Metaprogramming Applied to Numerical Problems

A Generic Implementation of Runge-Kutta Algorithms

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- numerical routines: Runge-Kutta Schemes
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Ordinary Differential Equations

ODEs are the typical way to describe physical, bioglogical, chemical, ... processes and thus play a fundamental role in mathematical modelling.

- Newton's equation of motion
- Reaction-diffusion systems
- Modelling of interacting neuronal networks

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Also, ODEs are used as approximations to Partial Differential Equations for numerical treatments.

Ordinary Differential Equations

A first order ODE is written in its most general form as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{x}(t) = \vec{f}(\vec{x}, t) \tag{1}$$

- $\vec{x}(t)$ is the function in demand (here: trajectory)
- t is the independent variable (here: time)
- $f(x, t)$ is the rhs, governing the behavior of x

Initial Value Problem (IVP):

$$\dot{x} = f(x, t), \qquad x(t = 0) = x_0 \tag{2}$$

Examples

- $\dot{x} = -\lambda x$ solution: $x(t) = x_0 \mathrm{e}^{-\lambda t}$
- $\ddot{x} = \omega^2 x \rightarrow \begin{cases} \dot{x} = p \\ \dot{p} = -\omega^2 x \end{cases}$ solution: $x(t) = A \sin(\omega t + \varphi_0)$.

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- Lorenz System: $\begin{aligned} \dot{x} &= \sigma(y - x) \\ \dot{y} &= x(R - z) - y \\ \dot{z} &= xy - \beta z. \end{aligned}$ solution: ?

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$\Longrightarrow$ numerical methods to solve ODEs are required for more complicated systems.

Runge-Kutta Scheme

One class of algorithms to solve IVP of ODEs.

- Discretized time $t \to t_n = t_0 + n \cdot h$ with (small) time step h
- Trajectory $x(t) \to x_n \approx x(t_n)$
- Iteration along trajectory: $x_0 \longrightarrow x_1 \longrightarrow x_2 \dots$
- One-step method: $x_1 = \Phi(x_0)$, $x_2 = \Phi(x_1)$, ...

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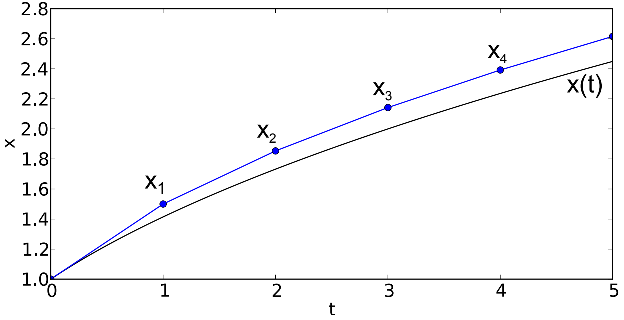

Runge-Kutta Scheme

Numerically solve the Initial Value Problem (IVP) of the ODE:

$$\dot{x}(t) = f(x,t), \qquad x(t=0) = x_0. \tag{3}$$

A Runge-Kutta scheme with s stages and parameters $c_1 \dots c_s$, $a_{21}, a_{31}, a_{32}, \dots, a_{ss-1}$ and $b_1 \dots b_s$ gives the approximate solution for $x_1 \approx x(h)$ starting at x_0 by computing:

$$x_1 = x_0 + h \sum_{i=1}^{s} b_i F_i \qquad \text{where} \qquad F_i = f(x_0 + h \sum_{j=1}^{i-1} a_{ij} F_j, hc_i). \tag{4}$$

This approximate solution x_1 is exact up to some order p.
Repeating the whole procedure brings you from x_1 to x_2, then to x_3 and so on.

At each stage i the following calculations have to be performed $(y_1 = x_0)$:

$$F_i = f(y_i, hc_i), \qquad y_{i+1} = x_0 + h\sum_{j=1}^{i} a_{i+1,j}F_j, \qquad i = 1\dots s-1$$

$$F_s = f(y_s, hc_s), \qquad x_1 = x_0 + h\sum_{j=1}^{s} b_jF_j.$$

The parameters a, b and c define the so-called Butcher tableau.

