



# Introduction to ODE solver and it's application in OpenFOAM

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# Introduction to ODE solver and its 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:

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

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)



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## Structure in OpenFOAM

*\$FOAM\_SRC/ODE*

Take a look at the subdirectory *\$FOAM\_SRC/ODE/ODESolvers*:

*KRR4/*

*RK/*

*SIBS/*

*ODESolver/*

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## 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
```

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## 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
)
```



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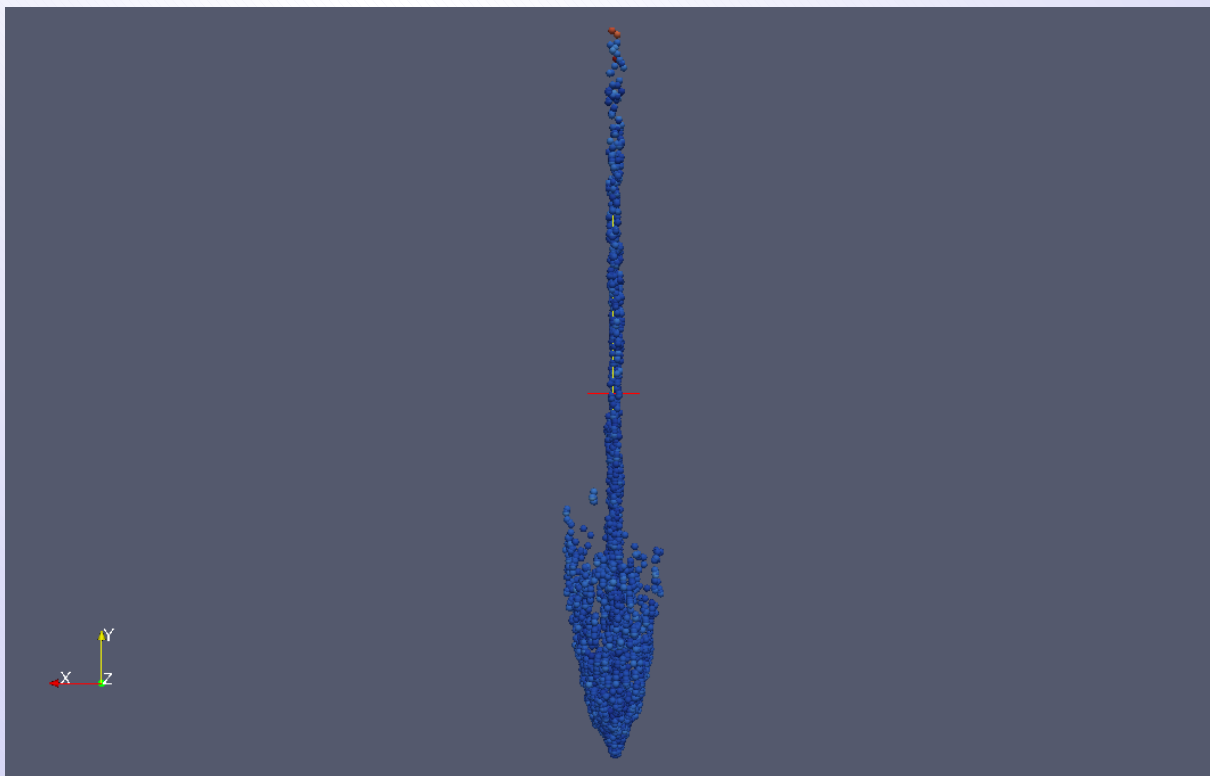
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## ODE in chemistry



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## 4. Solving Our Own ODE

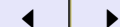
### 4.1. Our own test ODE

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

```
label nEqns() const
{
    return 2;
}
```

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## Solving Our Own ODE

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

void jacobian
{
    dfdx[0] = 0.0;
    dfdx[1] = 0.0;

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



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## 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:

$Y(1.0) = (1.1752 \ 1.5431)$

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## Solving Velocity ODE

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

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:

$$\begin{aligned} \frac{dy_1}{dx} &= y_2 \\ \frac{dy_2}{dx} &= -\frac{4y_1}{x^2} - \frac{y_2}{x} \end{aligned}$$

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

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**Thank you!**



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