Introduction to ODE solver and it's application in OpenFOAM

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1. Introduction

For the initial value ODE problem, there are three different kind of methods in OpenFOAM:

- RK: Runge-Kutta
- KRR4: Kaps-Rentrop
- SIBS: Semi-Implicit Bulirsh-Stoer

2. Mathematical Fundament

2.1. RK: Runge-Kutta

$$y' = f(t, y), y(t_0) = y_0$$

Then the Runge-Kutta methods is given by:

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i \tag{1}$$

Where the h is the time step and the the $\sum_{i=1}^{s} b_i k_i$ is an estimated slope:

$$k_1 = f(t_n, y_n)$$

$$k_2 = f(t_n + c_2 h, y_n + a_{21} h k_1)$$

$$k_s = f(t_n + c_s h, y_n + a_{s1} h k_1 + a_{s2} h k_2 + \cdots + a_{s,s-1} h k_{s-1})$$

For more information about the methods to solve ODE, one can read the book ”Introduction to Numerical Analysis” (New York: Springer-Verlag)

Structure in OpenFOAM

$FOAM_SRC/ODE

Take a look at the subdirectory *$FOAM_SRC/ODE/ODESolvers*:

KRR4/

RK/

SIBS/

ODESolver/

3. ODE in chemistry

There is an ode application in our standard tutorials:

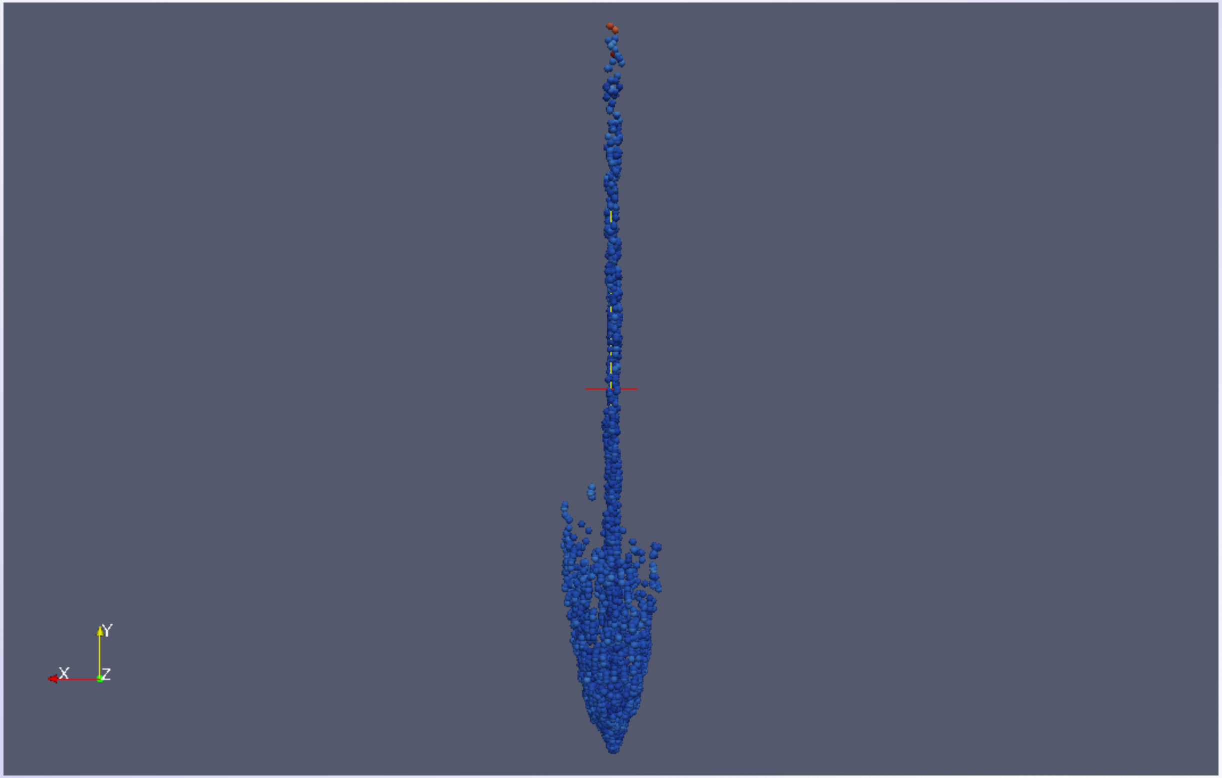
`$FOAM_SRC/thermophysicalModels /chemistryModel /chemistrySolver/ode/ode.C $FOAM_TUTORIALS//dieselFoam /aachenBomb/constant /chemistryProperties`

ODE in chemistry

```
(
    scalarField& c,
    const scalar T,
    const scalar p,
    const scalar t0,
    const scalar dt
)

    void derivatives
    (
        const scalar x,
        const scalarField& y,
        scalarField& dydx
    )
```

ODE in chemistry



4. Solving Our Own ODE

4.1. Our own test ODE

$$\frac{d^2y}{dx^2} = y, y(0) = 0, y'(0) = 1$$

```
label nEqns() const
    {

        return 2;
    }
```

Solving Our Own ODE

```
void derivatives
{
     dydx[0] = y[1];
     dydx[1] = y[0];

}

void jacobian
{
     dfdx[0] = 0.0;
     dfdx[0] = 0.0;

     dfdy[0][0] = 0.0;
     dfdy[0][1] = 1.0;
     dfdy[1][0] = 1.0;
     dfdy[1][1] = 0.0;


}
```

Solving Our Own ODE

```
Selecting ODE solver RK

Numerical:  y(1.0) = 2(1.17519 1.54307), hEst = 0.0736629
```

The same time we solve the ODE in MATLAB, we get:

```
Y(1.0) = (1.1752 1.5431)
```

Solving Velocity ODE

$$r\frac{d^2V_r}{dr^2} + \frac{dV_r}{dr} + \frac{4 \times V_r}{r} = 0$$

where $U_0 = U_\theta = 1$, $R = 1$ and $V_z = V_\theta = r$ in Walter Gyllenrams paper. Re-write the ODE into first-order ODE system we have:

$$\frac{dy_1}{dx} = y_2$$

$$\frac{dy_2}{dx} = -\frac{4y_1}{x^2} - \frac{y_2}{x}$$

with the boundary value $y_1(0) = y_1(1) = 0$

Thank you!