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# Parallel finite-element codes for the simulation of two-dimensional and three-dimensional solid-liquid phase-change systems with natural convection

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## Abstract

We present and distribute a FreeFem++ Toolbox for the parallel computing of two- or three-dimensional liquid-solid phase-change systems involving natural convection. FreeFem++ ([www.freefem.org](http://www.freefem.org)) is a free finite-element software available for all existing operating systems. We use the recent library `ffddm` that makes available in FreeFem++ state-of-the-art scalable Schwarz domain decomposition methods (DDM). The single domain approach used in our previous contribution [A. Rakotonrandisa, G. Sadaka, I. Danaila, A finite-element Toolbox for the simulation of solid-liquid phase-change systems with natural convection, Computer Physics Communications, DOI 10.1016/j.cpc.2020.107188, 2020] is adapted for the use of the DDM method. As a result, the computational time is considerably reduced for 2D configurations and furthermore 3D problems become affordable. The numerical method is based on an enthalpy-porosity model. The same set of equations is solved in both liquid and solid phases: the incompressible Navier-Stokes equations with Boussinesq approximation for thermal effects. A Carman-Kozeny-type penalty term is added to the momentum equations to bring progressively the velocity to zero into the solid. Model equations are discretized using Galerkin triangular or tetrahedral finite elements. The coupled system of equations is integrated in time using a second-order Gear implicit scheme. The resulting discrete equations are solved using a Newton algorithm. The DDM approach is based on an overlapping Schwarz method. The mesh is first split in subdomains using `Scotch` or `Metis` libraries. The final linear system is then solved in parallel using a GMRES Krylov method, with a Restricted Additive Schwarz (RAS) preconditioner. The mesh is adapted during the computation using metrics control. The 3D-mesh adaptivity uses the `mmg` ([www.mmgtools.org](http://www.mmgtools.org)) open source library. Parallel 2D and 3D computations of benchmark cases of increasing difficulty are presented: natural convection of air, natural convection of water, melting or solidification of a phase-change material, and, finally, a water freezing case. For each case, careful validations are provided and the performance of the code is assessed. The robustness of the Toolbox in 3D is also demonstrated by adapting the number of processors to the number of tetrahedra, which can considerably vary after the mesh adaptation.

**Keywords:** phase change, PCM, parallel computing, finite element, 3D melting, 3D solidification, mesh adaptivity, Navier-Stokes-Boussinesq, FreeFem.

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## Program summary

*Program Title:* PCM\_Toolbox\_DDM\_2D and PCM\_Toolbox\_DDM\_3D

*Catalogue identifier:*

*Program summary URL:*

*Program obtainable from:*

*Licensing provisions:* Apache License, 2.0 (Apache-2.0)

*No. of lines in distributed program, including test data, etc.:* 6820 (2D), 6382 (3D)

*No. of bytes in distributed program, including test data, etc.:* 3.6 Mo (2D and 3D)

*Distribution format:* .tar.gz

*Programming language:* FreeFem++ ([www.freefem.org](http://www.freefem.org)), mmg ([www.mmgtools.org](http://www.mmgtools.org))

*Computer:* PC, Mac, Super-computer.

*Operating system:* Mac OS, Linux.

*Nature of problem:* The software is scoped to parallel computations of 2D or 3D configurations of liquid-solid phase-change problems with convection in the liquid phase. Natural convection, melting and solidification processes are illustrated in the paper. The software can be easily modified to take into account different related physical models.

*Solution method:* We use a single domain approach, solving the incompressible Navier-Stokes equations with Boussinesq approximation in both liquid and solid phases. A Carman-Kozeny-type penalty term is added to the momentum equations to bring the velocity to zero into the solid phase. An enthalpy model is used in the energy equation to take into account the phase change. Discontinuous variables (latent heat, material properties) are regularized through an intermediate (mushy) region. Space discretization is based on Galerkin triangular/tetrahedral finite elements. A second order Gear implicit scheme is used for the time integration of the coupled system of equations. The resulting discrete equations are solved using a Newton algorithm. Piecewise quadratic (P2) finite-elements are used for the velocity and piecewise linear (P1) for the pressure. For the temperature both P2 or P1 discretization are possible. The mesh is first split in subdomains using *Scotch* or *Metis* libraries, which are interfaced with FreeFem++. Then, a Schwarz domain decomposition method is used through the FreeFem++ library *ffddm*. The final linear system is solved in parallel using a GMRES Krylov method, with a Restricted Additive Schwarz (RAS) preconditioner. Mesh adaptivity using metrics control makes possible the optimization of the distribution of mesh elements. For 3D case, the *mmg* open source library is used to adapt the mesh.

