Numerical Thermomechanical Viscous 2D Material Rheology Modelling Enhanced by Marker-in-Cell (MIC) Technique

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Abstract. The rheology of a material especially related to mechanical behaviour is an important characteristic. Rheology has wide applications for example in nanomaterials, engineering design, biology, and in a large scale case in geodynamics study. Rheology relies on several physical equations such as continuity equation, momentum equation, gravity potential, state equation, heat transfer, and advection equation. The equations seem to be simple, however, the application of those equations to a real case is not easy and causes many numerical problems. Marker-in-Cell (MIC) is a technique to solve a numerical rheology modelling problem especially diffusion of sharp gradients during the advection process. The technique successfully simulates the advection process for thermomechanical viscous material for a 2-dimensional case study. The model was initially set up two parts with laterally contrast difference of material characteristics. The lateral density difference of material induced gravitational force and generated circular movement of material. After the simulation was run for the 20-time step, the whole material moved more clockwise circulation. The model started to be stable when all denser material at the lower layer and lower density material at the upper part. The model was fully stable and become at a stationary state at a time more than 100-time steps. The final simulation result showed that the MIC algorithm successfully simulated the conversion process involving the thermomechanical mechanism with diffusion error control and without breaking the contrast density of the material.

Keywords: Material Rheology, 2D Thermomechanical Viscous, Marker-in-Cell

1. Introduction

The word of rheology from Greek word from Greek ἔωρηθένα, "flow" and -λογία, -logia, "study of". It means the study of a material's flow behavior under an applied deformation force. The material study in rheology in a liquid state, soft solids, and solids are deformed or flow in response to applied force or pressure. It is a part of material physics deal with deformation and flow of material in solids and liquids. The characteristic of the material which is obtained from experimental data is known as rheometry[1][2].

The experimental setup is applying to the material to understand the rheology of material indifference conditions for various purposes. Most of the laboratory experimental are qualitative modeling and limited to large or small size even for observation. The numerical modeling has more advantages for setup large scale and observes the whole location including inside the model shape without breaking running the model. However, the laboratory experiment is required for validation of the model. Besides understanding the physics of the material rheology, setup numerical modeling
require skill in mathematics, algorithm, and computer programming for implementing the algorithm[3][4]. Many algorithms are developed for solving various problems with a specific goal [5]. For instance, the frequent equation involves in rheology is the continuity equation. The continuity equation can be express as the Eulerian continuity equation which is written for a fixed point in space (not follow the movement of material)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,$$  \hspace{1cm} (1)

The continuity equation becomes simple for 1D with uniform and constant velocity:

$$\frac{\partial \rho}{\partial t} = -v \left( \frac{\partial \rho}{\partial x} \right)$$ \hspace{1cm} (2)

The one-dimensional advection equations (2) appear trivial, but this is an apparent simplicity. When we try to solve them numerically, we will be strangling with unexpected numerical problems. One of the problems in advection is the systematical numerical diffusion error of sharp gradients during the model simulation. The famous method for solving the partial differential equation is the finite difference method. Discretization of the equation (2) by selecting forward difference for the time and backward difference for spatial, we get computable recursive equation (3) which also call upwind differences[5], see figure 1a.

$$\frac{\Delta \rho}{\Delta t} = -v \frac{\Delta \rho}{\Delta x}$$

$$\rho_{n+1} - \rho_i = -v \frac{\Delta \rho}{\Delta x}$$

$$\rho_{n+1} = \rho_i - \Delta t \frac{\Delta \rho}{\Delta x}$$ \hspace{1cm} (3)

According to the computable recursive equation (3), we can write the stencil of the 1D grid as shown in figure 1a. A regular Eulerian 1D grid with constant spacing between the nodes (\(\Delta x = 1\)) and constant material velocity (\(v = 1\)) is applying. The main numerical computation is updating density directly for each time step. The implication of direct updating the density information will cost the numerical truncation error affect to the disturbing the density information. Figure 2b shows the diffusion pattern of disturbing density information after an 800-time step.