Butcher Tableau

Parameters a, b, and c are typically written as Butcher tableau:

$$
\begin{array}{c|ccccc}
c_1 & & & & & \\
c_2 & a_{2,1} & & & & \\
c_3 & a_{3,1} & a_{3,2} & & & \\
\vdots & \vdots & & \ddots & & \\
c_s & a_{s,1} & a_{s,2} & \dots & c_{s,s-1} & \\
\hline
 & b_1 & b_2 & \dots & b_{s-1} & b_s
\end{array}
$$

The Butcher Tableau fully defines the Runge-Kutta scheme.
Each line of the tableau represents one stage of the scheme.

Explicit Non-Generic Implementation

Given parameters `c_i` , `a_ij` , `b_i`

```
F_1 = f( x , t + c_1*dt );
x_tmp = x + dt*a_21 * F_1;

F_2 = f( x_tmp , t + c_2*dt );
x_tmp = x + dt*a_31 * F_1 + dt*a_32 * F_2;

// ...

F_s = f( x_tmp , t + c_s*dt );
x_end = x + dt*b_1 * F_1 + dt*b_2 * F_2 + ...
          + dt*b_s * F_s;
```

Not generic: Each stage written hard coded – you have to adjust the algorithm when implementing a new scheme.

Run Time Implementation

Given parameters `a[][]` , `b[]` , `c[]`.

```
F[0] = f( x , t + c[0]*dt );
x_tmp = x + dt*a[0][0] * F[0];

for( int i=1 ; i<s-1 ; ++i )
{
  F[i] = f( x_tmp , t + c[i]*dt );
  x_tmp = x;
  for( int j=0 ; j<i+1 : ++j )
    x_tmp += dt*a[i][j] * F[j];
}

F[s-1] = f( x_tmp , t + c[s-1]*dt );
x_end = x;
for( int j=0 ; j<s : ++j )
  x_end += dt*b[j] * F[j];
```

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    x_tmp += dt*a[i][j] * F[j];
}

F[s-1] = f( x_tmp , t + c[s-1]*dt );
x_end = x;
for( int j=0 ; j<s : ++j )
  x_end += dt*b[j] * F[j];
```

Generic, but factor 2 slower than explicit implementation!

Why Bad Performance

The run time generic code is hard to optimize for the compiler, because:

- Double `for` loop with inner bound depending on outer loop variable.
- 2D array `double** a` must be dynamically allocated:

```
a = new double*[s];
for( int i=0 ; i<s ; ++i )
  a[i] = new double[i+1];
a[0][0] = ...;
a[1][0] = ...; a[1][1] = ...;
...
```

  $\longrightarrow$ lives on heap, harder to be optimized compared to stack.

- Many more issues possible (optimizers are rather complex).

What to do?

Idea:

Use template engine to generate code that can be efficiently optimized by the Compiler.

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More specifically, we will use Template Metaprogramming to:

- Generate fixed size arrays: `a_1[1] , a_2[2] , ... , a_s[s]`
- Unroll the outer `for`-loop (over stages `s`) so the compiler sees sequential code.

As result, the code seen by the compiler/optimizer (after resolving templates) is very close to the non-generic version and thus as fast, hopefully.

Generic Runge-Kutta Algorithm

Idea:

- Write a Metaprogram that creates Runge-Kutta algorithms
- Metaprogram input: Parameters of the RK scheme (Butcher Tableau)
- Main objective: **Resulting program should be as fast as direct implementation**

With such a Metaprogram you can implement any new Runge-Kutta scheme by just providing the Butcher tableau.

- Decrease in programming time
- Less bugs
- Better maintainability

The Generic Implementation

Define a structure representing one stage of the Runge-Kutta scheme:

```
template< int i >
struct stage // general (intermediate) stage, i > 0
{
  double c; // parameter c_i
  array<double,i> a; // parameters a_i+1,i ... a_i,i
                     // b_1 .. b_j for the last stage
};
```

Given an instance of this stage with `c` and `a` set appropriately the corresponding Runge-Kutta stage can be calculated.

The Generic Implementation

