پروژه سوم درس انتقال در محیط متخلخل:

شبیه‌سازی ذوب مواد تغییرفازدهنده در محیط متخلخل به روش لتیس بولتزمن در محیط نرم‌افزار Palabos

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مقدمه

شبیه‌سازی

نتایج

energies

MDPI

Review

Phase Change Materials Energy Storage Enhancement Schemes and Implementing the Lattice Boltzmann Method for Simulations: A Review

Milad Shirbani [1], Majid Siavashi [1,*] and Mehdi Bidabadi [2]

Fabrication and Thermal Performance of PCMs

PCMs are categorized into three different types:

1. Organic PCMs
   - Paraffin
   - Non-paraffin
2. Inorganic PCMs
   - Salt hydrates
   - Metallics
3. Eutectics

Improvement of Energy Storage in PCMs

PCMs' low thermal conductivity prevents their use as pure PCMs in industrial applications.

1. Porous Media as Composite PCMs
   I. Metal Foam Composite PCMs
   II. Composite PCMs with Carbon Material
2. Nanoparticle-Enhanced PCMs
3. Adding Fins

معادلات حاکم ذوب مواد تغییرفازدهنده

The general governing equations for thermo-fluidic transport encountering phase changes (melting and solidification), assuming the flow to be Newtonian, laminar, and incompressible, are:

$$\nabla.(\boldsymbol{u}) = 0$$

$$\rho\left[\frac{\partial \boldsymbol{u}}{\partial t} + \nabla.(\boldsymbol{u}\boldsymbol{u})\right] = -\nabla p + \nabla.(\mu\nabla\boldsymbol{u}) + \rho\boldsymbol{f}$$

$$(\rho C_p)\left[\frac{\partial}{\partial t} + \nabla.(\boldsymbol{u}T)\right] = \nabla.(k\nabla T) + q$$

latent heat due to a phase transition

$$q = -\left[\frac{\partial(\rho\Delta H)}{\partial t} + \nabla.(\rho\boldsymbol{u}\Delta H)\right]$$

The second term may be omitted when the substance is pure

$$q = -\frac{\partial(\rho\Delta H)}{\partial t} = -\frac{\partial(\rho L f_l)}{\partial t}$$

$$\nabla.\boldsymbol{u}_f = 0 \qquad 6$$

$$\rho_f\left[\frac{\partial \boldsymbol{u}_f}{\partial t} + \nabla.\left(\boldsymbol{u}_f\boldsymbol{u}_f\right)\right] = -\nabla p_f + \mu_f\nabla^2\boldsymbol{u}_f + \rho_f g\beta\left(T - T_{ref}\right) \qquad 7$$

$$(\rho C_p)_f\left[\frac{\partial T_f}{\partial t} + \nabla.\left(\boldsymbol{u}_f T_f\right)\right] = \nabla.\left(k_f\nabla T_f\right) + q_{L_f} + q_{sf} \qquad 8a$$

$$(\rho C_p)_s\frac{\partial T_s}{\partial t} = \nabla.(k_s\nabla T_s) + q_{L_f} - q_{sf} \qquad 8b$$

معادلات حاکم ذوب مواد تغییرفازدهنده

The fluid and solid phases are addressed with the f and s subscripts. q_{sf} shows the transferred heat from two different phases, meaning solid to liquid, while q_{L_f} is the solid-liquid phase transition latent heat. From a more detailed point of view, a PCM could be considered a porous medium. Accordingly, melting and solidification would be distinguished by their initial porosity. For solidification, $\varepsilon_0 = 1$, would represent the liquid phase, and for melting, $\varepsilon_0 = 0$, represents the solid phase. Considering a PCM as a porous

$$q_{L_f} = -\frac{\partial \rho L_f \varepsilon}{\partial t} \quad (9) \qquad \varepsilon = \frac{V_f}{V_s + V_f} \quad (10)$$

temperature range for the melting of a PCM should be within $\Delta T_m = T_{m_{high}} - T_{m_{low}}$.

Otherwise, Equation (9) should be replaced with $C_{pm} = \frac{L_f}{\Delta T_m}$. Therefore, the momentum and energy equations would be reduced to:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla.(\boldsymbol{u}\boldsymbol{u}) = -\frac{1}{\rho_f}\nabla p_f + \nu_f \nabla^2 \boldsymbol{u} + \rho_f g \beta \left(T - T_{ref}\right) \quad (15)$$

$$\frac{\partial T}{\partial t} + \nabla.(\varepsilon \boldsymbol{u} T) = \alpha_m \nabla^2 T - \left(\frac{L_f}{C_{pm}}\right)\frac{\partial \varepsilon}{\partial t} \quad (16)$$

Based on the definition of porosity which was presented in Equation (10), the energy equations for the solid and liquid phases (Equations (8a,b)) could be merged:

$$[\varepsilon(\rho C_p)_f + (1-\varepsilon)(\rho C_p)_s]\left[\frac{\partial T}{\partial t} + \nabla.\left(\varepsilon \boldsymbol{u}_f T\right)\right] = [\varepsilon k_f + (1-\varepsilon)k_s]\nabla^2 T - [\varepsilon\left(\rho L_f\right)_f + (1-\varepsilon)\left(\rho L_f\right)_s]\frac{\partial \varepsilon}{\partial t} \quad (11)$$