*Running time:* For 2D cases: from seconds for the natural convection case to minutes or hours for PCM melting or solidification. Using only 6 MPI processes (cores or threads) on a personal computer, the parallel computation can bring a speed-up of 1.3 to 3.97, depending on the difficulty of the problem (see Table 1). For 3D cases, the running time depends on the size of the problem and the number of processes: from 55 minutes for the unsteady natural convection of air with  $Ra=1e4$  using 6 MPI processes to 1 day and 16h for the water freezing case using 224 MPI processes).

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## 1. Introduction

Accurate and efficient numerical simulations of solid-liquid phase-change problems are needed in many practical applications. Metal casting, Earth’s mantle formation and food freezing are well explored topics in this area. Recently, a great deal of attention was paid to the simulation of latent thermal energy storage (LTES) systems based on phase-change materials (PCM). Such devices are used for thermal energy storage (*e. g.* for solar power generation) or passive temperature control (*e. g.* for modern portable electronics) devices. For a review of various applications of PCMs, see recent reviews by [Agyenim et al. \(2010\)](#) and [Kalnæs and Jelle \(2015\)](#).

In all these problems, melting and solidification are fundamental processes that are difficult to simulate if accurate physical models are used. A sketch of the melting problem is shown in Fig. 1a. Buoyancy forces in the liquid (melted) phase generate a significant convective flow and thus deform the liquid-solid interface. Solidification is a similar process, but with a slower evolution and the possibility to generate several solid-liquid interfaces propagating simultaneously. Resolving all the scales in the liquid region using the Navier-Stokes-Boussinesq equations and accurately capturing the solid-liquid interfaces are the main challenges for a numerical system addressing these problems. In our recent contribution ([Rakotonrandisa et al., 2020](#)) we presented an in-depth review of physical and numerical models dealing with solid-liquid phase-change problems with convection. The approach retained in [Rakotonrandisa et al. \(2020\)](#) was based on the widely used enthalpy-porosity single-domain model, also called the fixed-domain model ([Brent et al., 1988](#)). In the present contribution, we extend this model to parallel computations using domain-decomposition (DD) methods, as illustrated in Fig. 1b.

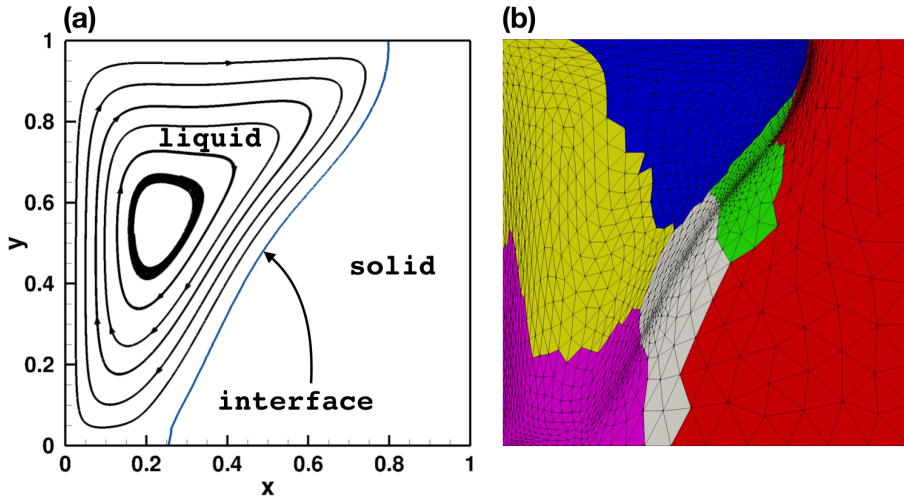


Figure 1: Sketch of the liquid-solid phase change problem considered in this paper. (a) Illustration of the melting, with convection in the liquid phase (streamlines of the velocity field) and a bent interface separating the two phases. (b) Illustration of the domain-decomposition used in present numerical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



The main advantage of the enthalpy-porosity single-domain model is that the solid-liquid interface is not explicitly tracked. The position of the interface is computed a posteriori by post-processing the obtained temperature field  $T$  (in Fig. 1b, the interface is represented by the iso-contour  $T = 0$ ). This makes the model appropriate for the use of domain decomposition models and parallel computing. Front tracking or front fixing deforming-grid methods (*e.g.* Stella and Giorgi (2004); Tenchev et al. (2005)) would obviously introduce an algorithmic complexity penalizing parallel computing performances. Note that a different category of models was recently suggested in the literature, based on the Lattice Boltzmann Method (Luo et al., 2015; Gong et al., 2015). Such methods based on non-deterministic models are also well adapted for parallel computations. For a comprehensive review of models for phase-change problems with convection, see Kowalewski and Gobin (2004).