```
// x , x_tmp , t , dt and F defined outside
template< int i >
void calc_stage( const stage< i > &stage )
{  // performs the calculation of the i-th stage
  if( i == 1 ) // first stage?
    F[i-1] = f( x , t + stage.c * dt );
  else
    F[i-1] = f( x_tmp , t + stage.c * dt );

  if( i < s ) { // intermediate stage?
    x_tmp = x;
    for( int j=0 ; j<i : ++j )
      x_tmp += dt*stage.a[j] * F[j];
  } else {   // last stage
    x_end = x;
    for( int j=0 ; j<i : ++j )
      x_end += dt*stage.a[j] * F[j];
  }
}
```

The Generic Implementation

Generate list of stage types: `stage<1> , stage<2>, ... , stage<s>` using Boost.MPL (MetaProgramming Library) and Boost.Fusion.

```
typedef mpl::range_c< int , 1 , s > stage_indices;

typedef typename fusion::result_of::as_vector
< typename mpl::push_back
  < typename mpl::copy
    < stage_indices ,
      mpl::inserter
      <
        mpl::vector0<> ,
        mpl::push_back< mpl::_1 , stage_wrapper< mpl::_2 , stage > >
      >
    >::type , stage< double , stage_count , last_stage >
  >::type
>::type stage_vector_base; //fusion::vector< stage<1> , stage<2> , ... , stage<s>

struct stage_vector : stage_vector_base
{
  // initializer methods
  stage_vector( const a_type &a , const b_type &b , const c_type &c )
  {
    // ...
  }
}
```

The Generic Implementation

Parameter types for `a`, `b` and `c`:

```
typedef typename fusion::result_of::as_vector
< typename mpl::copy
  < stage_indices ,
    mpl::inserter
    < mpl::vector0< > ,
      mpl::push_back< mpl::_1 ,
                      array_wrapper< double , mpl::_2 > >
    >
  >::type
>::type a_type; //fusion::vector< array<double,1> , array<double,2> , ... >

typedef array< double , s > b_type;
typedef array< double , s > c_type;
```

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typedef array< double , s > b_type;
typedef array< double , s > c_type;
```

Instead of a dynamically allocated `double**` the compiler/optimzier sees fixed size arrays: `array<double,1>` , `array<double,2>`, ...
$\longrightarrow$ **better optimization possibilities**

The Generic Implementation

The actual Runge-Kutta step (details ommited):

```
fusion::for_each( stages ,
                  calc_stage_caller( f , x , x_tmp , x_end , F , t , dt ) );
```

Remember: `stages` is `fusion::vector< stage<1> , stage<2> , ... >`
For each of the `stages`, `calc_stage` gets called, but the `for_each`-loop is **executed by the compiler!**

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For each of the `stages`, `calc_stage` gets called, but the `for_each`-loop is **executed by the compiler!**

The compiler/optimizer sees sequential code:

```
calc_stage( stage_1 ); // stage_1 is an
calc_stage( stage_2 ); // instance of stage<1>
...                    // similar for stage_2 ...
calc_stage( stage_s );
```

$\longrightarrow$ **better optimization possibilities**

The Generic Stepper

Provide some handy interface to the generic algorithm:

```cpp
template< int s >
class generic_runge_kutta
{
public:
  generic_runge_kutta( const coef_a_type &a ,
                       const coef_b_type &b ,
                       const coef_c_type &c )
    : m_stages( a , b , c )
  { }

  void do_step( System f , const state_type &x , const double t ,
                state_type &x_out , const double dt )
  {
    fusion::for_each( m_stages , calc_stage_caller( f , x , m_x_tmp , x_out ,
                                                    m_F , t , dt ) );
  }

private:
  stage_vector m_stages;
  state_type m_x_tmp;

protected:
  state_type m_F[s];
};
```

