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COMPARISON BETWEEN 3D FEM AND LBM FOR NUMERICAL SIMULATION OF PHASE CHANGE MATERIALS

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Abstract. The purpose of this work is to accurately assess the effectiveness of parallel finite element algorithms (FEM) and Lattice Boltzmann method (LBM) in the numerical simulation of phase change materials (PCM). A precise comparison between the two methods is presented, in order to give guidelines for the simulation of complex 3D systems involving PCM and natural convection.

Recent works [1, 2] have proven the capability of the FEM to accurately simulate liquid-solid phase change systems. The numerical method is based on a monolithic formulation with implicit interface capturing through the isoline of the fusion temperature. An enthalpy-porosity model has been derived and implemented. The parallelization is based on a domain decomposition approach, with additive Schwarz method for solving linear systems.

The LBM approach has been recently developed to further reduce the computational time. The model used for natural convection is directly applicable for LBM. An extensive comparison is then possible, in terms of accuracy, stability, ability to handle complex geometries and total execution time.

1 Introduction

Accurate and efficient numerical simulations of solid-liquid phase-change problems are needed in many practical applications such as latent thermal energy storage (LTES) systems which are based on phase-change materials (PCM). The fundamental processes are the melting and the solidification of PCM, which are difficult to simulate with accurate physical models. Buoyancy forces in the liquid (melted) phase generate a significant convective flow and thus deform the liquid-solid interface, as illustrated in Fig. 1a.

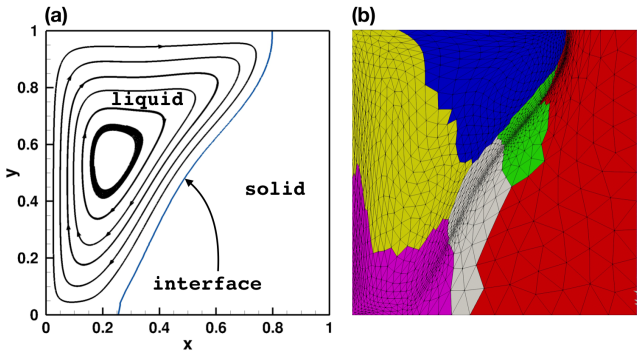

Figure 1: Sketch of the liquid-solid phase change problem considered in this paper. (a) Illustration of the melting, with convection in the liquid phase (streamlines of the velocity field) and a bent interface separating the two phases. (b) Illustration of the domain-decomposition used for numerical simulations. Note the adapted mesh, especially around the liquid-solid interface.

The main challenges for the numerical simulation of PCM are the resolution of all relevant scales of the liquid region and the accurate capture of the solid-liquid interface.

The basic configuration considered in this contribution is inspired by the experimental study of Okada [3]. It consists of a square cavity filled with an octadecane paraffin, with the following parameters: $Ra = 3.27\ 10^5$, $Pr = 56.2$ and $Ste = 0.045$.

2 Navier-Stokes-Boussinesq equations and enthalpy-porosity model

Previous works suggested a monolithic formulation of the problem, based on the Navier-Stokes equations with Boussinesq approximation for buoyancy effects, with a Carman-Kozeny penalty term to set the solid velocity to 0, see [1, 2]. These equations are coupled with an enthalpy model that avoids to track the interface. The dimensionless set of equations is:

$$\nabla \cdot \vec{u} = 0, \tag{1}$$

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} + \nabla p - \frac{1}{Re}\nabla^2 \vec{u} - f_B(\theta)\,\vec{e}_y - A_{mushy}(\theta)\vec{u} = 0, \tag{2}$$

$$\frac{\partial (C\theta)}{\partial t} + \nabla \cdot (C\theta \vec{u}) - \nabla \cdot \left(\frac{K}{RePr} \nabla \theta \right) + \frac{\partial (CS)}{\partial t} = 0. \tag{3}$$

$\vec{u}$, p and θ are the dimensionless velocity, pressure and temperature to be solved. The relevant dimensionless parameters are the Reynolds number Re, the Prandtl number Pr and the Raleigh number Ra. The solid-liquid interface is captured as the 0 iso-line of θ. K, C are the (possibly discontinuous) conductivity and specific heat (depending on θ). The phase changing process is taken into account through S, which is 0 in the solid region and $1/Ste$ in the liquid region, with Ste the Stefan number. Finally, f_B is the Boussinesq buoyancy force, proportional to θ. $A_{mushy}(\theta)$ is a penalty term which relaxes the velocity to 0 in the solid region.

