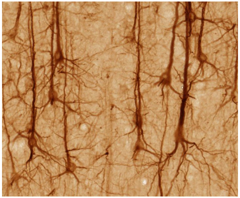
Newtons equations



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
- Accepted as Boost library – will be released with V. 1.53

Download

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

Modern C++

- Paradigms: Generic, Template-Meta programming, Functional
- 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.

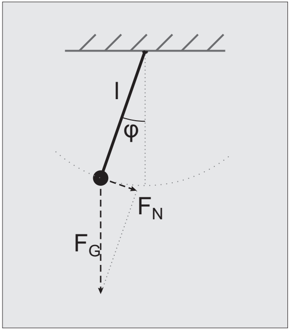
Existing libraries support only one state type!

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

Let's step into odeint

1. Introduction
2. Tutorial
3. Conclusion and Discussion

Example – Pendulum



Newtons law: $ma = F$

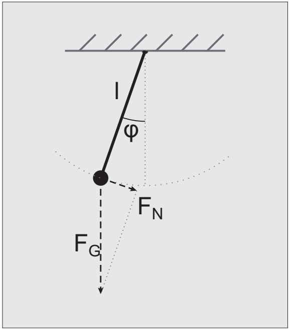
Acceleration: $a = l\ddot{\varphi} = \frac{d^2\varphi}{dt^2}$

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

$\Longrightarrow$ **ODE for** φ

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

Example – Pendulum



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

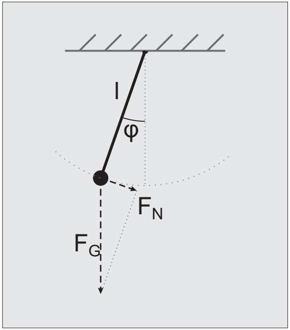
Small angle: $\sin \varphi \approx \varphi$

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

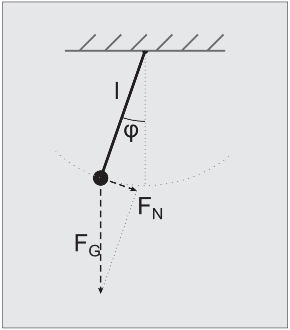
Pendulum with friction and external driving:

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

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

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

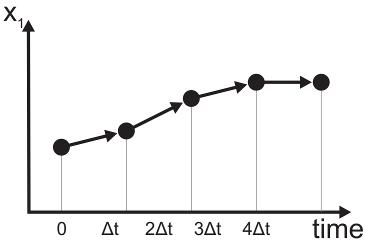
```
odeint::runge_kutta4< state_type > rk4;
pendulum p( 0.1 , 1.05 , 1.5 );

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;
```

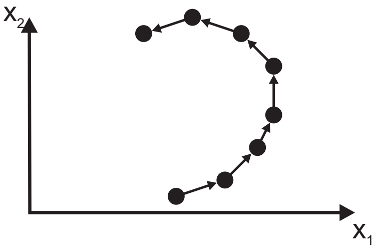
$$x(0) \mapsto x(\Delta t)$$

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";
}
```

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

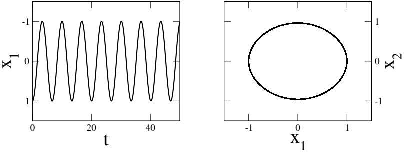




Simulation

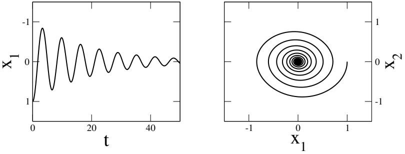
Oscillator

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



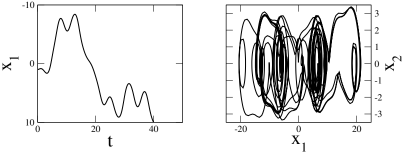
Damped oscillator:

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

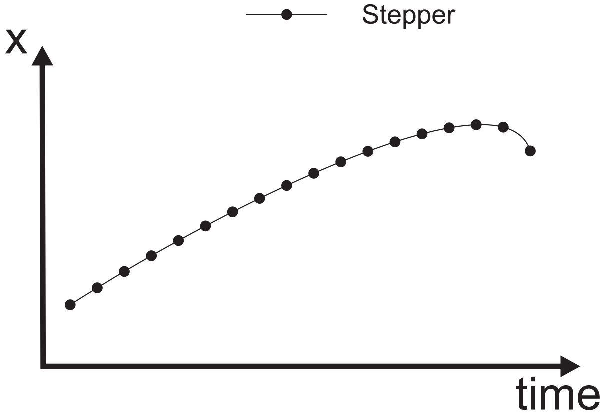


Damped, driven oscillator:

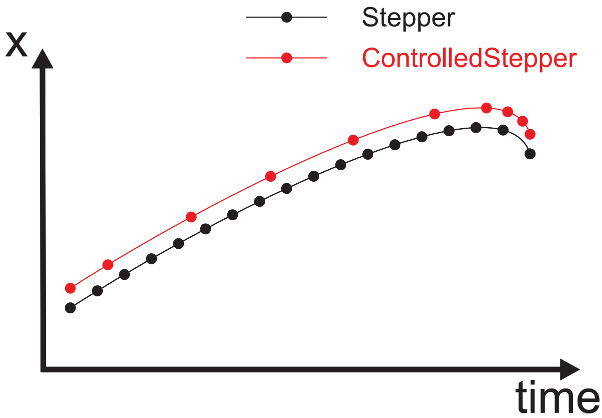
$\mu = 0.1\,,\ \omega_E = 1.05\,,\ \varepsilon = 1.5$



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 C++11 Lambdas):