معادلات حاکم ذوب مواد تغییرفازدهنده

For a flow in porous media that is laminar and incompressible in the absence of viscous dissipation, a chemical reaction, or radiative heat transfer and in the presence of natural convection, the Navier-Stokes equations are as follows

$$\nabla . \boldsymbol{u} = 0 \tag{17}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}.\nabla)\left(\frac{\boldsymbol{u}}{\varepsilon}\right) = -\frac{1}{\rho}\nabla(\varepsilon p) + \nu_e \nabla^2 \boldsymbol{u} + \boldsymbol{F} \tag{18}$$

These equations are the continuity and Darcy-Brinkmann-Forchheimer equations, respectively. $\nu_e \nabla^2 \boldsymbol{u}$ is responsible for representing the presence of solid boundaries and is called the Brinkmann term. ε, ν_e, and $\boldsymbol{F}$ are the porosity of the porous medium, effective viscosity, and the body force induced by the presence of the porous medium and other external forces, defined by:

$$\boldsymbol{F} = -\frac{\varepsilon \nu_f}{K}\boldsymbol{u} - \frac{\varepsilon F_\varepsilon}{\sqrt{K}}|\boldsymbol{u}|\boldsymbol{u} + \varepsilon \boldsymbol{G}, \quad K = \frac{\varepsilon^2 d_p^2}{150(1-\varepsilon)^2} \tag{19}$$

روش لتیس بولتزمن حرارتی برای ذوب مواد تغییرفازدهنده

The general LB equation is presented as follows

$$f_i(\vec{x}+\vec{e_i}\Delta t, t+\Delta t) - f_i(\vec{x},t) = -\Omega_{ij}\Delta t\left[f_j - f_j^{eq}\right](\vec{x},t) + S_i\Delta t \quad 26$$

In the above relation, $\Omega_{ij}\,\Delta t = 1/\tau_f$ where τ_f is the relaxation time of the fluid [115]. In Equation (26), the left-hand side is the collision term, and the first term on the right-hand side is called the streaming step. The discrete distribution function $f_i(\vec{x},t)$ is responsible for representing the moving of particles alongside the directions of the lattice. $\vec{c_i}$ indicates the discrete lattice speed along the i direction. To determine the direction, first, the LBM type should be

the key macroscopic quantities

$$\rho = m\sum_i f_i \ (mass\ density)$$
$$\rho u = m\sum_i f_i c_i (current\ density)$$
$$\rho T = m\sum_i f_i (c_i - u)^2 (temperature)$$
$$q = m\sum_i f_i (c_i - u)^3 (heat\ flux)$$

27

When the LB equation is applied to the phase change problem, the interaction of the fluid with the melting front is encoded by the source term S_i. Only a fraction $1 - r(\phi)$ is transmitted to the next link for any lattice site. This step is called reflection and is provided by [121]:

$$\tilde{f}_i(\vec{x}+\vec{e}_i\Delta t, t+\Delta t) = \left(1 - r(\vec{x},t)\right)f_i(\vec{x},t) + r(\vec{x},t) + r(\vec{x},t)f_{\bar{i}}(\vec{x},t) \quad (29)$$

روش لتیس بولتزمن حرارتی برای ذوب مواد تغییرفازدهنده

Multiple-Relaxation Time (MRT) Enthalpy-Based Model

In the MRT-LBM enthalpy-based model, the velocity field LBM governing equations are the same as SRT, while only the temperature field is obtained from the MRT-LBM. The MRT enthalpy-based equation for temperature distribution is [139]:

$$g_i(\vec{x}+\vec{e}_i\Delta t, t+\Delta t) - g_i(\vec{x}, t) = -\Lambda_{ik}\left[g_k - g_k^{eq}\right](\vec{x}, t) \tag{47}$$

where this time, there is a relaxation matrix $\Lambda = \Lambda_{ik}$ for the velocity field [9]. For the momentum space, the collision step is completed as:

$$\boldsymbol{m}(\boldsymbol{x}, t+\Delta t) = \boldsymbol{m}(\boldsymbol{x}, t) - \boldsymbol{s}[\boldsymbol{m}(\boldsymbol{x}, t) - \boldsymbol{m}^{eq}(\boldsymbol{x}, t)] \tag{48}$$

$$\begin{aligned} \boldsymbol{m} &= \boldsymbol{M}g_i = (m_0, m_1, \ldots, m_8)^T, \\ \boldsymbol{m}^{eq} &= \boldsymbol{M}g_i^{eq} = \left(m_0^{eq}, m_1^{eq}, \ldots, m_8^{eq}\right)^T \end{aligned} \tag{49}$$

$$\boldsymbol{S} = \boldsymbol{M}\boldsymbol{\Lambda}\boldsymbol{M}^{-1} \tag{50}$$

روش لتیس بولتزمن حرارتی برای ذوب مواد تغییرفازدهنده

$\boldsymbol{M}$ is the transformation matrix and is provided in:

$$\boldsymbol{M}=\begin{Bmatrix}1&1&1&1&1&1&1&1&1\\-4&-1&-1&-1&-1&2&2&2&2\\4&-2&-2&-2&-2&1&1&1&1\\0&1&0&-1&0&1&-1&-1&1\\0&-2&0&2&0&1&-1&-1&1\\0&0&1&0&-1&1&1&-1&-1\\0&0&-2&0&2&1&1&-1&-1\\0&1&-1&1&-1&0&0&0&0\\0&0&0&0&0&1&-1&1&-1\end{Bmatrix} \tag{51}$$

Also, $\boldsymbol{m}^{eq}$ is the equilibrium function in a momentum space and is obtained from [9,140]:

$$\boldsymbol{m}^{eq}=(H,-4H+2C_{p,ref}T+3C_pT\frac{u^2}{c^2},4H-3C_{p,ref}T \\ -3C_pT\frac{u^2}{c^2},C_pT\frac{u}{c},-C_pT\frac{u}{c},C_pT\frac{v}{c},-C_pT\frac{v}{c},C_pT\frac{u^2-v^2}{c^2},C_pT\frac{uv}{c^2})^T \tag{52}$$