**Figure 1.** (a) Stencil of a 1D grid for Eulerian advection equation for time forward different and spatial backward different. (b) Stencil of a 1D Eulerian grid (blue) -and Lagrangian grid (red) of the marker-in-cell technique for solving the advection equation[7].
To prevent the information of density distribution from numerical truncation error, we have to separate the preserving density distribution and calculated density distribution for numerical calculation. The preserving density is a Lagrangian coordinate system is moving coordinate (moving markers) following the material location. Whereas the calculated density is a Eulerian coordinate system refer to the non-moving space location (static nodes). The marker relatively denser then nodes as shown in figure 1b. The combination Eulerian-Lagrangian coordinate system for solving multi-material problems involving large material distortions is called the Particle-in-Cell method. The PIC method was initiated by Harlow and his co-workers in LANL [8][9]. The PIC method is a dual description method with both Lagrangian and Eulerian features: Lagrangian description to move the mass particles, while Eulerian descriptions to interpolate information between mass particles for Eulerian nodes[5].

As the case above case of study derived from equation (2), the mobile Lagrangian markers are moving constant velocity v and therefore MIC method successfully brings material density information including the gradient and sharp density shape as shown in figure 2b. Every time step the density for the Eulerian nodes is interpolated from markers density found around the nodes.

In the finite-differences method, the initial density value continues to change based on the recursive equation (3). But in the MIC method the initial density value does not change, but what changes is its location. Whereas the density value is the weighting average of the marker density by using a weighted-distance averaging such as the following linear interpolation algorithm.

\[ \rho_i^{t+\Delta t} = \frac{\sum m \rho_m w_m}{\sum m w_m}, \quad \text{where} \quad w_m = 1 - \frac{\Delta x m}{\Delta x}, \quad (4) \]

The pure advection MIC computation is not subjected to any diffusion process since markers always preserve their original density information and only change positions during the simulation. If we want to involve physical processes that would change the density distribution (e.g. thermal diffusion effect) then it can be a separate process with more rigorous calculation as 2D Viscous Thermomechanical discussion below.

2. Method

MIC method is an essential method for stability modelling in Thermomechanical Viscous material rheology modelling[10]. In this study we will discuss the 2D model with solving the momentum equation, adiabatic and shear heating, solving temperature and gravity. The Navier Stokes equation for slow-motion (ignoring the acceleration) and viscous incompressible flow in the uniform gravity field

\[ \frac{\partial \sigma_{ij}}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} - \frac{\partial p}{\partial x_i} = -\rho g_i \quad (5) \]

where the stress tensor related to strain tensor and viscosity
\[ \sigma_{ij} = 2\eta\ddot{\sigma}_{ij} = 2\eta \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \] (6)

and conservation of mass is controlled by the continuity equation

\[ \sum \frac{\partial v_i}{\partial x_i} = 0 \] (7)

The computation of temperature change in continuum media related to heat generation, advection, and conduction.

\[ \rho C_P \frac{dT}{dt} = \sum \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} \right) + H_j \] (8)

where \( k \ (\text{W/(m K)}) \) is the thermal conductivity, \( \rho \) is density \((\text{kg/m}^3)\); \( C_P \) is heat capacity at constant pressure \((\text{isobaric heat capacity, J/(kg K)})\); \( H_j \) is volumetric heat production/consumption \((\text{W/m}^3)\).

The total derivative of Temperature can be expressed with the chain rule

\[ \frac{dT}{dt} = \frac{\partial T}{\partial t} + \sum_i v_i \frac{\partial T}{\partial x_i} \] (9)

The staggered FD difference method is applicable for solving the above governing equation. The first step is to select a suitable discretization scheme and apply them to the staggered grid[11]. Following the discretization equation, we get the recursive equation which can be solved implicitly or explicitly. We select an implicit method for acceleration of computation while code running under Matlab. Besides selecting suitable discretization schemes, the adjustment of the associate time step is a critical factor for the stability of simulation. The whole step of numerical thermomechanical viscous 2D enhances by the MIC Technique as shown in figure 3.

According to flowchart figure 3, the first step is to interpolate physical properties from Lagrangian markers to Eulerian nodes. Modelling large scale material, such as geodynamics study, is required to determine self-gravity of the earth material itself by solving the Poisson equations in step 2. The
Navierstokes equation for calculated momentum and continuity equation on a staggered grid is done in step 3. The updated time step for marker movement based on maximum velocity at step 4. Shear and adiabatic heating terms are calculated at step 5 for the Eulerian nodes. The other updated time step for temperature equation at step 6 for solving temperature equation at step 7 and following the re-interpolate temperature change to makers point for step 8. Last step 9 is advected all markers point according to the calculated velocity field which produces in stem 2. After getting the values of the markers the step is to return to step 1 for interpolating the values of the nodes from markers values.