```
integrate_adaptive(s,ode,x,t_start,t_end,dt,
  []( const state_type &x , double t ) {
    cout << x[0] << " " << x[1] << "\n" } );
```

More integrate versions:

`integrate_const`, `integrate_times`, ...

Or even better: Use Iterators!

```
for_each(
  make_const_step_iterator_begin(rk4, ode, x, t1, t2, dt ),
  make_const_step_iterator_end(rk4, ode, x ),
  observer );
```

Ranges

```
boost::for_each(
  make_const_step_range(rk4, ode, x, t1, t2, dt ),
  observer );
```

- odeint's iterators are single-pass iterators
- Specializations for stepper concepts
- `const_step_iterator<>`, `adaptive_iterator<>`
- `const_step_time_iterator<>`, `adaptive_time_iterator<>` – value type is a pair of state and time of the ODE

Do fancy stuff with iterators!

Average of the *x*-component of the solution

```
double av = boost::accumulate(
  make_const_step_range(rk4, ode, x, t1, t2, dt),
  0.0, []( double sum , const state_type &x ) {
      return sum + x[0]; } );
```

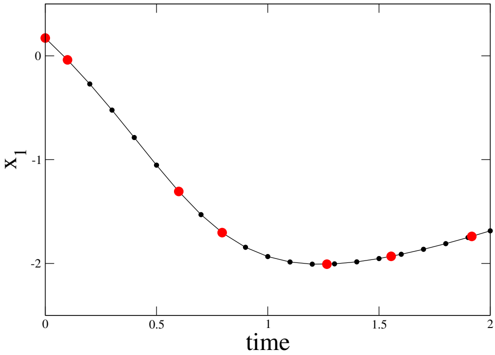
Find the first occurence of a threshold

```
auto iter = boost::find_if(
  make_const_step_time_range(rk4,ode, x, t1, t2, dt),
    [](const std::pair< state_type &, double> &x) {
      return ( x.first[0] < 0.0 ); } );
```

Adaptive step size vs. constant step size

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

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

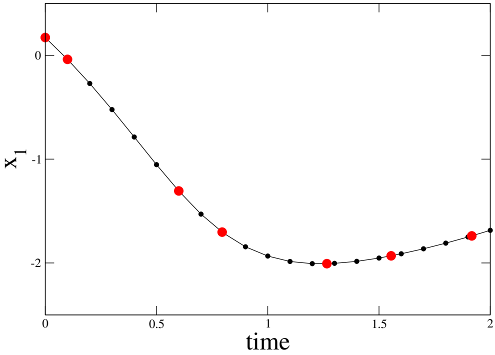


Problem: Equidistant observation with adaptive step size integration?

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!

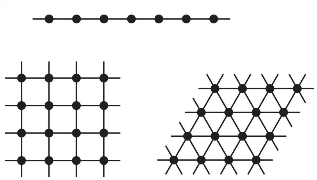
Small summary

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

Now, let's look at some advanced features!

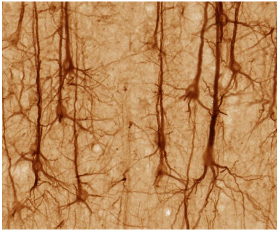
Large systems

Lattice systems

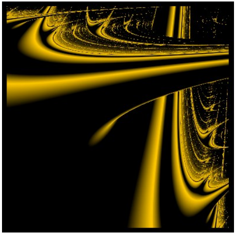


Discretiztations of PDEs

ODEs on graphs



Parameter studies



Phase compacton lattice

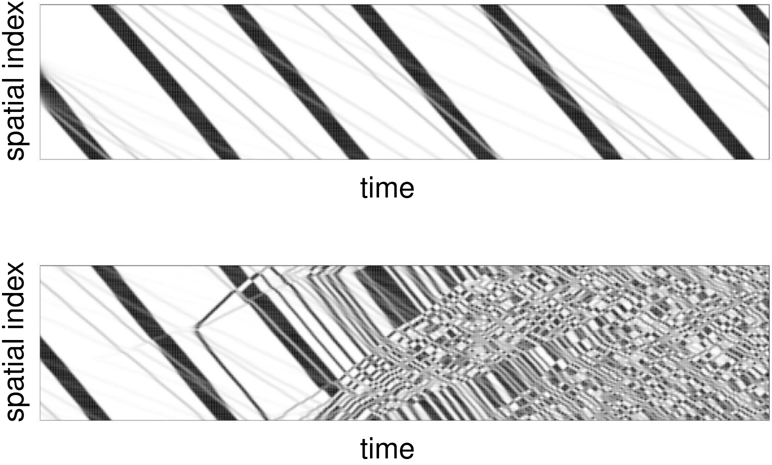
$$\dot{\varphi}_k = \cos \varphi_{k+1} - \cos \varphi_{k-1}$$

State space contains *N* variables

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

Simulation

Phase compacton lattice – Space-time plots



GPGPU technologies

General-purpose computing on graphics processing units

- CUDA
- OpenCL
- OpenMP
- OpenACC
- C++Amp

Large divergence of GPGPU technologies

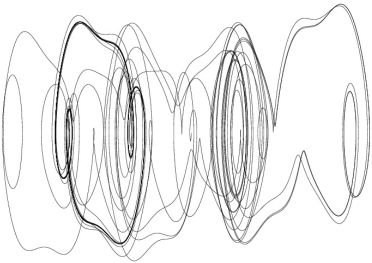
Solving ODEs with CUDA using Thrust

“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!”

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



Does one observe chaos over the whole parameter range?

Vary ε from 0 to 5.0 and ω_E from 0.5 to 1.5 and determine chaoticity!

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`

Intermezzo: Algebras and operations

Algebra has to have defined the following member functions:

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

`Operations` is a class with the following (static) functors:

- `scale_sum1` // *calculates* $y = a1*x1$
- `scale_sum2` // *calculates* $y = a1*x1 + a2*x2$
- ...

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

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

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 );
    }
  };
};
```