The relaxation matrix $\boldsymbol{S}$ in the momentum space is provided by [128]:

$$\boldsymbol{S}=diag(s_0,s_e,s_\varepsilon,s_j,s_q,s_j,s_q,s_e,s_e) \tag{53}$$

The diagonal matrix presented above should be in a way that its relaxation parameters satisfy $s_0=1$, $s_j=1/\tau_s$ and $0<s_{e,\varepsilon,q}<2$, where:

$$\tau_s=\begin{cases}3\dfrac{\lambda_{pcm}}{\rho_f c_{p,ref}}+0.5 & \text{in the PCM region}\\[2ex] 3\dfrac{\lambda_w}{\rho_f c_{p,ref}}+0.5 & \text{in the solid wall and fins}\end{cases} \tag{54}$$

For better numerical stability and to avoid numerical diffusion, the relaxation parameters should satisfy the following equation [9,139]:

$$\left(\frac{1}{s_e}-\frac{1}{2}\right)\left(\frac{1}{s_j}-\frac{1}{2}\right)=\frac{1}{4} \tag{55}$$

There is a function called the post-collision distribution, which is the result of a collision process in the velocity field. This function could be obtained from an inverse transformation as follows:

$$g_i(\boldsymbol{x},t+\Delta t)=\boldsymbol{M}^{-1}\boldsymbol{m}(\boldsymbol{x},t+\Delta t) \tag{56}$$

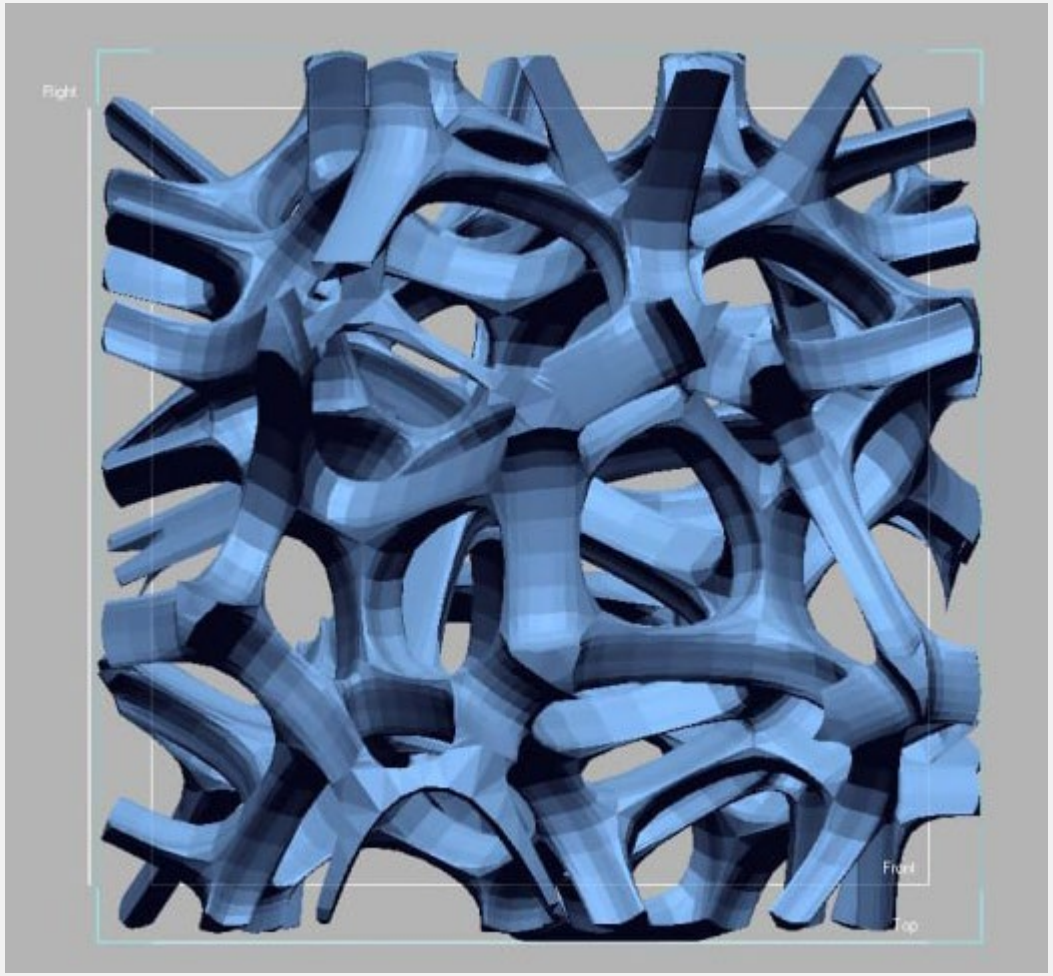
Then streaming process completes:

$$g_i(\boldsymbol{x}+\boldsymbol{e_i}\Delta \mathrm{t},\mathrm{t}+\Delta \mathrm{t})=g_i(\boldsymbol{x},t+\Delta t) \tag{57}$$