Another advantage of the enthalpy-porosity single-domain model is that the same Navier-Stokes-Boussinesq (NSB) system of equations is solved in both liquid and solid phases. Keeping in mind that the NSB equations are pertinent only in the liquid phase, their extension into the solid phase has to preserve the single-domain formulation. This is generally obtained by introducing in the momentum equations a penalization source term that brings the velocity to zero in the solid and do not affect the liquid. One of the most used expression of the penalization source term follows the Carman-Kozeny model for the permeability of a porous medium (Hannoun et al., 2003, 2005; Belhamadia et al., 2012), but other mathematically equivalent expressions were suggested (Angot et al., 1999; Favier et al., 2019). The energy equation is also modified to be valid in both phases using an enthalpy (temperature-transform) model introducing a regularized latent-heat term. Different formulations and implementations of the enthalpy-porosity model are presented in Kowalewski and Rebow (1999); Giorgi et al. (2000); Stella and Giorgi (2004).

The enthalpy-porosity single-domain model was implemented in Rakotondrandisa et al. (2020) using an adaptive finite-element method. The corresponding Toolbox for FreeFem++ (a free software under LGPL license)<sup>1</sup> was distributed with that paper. Extensive validation tests proved the ability of the numerical system to deal with melting and/or solidification problems of increasing difficulty. Problems with complex shapes of the computational domain or with multiple solid-liquid interfaces were successfully computed. The mesh adaptivity capabilities of the method ensured reasonable computational costs, since the mesh was refined only in the zones of large gradients of variables (artificial mushy region, boundary layers) and coarsened in the solid zones with low gradients. However, some cases, such as the water freezing or the melting-solidification cycle of a PCM, demanded hours or days on a personal computer to simulate physically pertinent time evolution.

Consequently, the main purpose of the present contribution is to extend the single-domain model of Rakotondrandisa et al. (2020) to parallel computing using domain-decomposition methods. For two-dimensional (2D) configurations, the new Toolbox can be used to reduce the computational time on personal computers with multi-core processors. Using high-performance computing (HPC) facilities, the Toolbox is well adapted to simulate 3D configuration of phase-change problems. It is important to note that very few 3D simulations with accurate capturing (mesh adaptivity) of the solid-liquid

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<sup>1</sup>FreeFem++ for different OS can be downloaded from <http://www.freefem.org/>.

interface were reported in this research area. Adaptive FE methods were suggested for classical two-phase Stefan problem in 2D and 3D (Belhamadia et al., 2004a,b). For phase-change systems with convection, adaptivity strategies were suggested and tested only for 2D problems (Belhamadia et al., 2012; Danaila et al., 2014; Belhamadia et al., 2019). An attempt to adapt the mesh in 3D simulations for melting phenomena was undertaken by Zimmerman and Kowalski (2018) using an AMR (Adaptive Mesh Refinement) technique based on a dual-weighted residual method. The method displayed a major drawback, since the mesh was refined during the advancement of the liquid-solid front, but never coarsened behind. As a consequence, only a very preliminary coarse grid simulation of the 3D melting was possible using the AMR method. We show in this contribution that our new method using domain decomposition and mesh adaptivity is perfectly suited to the accurately simulate 3D melting or solidification, in simple or complex-shape geometries.

The new parallel Toolbox is based on a single-domain enthalpy-porosity model for solid-liquid phase change problems with convection. For the energy conservation equation, a temperature-based formulation takes into account the latent heat by introducing a discontinuous source term. For the mass and momentum conservation equations, we solve in the entire domain the incompressible Navier-Stokes equations with Boussinesq approximation for buoyancy effects. To bring the velocity to zero in the solid phase, we introduce in the momentum equation a penalty term following the Carman-Kozeny model. The coupled system of momentum and energy equations is integrated in time using a second-order implicit Gear scheme. The resulting discretized equations are solved using a Newton method (Danaila et al., 2014). For the space discretization we use Taylor-Hood triangular finite elements, *i. e.*  $P_2$  for the velocity and temperature and  $P_1$  for the pressure. Temperature is discretized using  $P_2$  or  $P_1$  finite elements. Discontinuous variables (latent heat, thermal diffusivity, etc) at the solid-liquid interface are regularized through an intermediate artificial mushy region.

To enable parallel computing, we use the `ffddm` framework (Tournier et al., 2019), which is a set of FreeFem++ scripts implementing Schwarz domain-decomposition methods for the efficient solution of linear systems. The mesh is first split into subdomains using an automatic graph partitioning library, such as `Scotch` (Pellegrini and Roman, 1996) or `Metis` (Karypis and Kumar, 1998). Each subdomain is assigned to a MPI process. The linear systems are assembled and solved in parallel using a GMRES Krylov method with a Restricted Additive Schwarz (RAS) preconditioner (Dolean et al., 2015). Mesh adaptivity using metrics control makes possible the optimization of the distribution of mesh elements. For 3D cases, the mesh adaptivity is more involved: the metric is first computed using `mshmet`, which is a module inside FreeFem++ , and then used within the `mmg`<sup>2</sup> remeshing tool (Dapogny et al., 2014) to generate the adapted new mesh.