VexCL

Vector EXpression template library for OpenCL

Use expression template to write simple equations

```
vex::Context ctx( vex::Filter::Type(
    CL_DEVICE_TYPE_GPU) );
vex::vector< double > X( ctx.queue() , N );
vex::vector< double > Y( ctx.queue() , N );
vex::vector< double > Z( ctx.queue() , N );

// initialize X, Y, Z

Z = X + 2.0 * Y + cos( X );
```

Use VexCL for the ensemble of pendulums

Calculate an ensemble of pendulums

```
typedef vex::vector< double > vector_type;
typedef vex::multivector< double , 2 > state_type;
typedef runge_kutta4<state_type,double,state_type,double,
  vector_space_algebra,default_operations> stepper_type;

state_type X(ctx.queue(), N);
vector_type Eps(ctx.queue(), N);
vector_type Omega(ctx.queue(), N);

// initialize x, Eps, Omega
integrate_const(stepper(), ensemble(Eps, Omega, 0.1) ,
    X, 0.0, t_max, dt);
```

Memory layout:

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

Everything seems easy!

But how does `ensemble` look like?

Ensemble of nonlinear pendulums

```
struct ensemble
{
  const vector_type &m_eps;
  const vector_type &m_omega;
  double m_mu;

  ensemble(const vector_type &eps,const vector_type &omega,
    double mu)
      : m_eps(eps), m_omega(omega), m_mu(mu) { }

  void operator()(const state_type &x, state_type &dxdt,
    double t)
  {
    dxdt = std::make_tuple(
      x(1) ,
      -sin(x(0)) - m_mu*x(1) + m_eps*sin(m_omega*t)
      );
  }
};
```

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);
```

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);
```

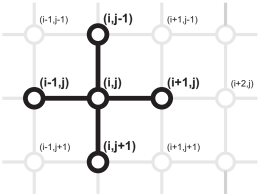
ODEs with complex numbers

Discrete Nonlinear Schrödinger equation

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

```
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;
```

Compile-time sequences and Boost.Units

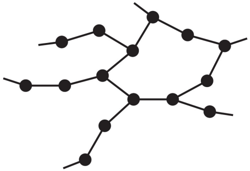
$$\begin{pmatrix} \dot{x} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} v \\ f(x,v) \end{pmatrix}$$

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

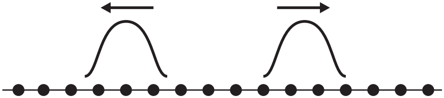
```
typedef units::quantity< si::time , double > time_type;
typedef units::quantity< si::length , double > length_type;
typedef units::quantity< si::velocity , double > velocity_type;
typedef units::quantity< si::acceleration , double > acceleration_type;

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



- Automatic memory management



Enlarge the lattice when waves hit the boundaries

- Arbitrary precision types, GMPXX

1 Introduction

2 Tutorial

3 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:

- ~~Boost Review process~~
- Implicit steppers
- HPX backend

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

Thank you!