3. Results and Discussion

The modelling of numerical thermomechanical viscous 2D is applying to the earth scale or namely geodynamics study. The model was initially set up two parts with laterally contrast difference of material characteristics. The left part material lighter and colder the right part of the material. The left part has properties with viscosity $\eta=10^{20}$ Pa s, density $\rho=3000\text{kg/m}^3$, thermal conductivity $k=1\text{W/m/K}$, thermal expansion $\alpha=3\cdot10^5$, heat capacity $C_p=1000$, and temperature $T=1000\text{K}$. The right part has parameter $\eta=10^{22}\text{Pa s}$, $\rho=3200\text{kg/m}^3$, $k=10\text{W/m/K}$, $\alpha=3\cdot10^5$, $C_p=1000$, and $T=1500\text{K}$.

![Figure 4. The evolution of mass density during the simulation for different time steps.](image)

The initial condition model of the density and temperature is shown in Figures 4a and 5a sequentially. The heaver material with the gravitational force pushes the lighter material to leave at the lower side as shown in figure 4b and 4c. After pushing the lighter material, at step 40 and 60 the
heaver material start fill lower side. Finally, at step 100 as shown in figure 4f, the model becomes a stationer condition in which all heaver material stays at lower and lighter at upper. He shape interface remains to exist without diffusion between them because of advantages applying the MIC method. However, the code is still not able to overcome the problem of boundary problems were in the lower left and right sides of the material still attached to the boundary as shown in Figures 4d and 4e. However, the boundary edge problem look disappears at time step 100 as shown in figure 4f.

![Figure 5](image_url)

Figure 5. The evolution of temperature distribution during the simulation for different time steps.

The initial condition as shown in figure 5a the right part of the material temperature is 1500K which hotter than the left part of the material temperature 1000K. During the process, the shear heating and adiabatic heating are contributed to the temperature. It appears the slightly change temperature at the left and right part of the material as shown in Figures 5b and 4c. In contrast with density evolution, the temperature distribution does not keep the sharp interface because of the computation of temperature distribution involving the thermal conduction process as shown in Figures 5d and 5e. Finally, at step 100, the hotter part associated with heaver material which fills the lower side and vice versa. In the initial condition, the coldest temperature is 1000K, but after the simulation the coldest temperature becomes 800K. The decreasing temperature or negative heat becomes from the adiabatic head process. Initially, the material at the left bottom corner fills compression and after it moves up the pressure decrease and produces negative heat exchange from an adiabatic heat process. The opposite happened, the material under increasing pressure will go to the lower side will produce positive heat exchange and increase the temperature.
The changing of temperature is mainly affected by shear heating and adiabatic heating as shown in Figure 6 and Figure 7 respectively. The shear heating is calculated from stress tensor for viscous deformation. Shear heating is always a positive value as shown in Figure 6. Because the shear heating comes from the shear deformation and stress thus it will work at the beginning of the simulation (Figure 6a) which dynamically active and become disappear when dynamically not active as shown in Figure 6c.

![Figure 6. Distribution of shear heating for time step 1, 20, dan 60](image)

The model setting, we applying to the algorithm has decreased and increased pressure changing during a simulation at the left and right parts respectively. According to the adiabatic heat process, the positive changing pressure will contribute positive heat, and vice versa as shown in figure 7a. At the initial step, the positive and negative adiabatic heat is symmetry. When the model going to the stationer condition, the changing pressure becomes slow and adiabatic heat becomes less as shown in figure 7c.

4. Conclusions
The advantage of the MIC method is that it combines two systems, both Eulerian and Lagrangian, seen from the side of a stationary space or a stationary material. The weakness of the finite difference
method is that the material is regarded as Eulerian so that computational errors in each calculation will have an impact on the value of the material itself in the form of diffusion and even increased fluctuation.

The simulation result shows that the MIC method successfully simulate the 2D thermomechanical viscous material and keep the contrast density interface between denser and lighter density. In this simulation, the thermodynamics process is contributed from shear heat and adiabatic heat. The adiabatic process will increase the temperature from the maximum of 1200K to 2500K. In other parts, the adiabatic heat will decrease temperature from the minimum 1000K to 800K.

The successfulness of this simulation which incorporates with MIC method is a step to geodynamics study[13] at a real earth scale for understanding tectonic activities such as Sumatran Fault[14][15] or for analogue scale such as for numerical modelling of sandbox simulation[16].

5. References
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Acknowledgments
This work is financially full supported by Hibah Laboratorium, Universitas Syiah Kuala contract No. 1641/UN11/SPK/PNBP/2019.