odeint

An advanced C++ framework for numerical integration of ordinary differential equations

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September 21, 2011

Outline

The interface problem in C/C++

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

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

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

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 {
```

Scalability 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)

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- Arbitrary precision types – GMP, MPFR
- Vectorial data types `float2d`, `float3d`

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Theoretical solution

GoF Design Pattern: Strategy, also known as Policy

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Numerical integration of ODEs

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

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

Example: Explicit Euler

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

General scheme of order s

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

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

odeint

Solving ordinary differential equations in C++

Open source

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

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Modern C++

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

First example – Lorenz system

```
#include <boost/numeric/odeint.hpp>
#include <tr1/array>

using namespace boost::numeric::odeint;

typedef std::tr1::array<double,3> state_type;

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

int main(int argc, char **argv) {
    state_type x = {{10.0, 10.0, 10.0}};
    typedef dense_output_runge_kutta<
        controlled_runge_kutta<
            runge_kutta_dopri5<state_type> > > stepper_type;
    integrate_const(stepper_type(), lorenz, x, 0.0, 10.0, 0.01);
    return 0;
}
```

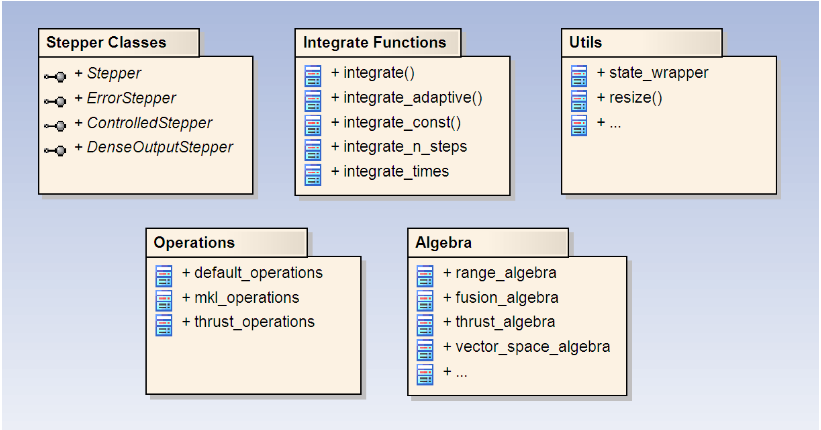
- The r.h.s. of the ODE is a simple function
- Methods with dense-output and/or step-size control
- Integrate functions
- Templates

Second example – Fermi-Pasta-Ulam lattice

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

struct fpu {
    double m_beta;
    fpu(double beta) : m_beta(beta) { }
    void operator()(const state_type &q, state_type &dpdt) const {
        // ...
    }
};

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

int main(int argc, char **argv) {
    state_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;
}
```

- Symplectic solver
- The ODE is now a functor, it can have parameters.
- Automatic memory managements
- Observer

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;
```

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

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General goal: Separation

- of how an vector is iterated
- of how the basic computations are performed

from the stepper

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    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

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    time_type, algebra, operations > stepper;
```

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

```
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..."

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

ODEs on GPUs

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

Frameworks

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

Applications:

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

odeint supports CUDA, through Thrust

Example: Parameter study of the Lorenz system

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

struct lorenz_system {

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

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

    size_t m_N;
    const state_type &m_beta;
};

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

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

    return 0;
}
```

Conclusion

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

An article about the used techniques exists at
`http://www.codeproject.com/KB/recipes/odeint.aspx`

Download and documentation
`http://headmyshoulder.github.com/odeint-v2/`

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

Contributions and feedback

are highly welcome