At last, the total enthalpy based on the boundary conditions could be derived from [9,141]:

$$\sum_0^8 g_i=H \tag{58}$$

تولید هندسه فوم فلزی متخلخل در نرم‌افزار geomagic design x



شکل ۱- هندسه محیط متخلخل

کد Reading_stl

steady.xml

Reading_stl > steady.xml

```
3   <!--
7
8   <geometry>
9       <!-- The name of the STL file that contains the representation of the object. -->
10      <file> B10PPI-0.9.stl </file>
11      <!-- Parameter to inflate the surface mesh before voxelization. -->
12      <inflationParameter> 0.1 </inflationParameter>
13      <!-- Precision for geometric operations (FLT, DBL, LDBL, INF). -->
14      <precision> DBL </precision>
15      <!-- Position of the center of the object in the simulation domain. -->
16      <center> <x> 4.5 </x> <y> 4.5 </y> <z> 4.5 </z> </center>
17      <!-- Size of the computational domain. -->
18      <domain> <x> 9 </x> <y> 9 </y> <z> 9 </z> </domain>
19  </geometry>
20
21
22  <numerics>
23      <!-- Length to define the resolution and the Reynolds number. -->
24      <characteristicLength> 0.5 </characteristicLength>
25      <!-- Grid resolution (number of nodes in the characteristicLength). -->
26      <resolution> 6 </resolution>
27  </numerics>
```

شکل ۲- ورودی‌های کد Reading_stl

تغییر Flagها


```
jupytertest.ipynb
jupytertest2 > jupytertest.ipynb
+ Code + Markdown ···

with open("B10PPI-0.9.txt", "r") as data_file:
        #data=data_file.readlines()
        data=data_file.read()
        #data=list(map(lambda x: x.replace("\n", ""),data))
        # data=list(map(lambda x: x.replace("2", "3"),data))
        # data=list(map(lambda x: x.replace("4", "3"),data))
        # data=list(map(lambda x: x.replace("5", "3"),data))
        #data=list(map(lambda x: x.split(), data))
        data= data.replace("2", "3")
        data= data.replace("4", "3")
        data= data.replace("5", "3")
        #without foam
       # data= data.replace("3", "1")

[1]

with open("out_B10PPI-0.9.txt", "w") as out_file:

    out_file.write(data)
```

```
T PCMfluidflag=0, PCMsolidflag=1 , wallflag=2 ,  metalsolidflag=3;
// T isolateSolidFlag=2 , boundarySolidFlag=1, fluidFlag=0;
```

شکل ۳- کد پایتون تغییر flagها در محیط Jupyter

کد اصلی

وارد کردن پارامترهای ورودی

simulation-parameter.xml

PCM > simulation-parameter.xml

```
<geometry>
    <!-- The name of the geometry file that contains the 0 1 data. -->
    <file> out_B10PPI-0.9.txt </file>
    <!-- Size of the computational domain. [m]-->
    <domain> <dx_real> 1e-4 </dx_real>  </domain>
    <!-- number of lattice in computational domain. -->
    <numDomain> <nx> 91 </nx> <ny> 91 </ny> <nz> 91 </nz> </numDomain>
</geometry>
```

```
  <leftwall_temp_real> 100.0 </leftwall_temp_real>
  <rightwall_temp_real> 25.0 </rightwall_temp_real>
```

```
    <Prandtl> 3.2 </Prandtl>
```

```
    <!-- omega Gas. -->
    <omegaT> 0.86 </omegaT>
```

شکل ۴- در نظر گرفتن عدد پرانتل برابر ۳,۲ و بدست آوردن امگا حرارتی متناسب با آن

کد اصلی

محاسبات به دست آوردن omegaT

```
alpha_l= (1.0/omegaT-0.5)/3.0;
omegaT = ((omega – 0.5)/Pr)+0.5
nu_l=(1.0/omega-0.5)/3.0;
C_nu=nu_r/nu_l;
omega= 1.0/(nu_l*3+0.5);  //omega fluid
lx_r= dx_r*(nx-1);
rho_l=1.0;
```

Sorption modeling parametrs and unit converstion coefficient

```
Number of node in x direction :      nx  =91
Number of node in y direction :      ny  =91
Number of node in y direction :      nz  =91
```

NonDimentional parametrs

```
Prandtl Number:                      Pr=3.2
Stefan Number:                       St=20
Rayleigh Number:                     Ra=100000
gbeta for lattice Number:            gbeta_l=0.00102932
```

real parametrs

```
left wall temperature real :         leftwall_temp_r=100
right wall temperature real :        rightwall_temp_r=25
real length:                         lx_r=0.009
real density:                        rho_r=900
Alpha_real:                          alpha_r=0.0377562
Alpha_solid_real:                    alpha_solid_r=2.12711
k_solid_real:                        k_solid_r=400
real nu:                             nu_r=0.006
real time step:                      dt_r=5.85149e-08
```

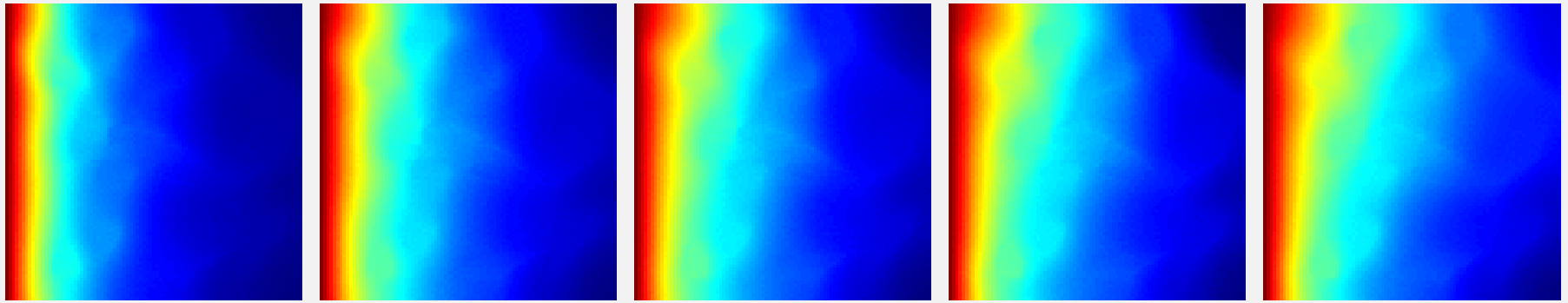
unit convertors

```
convertor length:                    C_l=0.0001
convertor density:                   C_rho=900
convertor mass:                      C_m=9e-10
convertor alpha:                     C_alpha=0.170897
convertor time:                      C_s=5.85149e-08
convertor temperature:               C_temp=100
convertor gbeta:                     C_gbeta=2.92056e+08
```