The paper is organized as follows. Section 2 introduces the enthalpy-porosity single domain model based on the Navier-Stokes-Boussinesq equations. Section 3 presents the adaptive finite-element numerical method using a Newton algorithm for the non-linear discretized equations. We also discuss in this section the Schwarz domain decomposition method used for parallel computations and the algorithm for mesh adaptivity (with emphasis on the 3D adaptivity technique). A description of the programs contained in the provided 2D and 3D toolboxes is given in Section 4. The next two sections are devoted to

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<sup>2</sup><http://www.mmgtools.org/>.

extensive numerical validations of the method for 2D benchmarks (§5) and corresponding 3D configurations (§6). The robustness of the algorithm is demonstrated by comparing our results with reference data available in the literature. The capabilities of the Toolbox to deal with complex geometries is also illustrated. The main features of the software and possible extensions are summarized in Section 7.

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

We consider a solid-liquid system placed in a 2D or 3D domain  $\Omega$ . The dimensionless system of equations to be solved in both liquid and solid regions is based on the incompressible Navier-Stokes equations, with Boussinesq approximation for buoyancy effects, and a temperature transforming model for the energy equation (Voller et al., 1987; Cao et al., 1989):

$$\nabla \cdot \mathbf{u} = 0, \quad (1)$$

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

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

Non-dimensional space, velocity, temperature and time variables in (1)-(3) were obtained from physical ones after applying the following scaling:

$$\mathbf{x} \rightarrow \frac{\mathbf{x}}{H}, \quad \mathbf{u} \rightarrow \frac{\mathbf{u}}{V_{ref}}, \quad \theta = \frac{T - T_{ref}}{\delta T}, \quad t \rightarrow \frac{V_{ref}}{H} t, \quad (4)$$

where  $H$  is the reference length (usually the height of the cavity when a rectangular domain is considered) and  $V_{ref}$  a reference velocity that will be defined differently for melting and solidification problems.  $T_{ref}$  is the reference temperature and in most cases  $T_{ref} = T_f$  (the temperature of fusion), unless otherwise specified. Consequently, the non-dimensional temperature of fusion is set to  $\theta_f = 0$ . Temperature difference  $\delta T$  defines a temperature scale, that will be set differently for melting and solidification cases.

The linearized Boussinesq buoyancy force ( $f_B$ ), the Reynolds ( $Re$ ) and Prandtl ( $Pr$ ) numbers are defined as (subscripts  $s$  and  $l$  refer to the solid and the liquid phases, respectively):

$$f_B(\theta) = \frac{Ra}{PrRe^2} \theta, \quad Re = \frac{\rho V_{ref} H}{\mu_l} = \frac{V_{ref} H}{\nu_l}, \quad Pr = \frac{\nu_l}{\alpha_l}, \quad (5)$$

with  $\nu$  the kinematic viscosity and  $\alpha = k/(\rho c)$  the thermal diffusivity. In the expression of  $f_B$ , the Rayleigh number of the flow is defined as:

$$Ra = \frac{g\beta H^3 \delta T}{\nu_l \alpha_l}, \quad (6)$$

with  $\beta$  the thermal expansion coefficient and  $g$  the gravitational acceleration.

If previous non-dimensional numbers are pertinent only in the liquid phase, the non-dimensional conductivity  $K$  and specific heat  $C$  are defined in both phases:

$$K(\theta) = \frac{k}{k_l} = \begin{cases} 1, & \theta \geq \theta_f, \\ k_s/k_l, & \theta < \theta_f, \end{cases}, \quad C(\theta) = \frac{c}{c_l} = \begin{cases} 1, & \theta \geq \theta_f, \\ c_s/c_l, & \theta < \theta_f. \end{cases} \quad (7)$$

The non-dimensional function  $S = s/s_l$  in the energy equation (3) takes a similar non-dimensional form:

$$S(\theta) = \frac{s}{s_l} = \begin{cases} \frac{h_{sl}/c_l}{\delta T} = \frac{1}{Ste}, & \theta \geq \theta_f, \\ 0, & \theta < \theta_f, \end{cases} \quad (8)$$

with  $h_{sl}$  the latent heat of fusion and  $Ste$  the Stefan number.

