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The AMR technique for simulating dissolution processes with a diffuse interface model

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1. Introduction

Dissolution of solids or porous media, for example underground cavities, poses many practical engineering problems, which may be better understood through numerical simulations. There are mainly two ways for such simulations: first, a direct treatment of the moving interface, for instance using an ALE technique ; second, using a diffuse interface model (referred to as DIM in the paper sequel) to smooth the interface with continuous quantities . Recently, Luo et al. [3] presented a Darcy-scale local non-equilibrium diffuse interface model (DIM) obtained with the help of a volume averaging theory [1]. Numerical computations over various dissolution problems showed that it is more convenient and efficient to use a DIM model rather than an ALE technique, as the DIM model provides global control equations such that the 'artificial interfaces' can move freely among different meshes without the need for re-meshing.

Since there are sharp fronts in this problem, the further advantage of the DIM model is that it enables us to introduce adaptive mesh refinement (AMR) technique to this problem in a relative straightforward manner. The AMR technique [2] improves the computational efficiency by using an adaptive mesh system instead of a fixed fine grid. The grid system is automatically generated according to pre-defined refinement criteria, with fine grids near the fronts and coarse grids where the quantities vary slowly. In this paper, the AMR technique is applied to the simulation of solid/liquid dissolution problems with a DIM model. Besides algorithmic difficulties, the major problem is the design of accurate interpolation schemes between the different grids. For instance, the pressure interpolation at the interface must take into account gravity effects. Pressure values are therefore predicted by integration over the grid, based on the used momentum equation (Darcy's law for a porous medium problem). In the following sections, we present the control equations of the DIM model, the AMR algorithm, and numerical examples showing its efficiency and accuracy.

2. Mathematical model (DIM)

According to [3], the Darcy-scale diffuse interface model for Solid/Liquid dissolution problems in a binary system includes the following 3 balance equations (1)-(3): the mass balance for the σ -phase, the mass balance for the β -phase, the mass balance for species A.

$$\rho_\sigma \frac{\partial \varepsilon_\beta}{\partial t} = \rho_\beta^* \alpha (\omega_{eq} - \Omega_{A\beta}) \quad (1)$$

$$\frac{\partial \varepsilon_\beta \rho_\beta^*}{\partial t} + \nabla \cdot (\rho_\beta^* \mathbf{V}_\beta) = \rho_\beta^* \alpha (\omega_{eq} - \Omega_{A\beta}) \quad (2)$$

$$\varepsilon_\beta \rho_\beta^* \frac{\partial \Omega_{A\beta}}{\partial t} + \rho_\beta^* \mathbf{V}_\beta \cdot \nabla \Omega_{A\beta} = \nabla \cdot (\varepsilon_\beta \rho_\beta^* \mathbf{D}_{A\beta}^* \cdot \nabla \Omega_{A\beta}) + \rho_\beta^* \alpha (1 - \Omega_{A\beta}) (\omega_{eq} - \Omega_{A\beta}) \quad (3)$$

where ε_β is the volume fraction of β -phase, $\Omega_{A\beta}$ is the mass fraction of species A in the β -phase, ω_{eq} is the equilibrium mass fraction at the $\sigma - \beta$ interface, α is the mass exchange term, ρ_β^* and ρ_σ are

respectively the β -phase and σ -phase densities, and $D_{A\beta}^*$ is the effective diffusion tensor for species A. Velocity, V_β , is obtained from Darcy's Law

$$V_\beta = -\frac{K}{\mu} (\nabla P_\beta - \rho_\beta \mathbf{g}) \quad (4)$$

with K the permeability, μ the viscosity and \mathbf{g} the gravity vector. α , $D_{A\beta}^*$, and K are functions of ε_β .

3. AMR algorithm

After discretizing the control equations in the previous section, one could follow the steps below to implement the AMR algorithm: (1) Re-gridding (the grid system, which is composed of the active meshes of the different levels, is determined according to a refinement criterion, for instance maximum values of the deviation or gradient of certain front-indicating variables inside a coarse grid, e.g., ε_β , $\Omega_{A\beta}$, etc...), (2) Refining (interpolation process to obtain the values inside a fine mesh from coarse meshes), (3) Coarsening (assignment of values for a coarse grid using some averaging technique), (4) full-domain solution, (5) iteration of the above steps to reach final simulation time.

As an illustration of the AMR algorithm, we show Fig. 1 the dissolution of a NaCl block localized at the center top of a tube (tube dimensions: $20\text{mm} \times 10\text{mm} \times 5\text{mm}$). Fresh water is injected from the left boundary with a constant velocity ($Pe=10$) and flows out at the right boundary with a constant pressure at the top. The four lateral boundaries are impervious. The used spatial fine meshes are $64 \times 32 \times 16=32768$. Fig 1 shows the computational results at the central-section using both the AMR and fine-grid numerical models. It is shown that the heavy liquid tends to spread downward due to the gravity effects. The computational times were 1h50min and 35h20min respectively under the same CPU. The total grid numbers used by AMR algorithm range from 3678 at $t=0\text{s}$ to 10501 at $t=2000\text{s}$.

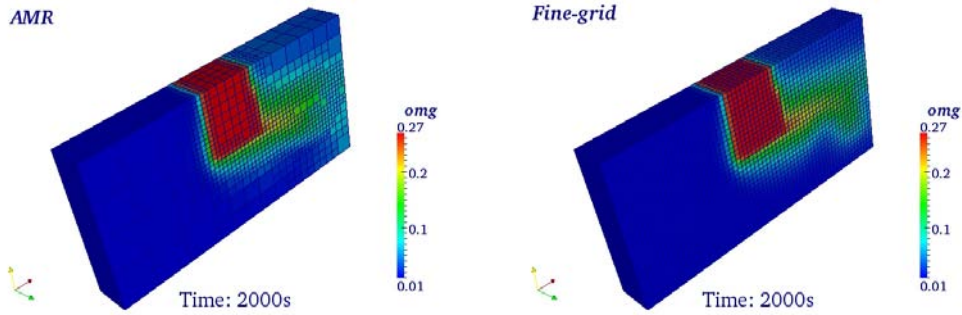


Figure 1: Comparison of $\Omega_{A\beta}$ at $t=2000\text{s}$ using AMR and Fine-grid.

4. Conclusions and perspectives

The performed numerical tests showed that the AMR results and the fine-grid results are in very good agreement, while the computational efficiency obtains a significant enhancement with the AMR technique, as expected. In future work, we will focus on the simulations for large (reservoir) scale. As a consequence, larger mesh numbers will be adopted, which will require a parallelized implementation.

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