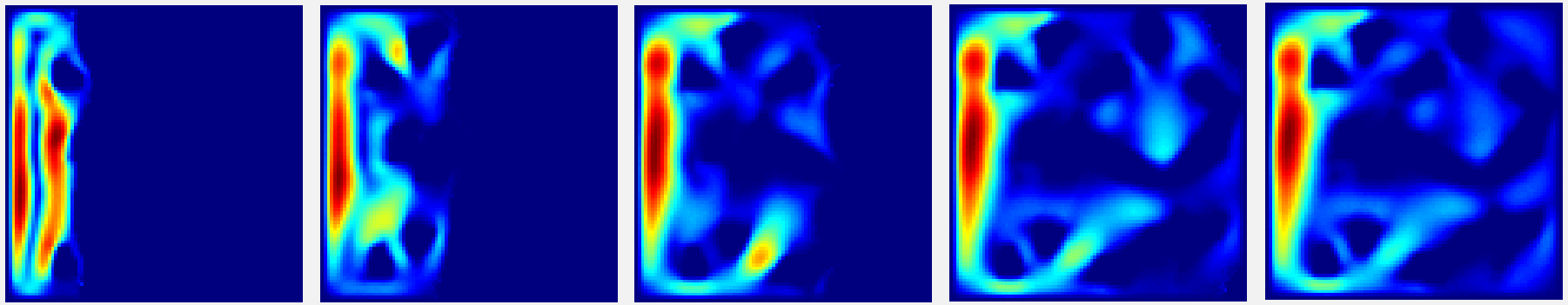
lattice parametrs

```
number of lattice in X direction:    Nx_l=91
number of lattice in Y direction:    Ny_l=91
number of lattice in z direction:    Nz_l=91
lattice diffusion fre for fluid:     omegaT_fluid=0.86
lattice diffusion fre for solid:     omegaT_solid=0.0264268
lattice flow fre:                    omega=1.652
Alpha_lattice:                       alpha_l=0.22093
Alpha_solid_lattice:                 alpha_solid_l=12.4468
kinematic viscosity:                 Nu_l=0.035109
lattice density:                     rho_l=1
lattice time step:                   dt_l=1
maximum Iteration:                   maxIter=150000
```