Discontinuous step-functions defined in (7) and (8) are replaced by continuous and differentiable hyperbolic-tangent functions, generically defined for all  $\theta$  by the formula (Danaila et al., 2014):

$$F(\theta; a_s, \theta_s, R_s) = f_l + \frac{f_s - f_l}{2} \left\{ 1 + \tanh \left( a_s \left( \frac{\theta_s - \theta}{R_s} \right) \right) \right\}, \quad (9)$$

where  $f_l, f_s$  are the imposed values in the liquid and solid phases,  $a_s$  a smoothing parameter,  $\theta_s$  the central value (around which we regularize) and  $R_s$  the smoothing radius. For example, we use for the non-dimensional source term in (3) the following regularization over the artificial mushy region  $\theta \in [-\varepsilon, \varepsilon]$ :

$$S(\theta) = \frac{1}{Ste} - \frac{1}{2Ste} \left\{ 1 + \tanh \left( \frac{\theta_r - \theta}{R_s} \right) \right\}, \quad (10)$$

where  $\theta_r$  is the central value around which we regularize (typically  $\theta_r = \theta_f = 0$ ) and  $R_s$  the smoothing radius (typically  $R_s = \varepsilon$ ).

Finally, the penalty term  $A_{mushy}(\theta)\mathbf{u}$  in momentum equation (2) follows from the Carman-Kozeny model (Voller et al., 1987; Belhamadia et al., 2012; Kheirabadi and Groulx, 2015):

$$A_{mushy}(\theta) = -\frac{C_{CK}(1 - L_f(\theta))^2}{L_f(\theta)^3 + b}, \quad (11)$$

where  $L_f(\theta)$  is the local liquid fraction, which is 1 in the fluid region and 0 in the solid.  $L_f$  is regularized inside the artificial mushy-region using a hyperbolic-tangent similar to (10). The Carman-Kozeny constant  $C_{CK}$  is set to a large value ( $10^6$ ) and the constant  $b = 10^{-6}$  is introduced to avoid divisions by zero.

### 3. Numerical method

#### 3.1. Finite-element formulation

Finite-element methods for solving Navier-Stokes type systems of equations like (1)-(3) are generally based on a separate discretization of the temporal derivative (using finite differences, splitting or characteristics methods) and the generalization of the Stokes problem for the resulting system (Temam, 1983; Girault and Raviart, 1986; Quarteroni and Valli, 1994). To simplify the presentation, we consider in the following that  $C = 1$ . For the phase-change problems considered in this paper, this is a physically valid assumption.

For the time integration, we use a second-order Gear (BDF2) finite-difference scheme (see also Belhamadia et al. (2012)):

$$\frac{d\phi}{dt} \simeq \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{7\delta t}, \quad (12)$$

computing the solution  $\phi^{n+1}$  at time  $t_{n+1} = (n+1)\delta t$  by using two previous states  $(\phi^n, \phi^{n-1})$ . We use this scheme to advance in time both velocity ( $\phi = \mathbf{u}$ ) and temperature fields ( $\phi = \theta$ ). The other terms in equations (1)-(3) are treated implicitly. We obtain the following implicit semi-discretization in time of the single-domain model (1)-(3):

$$\nabla \cdot \mathbf{u}^{n+1} = 0, \quad (13)$$

$$\begin{aligned} \frac{3}{2} \frac{\mathbf{u}^{n+1}}{\delta t} + (\mathbf{u}^{n+1} \cdot \nabla) \mathbf{u}^{n+1} + \nabla p^{n+1} - \frac{1}{Re} \nabla^2 \mathbf{u}^{n+1} \\ - A_{mushy}(\theta^{n+1}) \mathbf{u}^{n+1} - f_B(\theta^{n+1}) \mathbf{e}_y = \\ 2 \frac{\mathbf{u}^n}{\delta t} - \frac{\mathbf{u}^{n-1}}{2\delta t}, \end{aligned} \quad (14)$$

$$\begin{aligned} \frac{3}{2} \frac{\theta^{n+1} + S(\theta^{n+1})}{\delta t} + \nabla \cdot (\mathbf{u}^{n+1} \theta^{n+1}) - \nabla \cdot \left( \frac{K(\theta^{n+1})}{RePr} \nabla \theta^{n+1} \right) = \\ 2 \frac{\theta^n + S(\theta^n)}{\delta t} - \frac{\theta^{n-1} + S(\theta^{n-1})}{2\delta t}. \end{aligned} \quad (15)$$

To solve the system of equations (13)-(15) we use a classical Galerkin finite-element method. We consider homogeneous Dirichlet boundary conditions for the velocity, *i. e.*  $\mathbf{u} = 0$  on  $\partial\Omega$ , and set the classical Hilbert spaces for the velocity and pressure:

$$\mathbf{V} = \mathbf{V} \times V, \quad V = H_0^1(\Omega), \quad Q = \left\{ q \in L^2(\Omega) \mid \int_{\Omega} q = 0 \right\} \quad (16)$$

