Documentation on `modelEqn`

Numerical approach for a temperature distribution

Contents

1 1D spherical equations

1.1 Basic approach and scope

- Calculate a target property field as a function of time and physical space in a spherical particle
- Discretization for various boundary conditions

1.2 Overview of the Problem

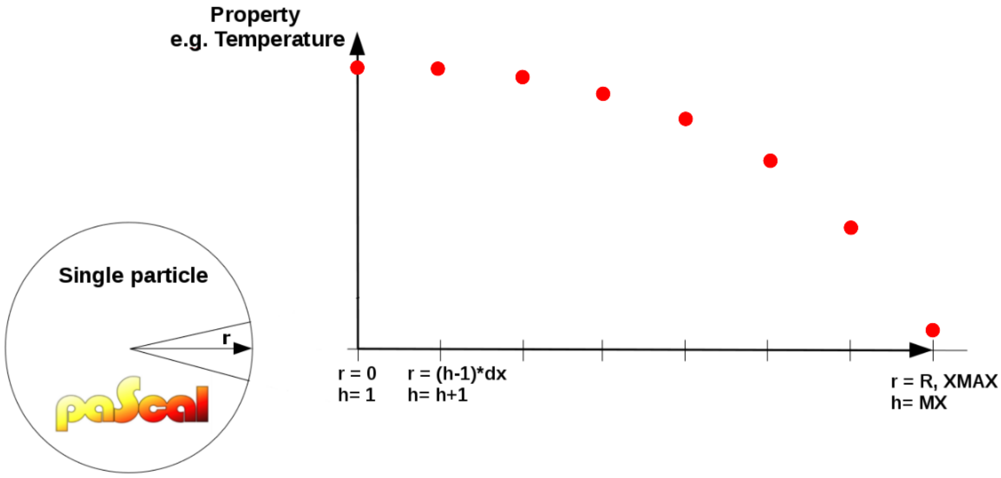

Figure 1: Overview

- Half of particle is discretized starting at $r = 0, h = 1$
- Every point coordinate until $h = MX$ ($MX=$ number of grid points to be set in input script using e.g. `particle_mesh nGridPoints 20`) can be obtained using $r = (h-1) \cdot \triangle r$ with $\triangle r = \dfrac{XMAX}{MX-1}$ with XMAX to be set in input script using e.g. `xmax 1.e-3`
- Value of target properties (e.g. temperature) obtained from discretization in physical space and integrating governing equations over time

1.3 Numerical approach and governing equations

- Fourier differential equation in spherical coordinates with $\lambda_{eff} = const.$ and no inner heat sources
- Eqn. (2) to Eqn. (3): transport of thermal energy in nothing but radial direction

$$\rho\, c_p \, \frac{\partial T}{\partial t} = div(\lambda_{eff}\, grad\, T) + \dot{q} \tag{1}$$

$$\rho\, c_p \, \frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(\lambda_{eff}\, r^2 \frac{\partial T}{\partial r}\right) + \frac{1}{r^2\, sin^2\varphi}\frac{\partial}{\partial \psi}\left(\lambda_{eff}\frac{\partial T}{\partial \psi}\right) + \frac{1}{r^2\, sin^2\varphi}\frac{\partial}{\partial \varphi}\left(\lambda_{eff}\frac{\partial T}{\partial \varphi}\right) + \dot{q} \tag{2}$$

$$\rho\, c_p \, \frac{\partial T}{\partial t} = \lambda_{eff}\left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r}\right) \tag{3}$$

with thermal diffusivity

$$a = \frac{\lambda_{eff}}{\rho\, c_p} \tag{4}$$

$$\frac{\partial T}{\partial t} = a \cdot \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r}\right) \tag{5}$$

1.4 Discretization in physical space

- CDS - second order scheme

$$\frac{\partial T}{\partial r} = \frac{T_{h+1} - T_{h-1}}{2\, \triangle\, r} + O(\triangle r^2) \tag{6}$$

$$\frac{\partial^2 T}{\partial r^2} = \frac{T_{h+1} + T_{h-1} - 2T_h}{\triangle r^2} + O(\triangle r^2) \tag{7}$$

1.5 Boundary conditions

1.5.1 Middle of sphere

- Singularity in spherical coordinates at $r = 0$, symmetry
- First derivative of temperature after radius divided by radius is replaced by second derivative of temperature after radius (L'hopital)

$$\frac{\partial T}{\partial t} = 3\,a\,\frac{\partial^2 T}{\partial r^2} \tag{8}$$

with:

$$\frac{\partial^2 T}{\partial r^2} = \frac{T_{h+1} + T_{h-1} - 2T_h}{\triangle r^2} + O(\triangle r^2) \tag{9}$$

and T_{0-1} results of *auxiliary point method* and boundary condition second order at $r = 0, h = 1$ with T_{0-1}=T_{0+1}

$$\frac{\partial T}{\partial t} = 6\,a\,\frac{T_{0+1} - T_0}{\triangle r^2} \tag{10}$$