نتایج و خروجی کد

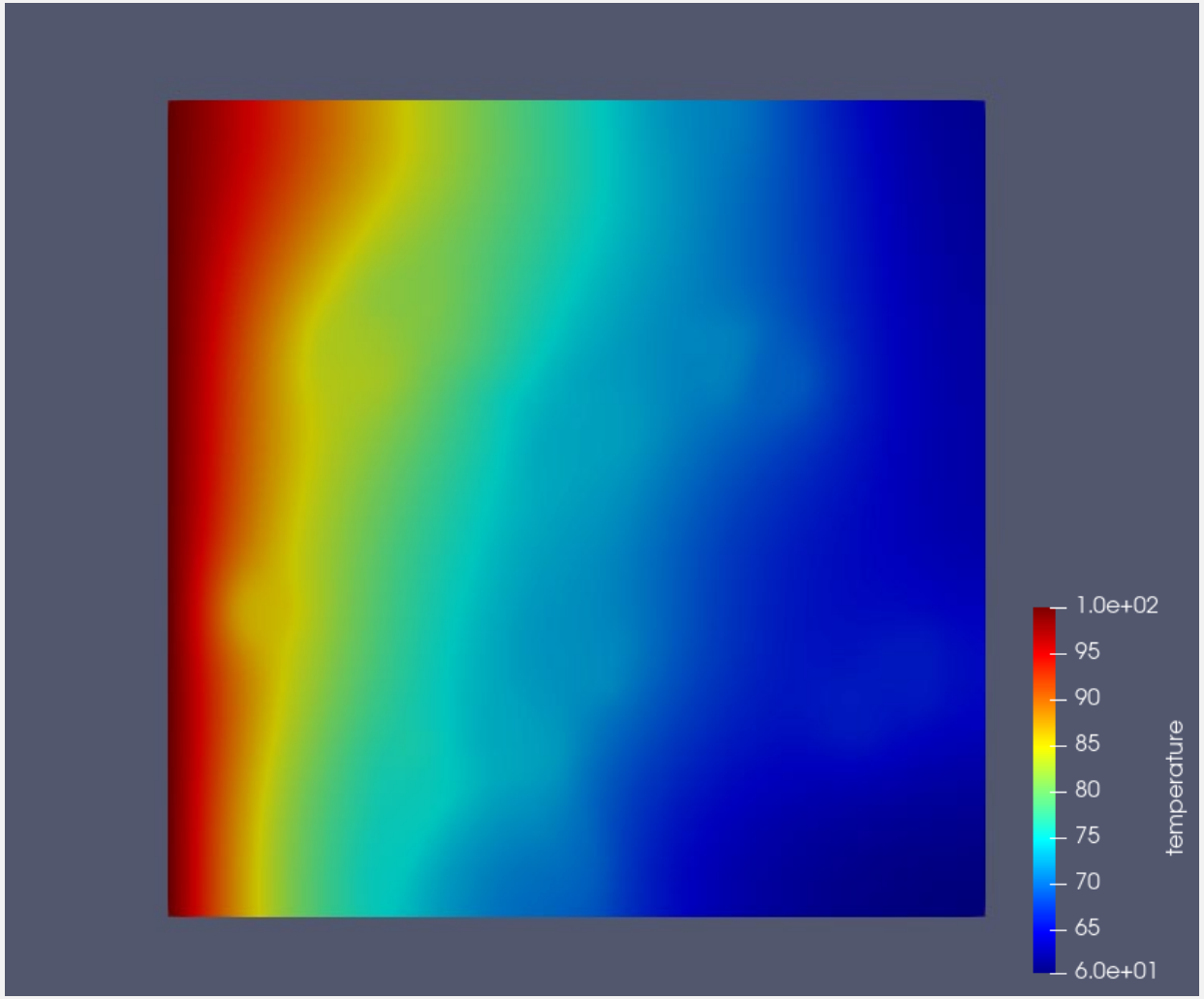


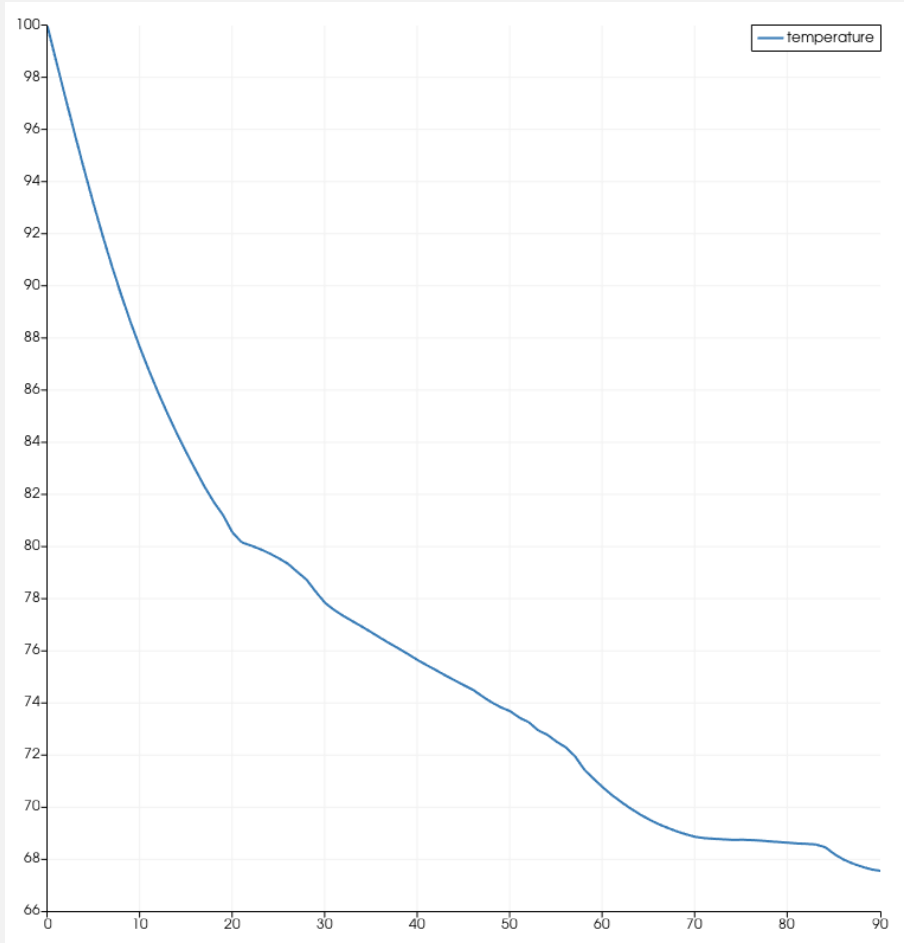
شکل ۵- توزیع دما در هر ۱۰۰۰ ایتریشن



شکل ۶- توزیع دما در هر ۱۰۰۰ ایتریشن