Following the generalization of the Stokes problem (Temam, 1983; Girault and Raviart, 1986; Quarteroni and Valli, 1994), the weak formulation of the system (13)-(15) can be written as: find  $(\mathbf{u}^{n+1}, p^{n+1}, \theta^{n+1}) \in \mathbf{V} \times Q \times V$ , such that:

$$b(\mathbf{u}^{n+1}, q) - \gamma(p^{n+1}, q) = 0, \quad \forall q \in Q \quad (17)$$

$$\begin{aligned} \frac{3}{2\delta t} (\mathbf{u}^{n+1}, \mathbf{v}) + c(\mathbf{u}^{n+1}; \mathbf{u}^{n+1}, \mathbf{v}) + \frac{1}{Re} a(\mathbf{u}^{n+1}, \mathbf{v}) \\ - (A_{mushy}(\theta^{n+1}) \mathbf{u}^{n+1}, \mathbf{v}) + b(\mathbf{v}, p^{n+1}) - (f_B(\theta^{n+1}) \mathbf{e}_y, \mathbf{v}) \\ = \frac{2}{\delta t} (\mathbf{u}^n, \mathbf{v}) - \frac{1}{2\delta t} (\mathbf{u}^{n-1}, \mathbf{v}), \quad \forall \mathbf{v} \in \mathbf{V} \end{aligned} \quad (18)$$

$$\begin{aligned} \frac{3}{2\delta t} (\theta^{n+1} + S(\theta^{n+1}), \phi) + (\mathbf{u}^{n+1} \cdot \nabla \theta^{n+1}, \phi) + \left( \frac{K(\theta^{n+1})}{RePr} \nabla \theta^{n+1}, \nabla \phi \right) \\ = \frac{2}{\delta t} (\theta^n + S(\theta^n), \phi) - \frac{1}{2\delta t} (\theta^{n-1} + S(\theta^{n-1}), \phi), \quad \forall \phi \in V, \end{aligned} \quad (19)$$

where  $(u, v) = \int_{\Omega} u \cdot v$  denotes the scalar product in  $L^2(\Omega)$  or  $(L^2(\Omega))^2$ ; the bilinear forms  $a, b$  and trilinear form  $c$  are defined as (Girault and Raviart, 1986; Quarteroni and Valli,

1994):

$$\begin{aligned}
a : \mathbf{V} \times \mathbf{V} &\rightarrow \mathbb{R}, & a(\mathbf{u}, \mathbf{v}) &= \int_{\Omega} \nabla^t \mathbf{u} : \nabla \mathbf{v} = \sum_{i,j=1}^2 \int_{\Omega} \partial_j u_j \cdot \partial_j v_i, \\
b : \mathbf{V} \times Q &\rightarrow \mathbb{R}, & b(\mathbf{u}, q) &= - \int_{\Omega} \nabla \cdot \mathbf{u} q = - \sum_{i=1}^2 \int_{\Omega} \partial_i u_i \cdot q, \\
c : \mathbf{V} \times \mathbf{V} \times \mathbf{V} &\rightarrow \mathbb{R}, & c(\mathbf{w}; \mathbf{z}, \mathbf{v}) &= \int_{\Omega} [(\mathbf{w} \cdot \nabla) \mathbf{z}] \cdot \mathbf{v} = \sum_{i,j=1}^2 \int_{\Omega} w_j (\partial_j z_i) v_i.
\end{aligned}$$

Note that we introduced in Eq. (17) a penalty term on the pressure. An extensive discussion of the role of this parameter in reinforcing the incompressibility constraint and in the stabilization of the method is provided in Rakotondrandisa et al. (2020). We recall the main lines of this discussion. Following the incompressibility constraint (13), the pressure is defined up to an additive constant and imposing that  $p^{n+1} \in Q$  removes this uncertainty. Equation (17) numerically ensure that the pressure field is of zero average in  $\Omega$ . The penalty term in (17) acts at an algebraic level, by modifying the matrix of the final system (a zero lower diagonal block is avoided). Since in the present toolbox we use only iterative solvers (GMRES), this modification is not essential. It is in exchange important when LU-type direct solvers without pivoting are used, essentially for 2D calculations (UMFPACK solver in Rakotondrandisa et al. (2020); Aldbaissy et al. (2018), SuperLU in Woodfield et al. (2019)). Finally, the penalty constant  $\gamma$  has no role in stabilizing the method. Since the Taylor-Hood finite elements used in our simulations satisfy the inf-sup condition, this technique is assimilated to a *stable penalty*, or, in other words, just a computational trick to obtain a good solution (Brezzi and Fortin, 1991; Boffi et al., 2013). Note that, compared to classical penalty methods, we use in our calculations very low values of the penalty parameter ( $\gamma = 10^{-7}$ ). This ensures very low values of the average on  $\Omega$  for the pressure and also for the divergence of the velocity field.