Example: Runge-Kutta 4

Butcher Tableau:
$$\begin{array}{c|cccc}
0 & & & & \\
0.5 & 0.5 & & & \\
0.5 & 0 & 0.5 & & \\
1.0 & 0 & 0 & 1.0 & \\
\hline
 & 1/6 & 1/3 & 1/3 & 1/6
\end{array}$$

```
 // define the butcher array
const array< double , 1 > a1 = {{ 0.5 }};
const array< double , 2 > a2 = {{ 0.0 , 0.5 }};
const array< double , 3 > a3 = {{ 0.0 , 0.0 , 1.0 }};

const a_type a = fusion::make_vector( a1 , a2 , a3 );
const b_type b = {{ 1.0/6.0 , 1.0/3.0 , 1.0/3.0 , 1.0/6.0 }};
const c_type c = {{ 0.0 , 0.5 , 0.5 , 1.0 }};

// create the stages with the rk4 parameters a,b,c
generic_runge_kutta< 4 > rk4( a , b , c );
// do one rk4 step
rk4.do_step( lorenz , x , 0.0 , x , 0.1 );
```

Performance

Did we achieve our aim? Test RK4 on Lorenz System!

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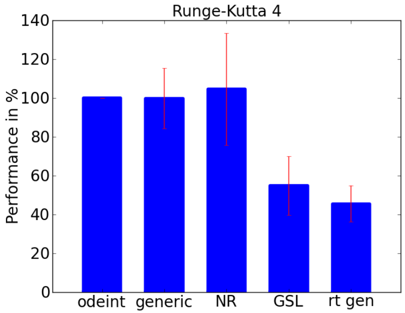

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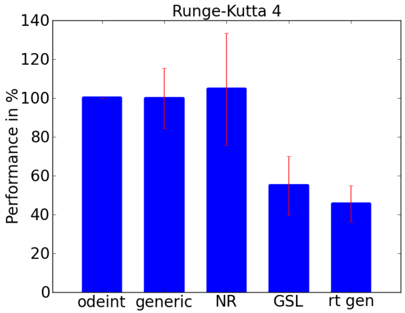

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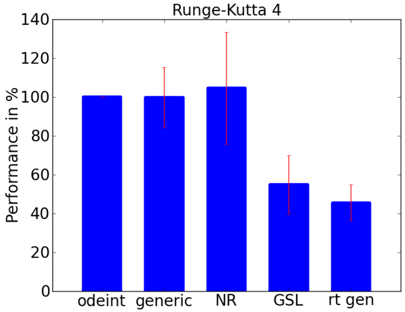

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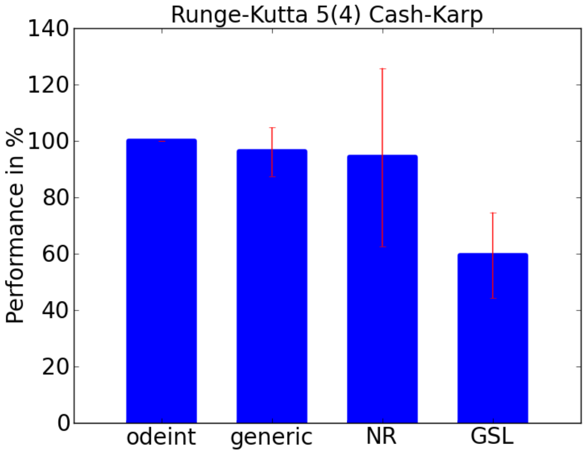
Yes!

- On modern compilers (Intel 12, gcc 4.5/4.6) as fast as explicit code.
- Older compilers might produce slightly worse performant code.
- Always factor 2 better than run time generic implementation.

Performace

Second test with a different scheme: Runge-Kutta Cash-Karp 5(4)



Conclusions

We implemented a generic Runge-Kutta algorithm that executes **any** RK scheme and has the following properties:

- Parameters (Butcher Tableau) can be defined in a natural way as C++ Arrays
- By virtue of Template Metaprogramming our code is as fast as direct implementation of the specific scheme
- **Major improvement (factor 2) compared to generic run time implementation** (but some increase in compile time)
- Embedded methods with error estimate can also be easily covered in a generic way
- This technique can be applied to other numerical problems, e.g. spline fitting, ...

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Thank you

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