1.5.2 Surface of sphere, r = XMAX

1.5.3 NEUMANN

- Fixed heat flux

$$\dot{q} = -\lambda_{eff}\,\frac{\partial T}{\partial r} \tag{11}$$

$$\dot{q} = -\lambda_{eff}\,\frac{T_{h+1} - T_{h-1}}{2\,\triangle\,r} \tag{12}$$

$$T_{h+1} = T_{h-1} - \frac{2\,\dot{q}\,\triangle\,r}{\lambda_{eff}} \tag{13}$$

$$\frac{\partial^2 T}{\partial r^2} = \frac{T_{h-1} - \dfrac{2\,\dot{q}\,\triangle\,r}{\lambda_{eff}} + T_{h-1} - 2\,Th}{\triangle r^2} \tag{14}$$

$$= \frac{2\left(T_{h-1} - \dfrac{\dot{q}\,\triangle\,r}{\lambda_{eff}} - T_h\right)}{\triangle r^2} \tag{15}$$

$$\frac{\partial T}{\partial r} = \frac{T_{h+1} - \dfrac{2\,\dot{q} \bigtriangleup r}{\lambda_{eff}} - Th - 1}{2 \bigtriangleup r} \tag{16}$$

$$= -\frac{2\,\dot{q} \bigtriangleup r}{2 \bigtriangleup r \lambda_{eff}} \tag{17}$$

$$= -\frac{\dot{q}}{\lambda_{eff}} \tag{18}$$

$$\frac{\partial T}{\partial t} = \frac{2\left(T_{h-1} - \dfrac{\dot{q} \bigtriangleup r}{\lambda_{eff}} - T_h\right)}{\bigtriangleup r^2} - \frac{2\,\dot{q}}{R\,\lambda_{eff}} \tag{19}$$

1.5.4 DIRICHLET

- Fixed wall temperature T_w

$$T_h = T_{wall} \tag{20}$$

1.5.5 CONVECTIVE

- Convective heat transfer at the surface of the particle

$$\alpha \cdot (T_h - T_{enviro}) = -\lambda_{eff} \frac{\partial T}{\partial r} \tag{21}$$

- Calculation of *auxiliary point*

$$\alpha \cdot (T_h - T_{enviro}) = -\lambda_{eff} \frac{T_{h+1} - T_{h-1}}{2 \bigtriangleup r} \tag{22}$$

with Biot number

$$Bi = \frac{\alpha \bigtriangleup r}{\lambda_{eff}} \tag{23}$$

$$T_{h+1} = -2\,Bi\,(T_h - T_{enviro}) + T_{h-1} \tag{24}$$

with T_{h+1} at $x = R, XMAX$

$$\frac{\partial T}{\partial t} = a \cdot \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{R}\frac{\partial T}{\partial r}\right) \tag{25}$$

results in

$$\begin{aligned}\frac{\partial T}{\partial t} =& \frac{a}{\bigtriangleup r^2}(-2\,Bi\,(T_h - T_{enviro}) + T_{h-1} + T_{h-1} - 2\,T_h) + \\ & \frac{2\,a}{2\,R \bigtriangleup r}\,(-2\,Bi\,(T_h - T_{enviro}) + T_{h-1} - T_{h-1})\end{aligned} \tag{26}$$

$$
\begin{aligned}
\frac{\partial T}{\partial t} =& \frac{2\,a}{\triangle r^2}(-\,Bi\,(T_h - T_{enviro}) + T_{h-1} - T_h) + \\
& \frac{a}{R\,\triangle\,r}\,(-\,2\,Bi\,(T_h - T_{enviro})) = f(RHS - RightHandSide)
\end{aligned}
\tag{27}
$$

If a heat flux from `LIGGGHTS` is pulled trough a coupling model it acts as a thermal source term and is added for the outer grid point which results in

$$
\begin{aligned}
&\frac{\partial T}{\partial t} = \frac{2\,a}{\triangle r^2}\,(-\,Bi\,(T_h - T_{enviro}) + T_{h-1} - T_h) + \\
&\frac{a}{R\,\triangle\,r}\,(-\,2\,Bi\,(T_h - T_{enviro})) + \frac{\dot{q}}{\rho_{eff}\,c_{p,eff}} = f(\text{RHS - Right Hand Side})
\end{aligned}
\tag{28}
$$

1.6 Jacobian matrix coefficients

- Function `returnJac` in `modeleqn1Dspherical`
- Represents the derivation of RHS by every single component (e.g. $T_h, T_{h+1}, ...$)

1.6.1 Middle of sphere

based on Eqn. (10)

$$
\frac{\partial f}{\partial T_0} = -\frac{6\,a}{\triangle r^2}
\tag{29}
$$

$$
\frac{\partial f}{\partial T_{0+1}} = \frac{6\,a}{\triangle r^2}
\tag{30}
$$

1.6.2 Between middle and surface

- Used for $1 < h < MX$
- Based on Eqn. (6), (7) and (5)

$$
\frac{\partial f}{\partial T_h} = -\frac{2\,a}{\triangle r^2}
\tag{31}
$$

$$
\frac{\partial f}{\partial T_{h-1}} = \frac{a}{\triangle r}\left(\frac{1}{\triangle r} - \frac{1}{x}\right)
\tag{32}
$$

$$
\frac{\partial f}{\partial T_{h+1}} = \frac{a}{\triangle r}\left(\frac{1}{\triangle r} + \frac{1}{x}\right)
\tag{33}
$$