The system of non-linear equations (17)-(19) is solved using a Newton method. To advance the solution from time  $t_n$  to  $t_{n+1}$ , we start from an initial guess  $\mathbf{w}_0 = (\mathbf{u}^n, p^n, \theta^n)$  (which is the solution at  $t_n$ ), and construct the Newton sequence  $\mathbf{w}_k = (u_k, p_k, \theta_k)$  by solving for each inner iteration  $k$ :

$$b(\mathbf{u}_{k+1}, q) - \gamma(p_{k+1}, q) = 0, \quad (20)$$

$$\begin{aligned}
& \frac{3}{2\delta t} (\mathbf{u}_{k+1}, \mathbf{v}) + c(\mathbf{u}_{k+1}; \mathbf{u}_k, \mathbf{v}) + c(\mathbf{u}_k; \mathbf{u}_{k+1}, \mathbf{v}) \\
& + \frac{1}{Re} a(\mathbf{u}_{k+1}, \mathbf{v}) - \left( \frac{dA_{mushy}}{d\theta}(\theta_k) \theta_{k+1} \mathbf{u}_k, \mathbf{v} \right) - (A_{mushy}(\theta_k) \mathbf{u}_{k+1}, \mathbf{v}) + b(\mathbf{v}, p_{k+1}) \\
& - \left( \frac{df_B}{d\theta}(\theta_k) \theta_{k+1} \mathbf{e}_y, \mathbf{v} \right) = \frac{1}{\delta t} \left( 2\mathbf{u}^n - \frac{1}{2}\mathbf{u}^{n-1}, \mathbf{v} \right) \\
& + c(\mathbf{u}_k; \mathbf{u}_k, \mathbf{v}) - \left( \frac{dA_{mushy}}{d\theta}(\theta_k) \theta_k \mathbf{u}_k, \mathbf{v} \right) - \left( \left( \frac{df_B}{d\theta}(\theta_k) \theta_k - f_B(\theta_k) \right) \mathbf{e}_y, \mathbf{v} \right), \quad (21) \\
& \frac{3}{2\delta t} \left( \theta_{k+1} + \frac{dS}{d\theta}(\theta_k) \theta_{k+1}, \phi \right) + (\mathbf{u}_k \cdot \nabla \theta_{k+1}, \phi) + (\mathbf{u}_{k+1} \cdot \nabla \theta_k, \phi) + \left( \frac{K(\theta_k)}{RePr} \nabla \theta_{k+1}, \nabla \phi \right) \\
& + \left( \frac{dK}{d\theta}(\theta_k) \frac{\theta_{k+1}}{RePr} \nabla \theta_k, \nabla \phi \right) = \frac{2}{\delta t} (\theta^n + S(\theta^n), \phi) + \frac{3}{2\delta t} \left( \frac{dS}{d\theta}(\theta_k) \theta_k - S(\theta_k), \phi \right) \\
& (\mathbf{u}_k \cdot \nabla \theta_k, \phi) - \frac{1}{2\delta t} (\theta^{n-1} + S(\theta^{n-1}), \phi) + \left( \frac{dK}{d\theta}(\theta_k) \frac{\theta_k}{RePr} \nabla \theta_k, \nabla \phi \right). \quad (22)
\end{aligned}$$

Note that the last term of Eq. (21) cancels in the case of a linear Boussinesq force  $f_B$  (see Eq. (5)); this is not the case when non-linear variations of the density of the liquid are considered (convection or solidification of water). Note also that the previous system of equations (20)-(22) depends only on  $\mathbf{u}^n$ ,  $\mathbf{u}^{n-1}$ ,  $\theta^n$  and  $\theta^{n-1}$  and is independent of  $p^n$ , the pressure being in this approach a Lagrange multiplier for the divergence free constraint.