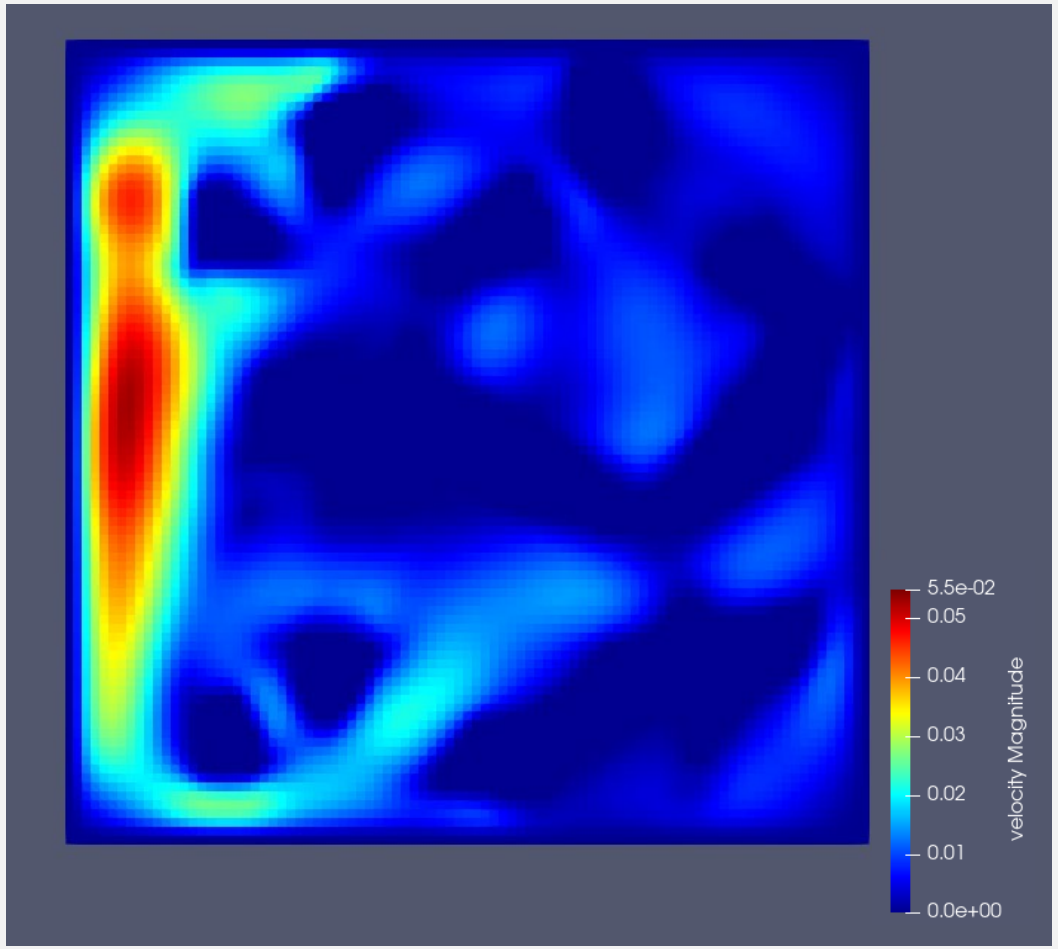
تحلیل نتایج با استفاده از Paraview

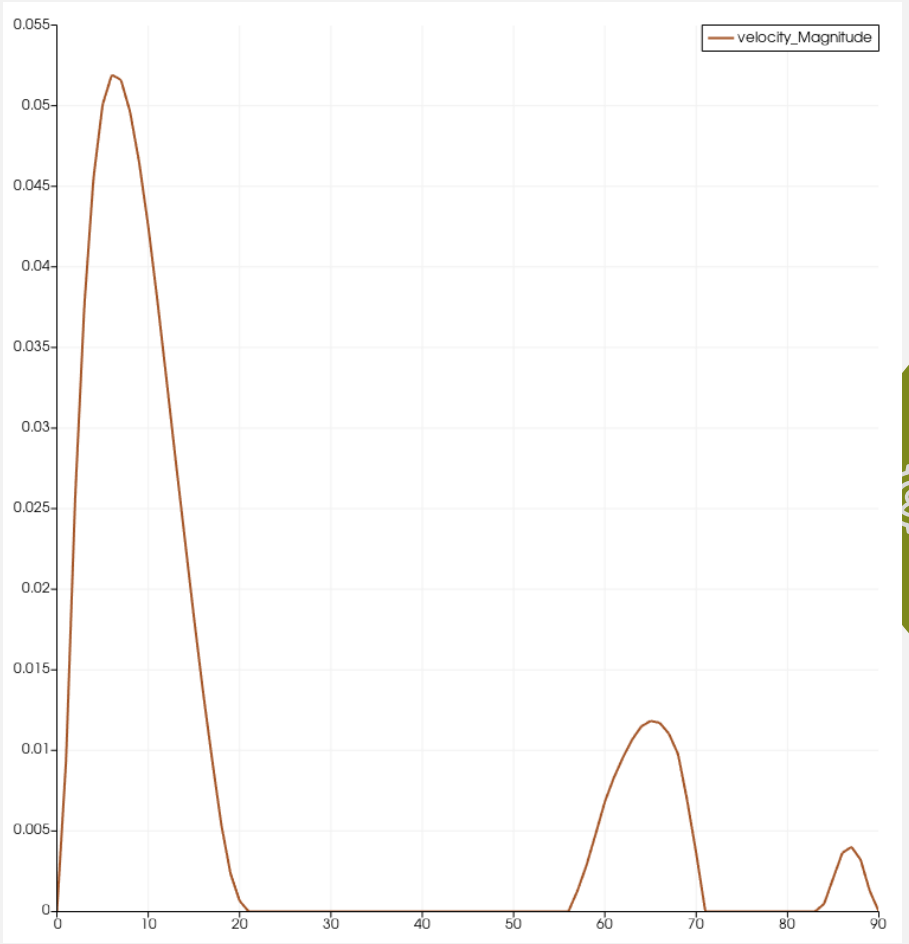




شکل ۷- توزیع دما نهایی

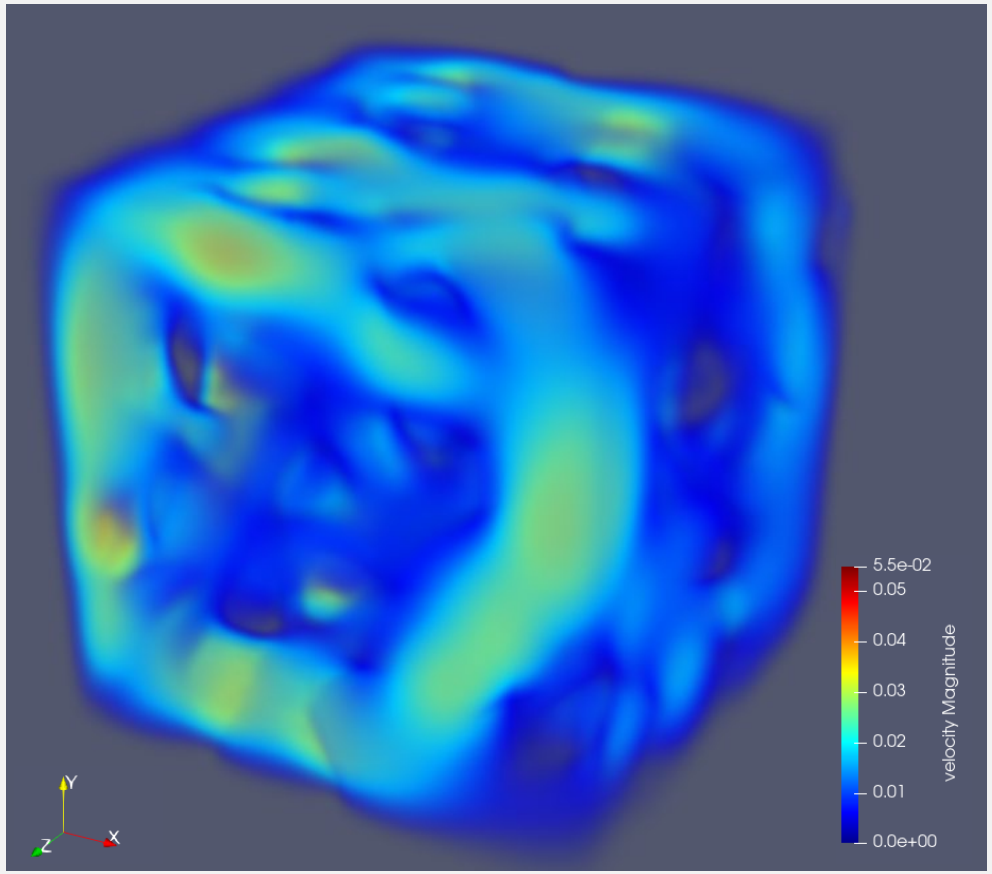
تحلیل نتایج با استفاده از Paraview