3 Finite element approach

In our FEM approach, the coupled system (1)-(2)-(3) is integrated in time using a second-order implicit Gear scheme. The resulting equations are then solved using a Newton method. The space discretization relies on the Taylor-Hood triangulate finite element, i.e. P_1 for the pressure and P_2 for the velocity. Temperature can be discretized using P_1 or P_2 finite elements. All the discontinuous coefficients (K, C, S...) are regularized through an intermediate artificial mushy region.

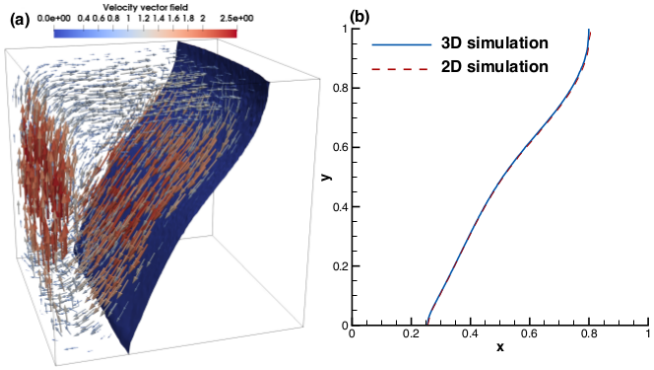

Figure 2: Melting of a cubic PCM [3]. Configuration at $t = 80.1$, computed using 224 MPI processes with P2 for the temperature. (a) 3D velocity vectors and isosurface $T = 0$ representing the liquid-solid interface. (b) Position of the interface in the central plane ($y = 0.5$): comparison between 2D and 3D simulations (both using P_2 finite elements for the temperature). Execution time: 8h on 224 MPI processes.

The algorithm has been implemented using the open-source software FreeFem++ [4]. An adaptive refinement is performed at each time step, in order to accurately capture the physical phenomena with a reasonable computational time. One of the main consuming parts of the algorithm is the resolution of resulting linear systems. We rely on the parallel framework `ffddm` [5]; linear systems are solved using a domain decomposition approach, with a parallel GMRES algorithm and a Restricted Additive Schwarz preconditioner.

4 Lattice Boltzmann method for natural convection

FEM has been proven to be reliable, accurate and affordable for 3D systems. Nonetheless, the parallel efficiency of LBM may increase the ability of simulating complex cases of PCM. In order to achieve this goal, an extensive and accurate comparison of LBM with FEM is necessary. Before tackling the simulation of a PCM, the first mandatory step is to validate LBM on natural convection.

In this case, the system of equations (1)-(2)-(3) with $A_{mushy} \equiv 0$ and $S \equiv 0$ can be directly casted in a LBM setting. $\vec{u}$ is recovered as the first order moment of a distribution function f_i, while θ is the zeroth order moment of a second distribution function g_i. A D2Q9 (in 2D) or D3Q19 (in 3D) stencil is used. The Boussinesq term is introduced as a source term in the collision step for f_i. The two-ways coupling is completed by using $\vec{u}$

in the first order moment of the equilibrium distribution g_i^{eq}.

FEM and LBM are compared using the diffusive scale for LBM (or acoustic scale at high Re). The focus is on the resources (computational time, computational resources, resolution) needed to reach a desired accuracy, and relies on the links between the relaxation rates of the LBM scheme and the relevant dimensionless parameters. The parallelization is handled through the multiphysics framework waLBerla [6].

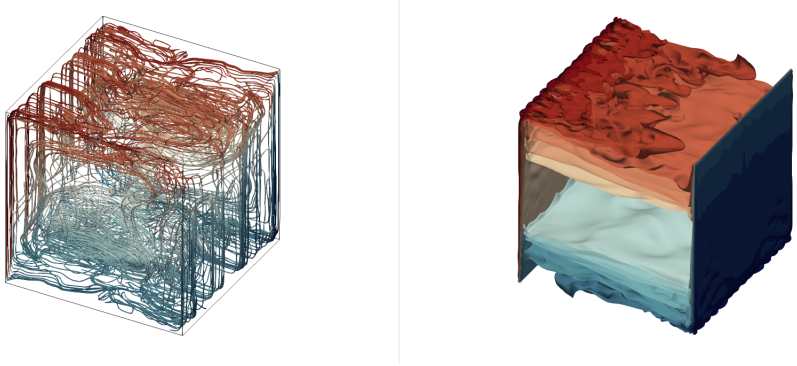

Figure 3: Natural convection in a differentially heated cavity. Unsteady field at $Ra = 10^9$. Computation using LBM approach on a 250^3 lattice with the multiphysics framework waLBerla [6]. (left) Streamlines of the velocity field. (right) Isocontours of θ.

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