1.6.3 Surface of sphere, r = XMAX

1.6.4 DIRICHLET

based on Eqn. (20)

$$\frac{\partial f}{\partial T_h} = 0 \tag{34}$$

1.6.5 NEUMANN

based on Eqn. (19)

$$\frac{\partial f}{\partial T_h} = -\frac{2}{\triangle r^2} \tag{35}$$

$$\frac{\partial f}{\partial T_{h-1}} = \frac{2}{\triangle r^2} \tag{36}$$

1.6.6 CONVECTIVE

based on Eqn. (27)

$$\frac{\partial f}{\partial T_h} = -\frac{2\,a}{\triangle r}\left(\frac{Bi}{R} + \frac{Bi}{\triangle r} - \frac{1}{\triangle r}\right) \tag{37}$$

$$\frac{\partial f}{\partial T_{h-1}} = \frac{2\,a}{\triangle r^2} \tag{38}$$

1.7 Calculating of average values

- Need to compute volume averaged particle properties
- Volume shells defined at every location i with r ranging from $0 \leq i < MX$

$$\overline{y} = \frac{\sum_0^i \triangle V\, y_i}{\sum_0^i \triangle V} \tag{39}$$

with

$$\begin{aligned}\triangle V &= \frac{\pi}{6}\left(r_a^3 - r_i^3\right) &(40)\\ &= \frac{\pi dx^3}{6}\left[(i+0.5)^3 - (i-0.5)^3\right] &(41)\end{aligned}$$

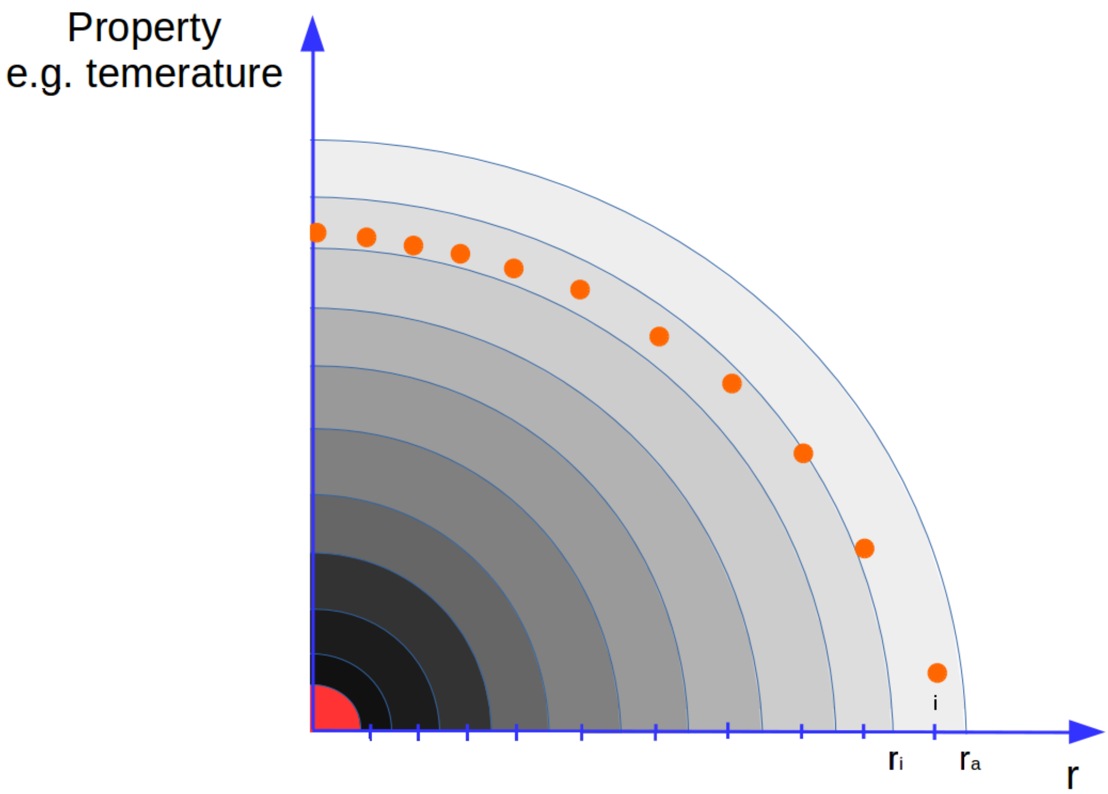

Figure 2: Averaging shells with $r_a = i + 0.5$ and $r_i = i - 0.5$ and $0 \leq i < MX$