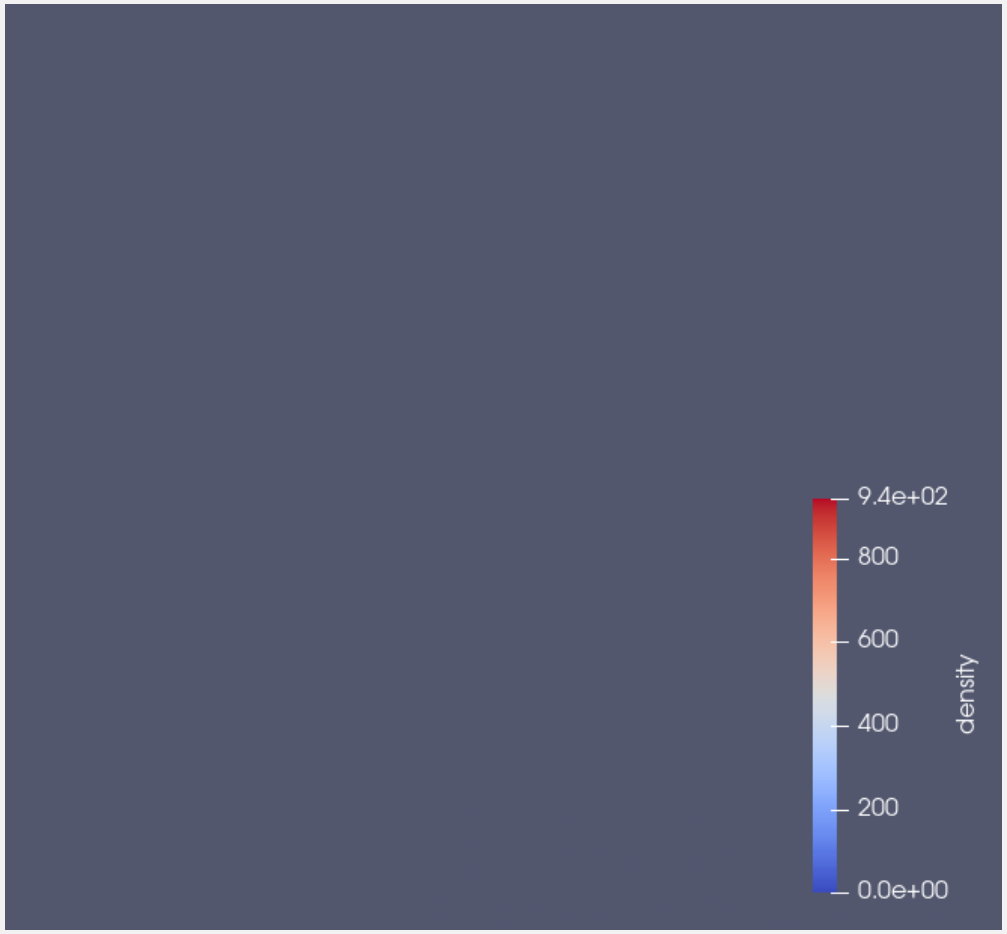


شکل ۸- توزیع اندازه سرعت نهایی

تحلیل نتایج با استفاده از Paraview



شکل ۹- پروفیل اندازه سرعت ۳ بعدی



شکل ۱۰- انیمیشن (گیف) نحوه ذوب PCM