The Newton loop (following  $k$ ) has to be iterated until convergence for each time step  $\delta t$  following the algorithm:

$$\left\| \begin{array}{l} \text{Navier-Stokes time loop following } n \\ \text{set } \mathbf{w}_0 = (\mathbf{u}^n, p^n, \theta^n) \\ \left\| \begin{array}{l} \text{Newton iterations following } k \\ \text{solve (20) to get } \mathbf{w}_{k+1} \\ \text{stop when } \|\mathbf{w}_{k+1} - \mathbf{w}_k\| < \xi_N \\ \text{actualize } (\mathbf{u}^{n+1}, p^{n+1}, \theta^{n+1}) = \mathbf{w}_{k+1} \end{array} \right. \end{array} \right. \quad (23)$$

For the space discretization of the system (20)-(22) we use standard Taylor-Hood finite elements (Taylor and Hood, 1973), approximating the velocity with  $P_2$  (piecewise quadratic) finite elements ( $\mathbf{V}_h$  space), and the the pressure with the  $P_1$  (piecewise linear) finite elements ( $Q_h$  space):

$$\mathbf{V}_h = \{ \mathbf{v} \in C^0(\bar{\Omega})^2 \mid \forall K \in \mathcal{T}_h, \quad \mathbf{v}|_K \in P_2 \}, \quad (24)$$

$$Q_h = \{ v \in C^0(\bar{\Omega}) \mid \forall K \in \mathcal{T}_h, \quad v|_K \in P_1 \}, \quad (25)$$

where  $K$  is an element of the triangulation  $\mathcal{T}_h$ , with characteristic mesh size  $h$ . Temperature and enthalpy variables are discretized using either  $P_1$  or  $P_2$  finite elements.

This algorithm was implemented using the open-source software FreeFem++ (Hecht et al., 2007; Hecht, 2012). The FreeFem++ programming framework offers the advantage to hide all technical issues related to the finite element method. The high level programming language with syntax close to mathematical formulations, makes the implementation of the present numerical algorithm very easy. Similar algorithms based on FreeFem++ were successfully used for solving different systems of equations with locally sharp variation of the solution, such as Gross-Pitaevskii equation (Danaila and Hecht, 2010; Vergez et al., 2016) or Laplace equations with nonlinear source terms (Zhang and Danaila, 2013).

The FreeFem++ syntax to implement the Newton algorithm is very close to the mathematical formulation given above. After defining a vector finite-element space `fespace Wh(Th, [P2,P2,P1,P2])`, associated to the mesh `Th`, we define the velocity, pressure and temperature variables in a compact manner by declaring: `Wh [u1,u2,p,T];`. Corresponding test functions are defined similarly. It is then convenient to define a `varf` weak (variational) formulation in FreeFem++ to build the matrices and the rhs-vectors resulting from the algorithm (20)-(22). The use of the `macro` environment (which is used as a pre-processor command for a simple syntax replacement in the script) makes the reading of the programs very intuitive by comparing each term to its mathematical expression. For example, the following `macros` define the necessary operators for the variational formulation (20)-(22) in 2D (`#` is the concatenation operator):

```
macro grad(u) [dx(u),dy(u)]//
macro Grad(u) [grad(u#1),grad(u#2)]//
macro div(u) (dx(u#1)+dy(u#2))//
```

```

macro ugrad(u,v) ([u#1,u#2] '*grad(v)) //
macro UgradV(u,v) [ugrad(u,v#1),ugrad(u,v#2)] //
macro c(w,Z,v) (UgradV(w,Z) '*[v#1,v#2]) //

```

The variational formulations used to build the matrix and the rhs-vector of the final system follows closely the mathematical formulation (20)-(22). For example, the simple case of the stationary convection of air is defined by the following macros (the syntax +bcu1+ ... is used to prescribe Dirichlet boundary conditions):

```

macro VarfStatNATCONV(varfName, meshName, VhName)
varf varfName([uw1,uw2,pw,Tw],[v1,v2,q,TT])
= int2d(meshName,qforder=ord)( b(uw,q) - gamma*pw*q
+ c(uw,u,v) + c(u,uw,v) + IRe*a(uw,v) + b(v,pw) - coef*dfB(T
)*Tw*v2
+ ugrad(u,Tw)*TT + ugrad(uw,T)*TT + grad(Tw) '*grad(TT)*IPr )
+ bcu1 + bcu2 + bcT;
// EOM

macro VarfrhsStatNATCONV(varfName, meshName, VhName)
varf varfName([uw1,uw2,pw,Tw],[v1,v2,q,TT])
= int2d(meshName,qforder=ord)( c(u,u,v) + ugrad(u,T)*TT
- coef*dfB(T)*T*v2 + coef*fB(T)*v2 )
+ bcu1 + bcu2 + bcT;
// EOM

```

New terms can be added to the variational formulation expressed in the **varf** structure, without affecting other parts of the program. The implementation of new models or numerical methods for this problem is greatly facilitated by this modular structure of programs. Moreover, the switch from 2D to 3D computations is automatically operated in FreeFem++ depending of the 2D or 3D definition of the mesh object **Th**. Consequently, the FreeFem++ syntax for the implementation of the Newton algorithm is the same for both 2D and 3D problems. For the example of the stationary natural convection of air, the only modifications to switch from 2D to 3D settings concern the add of the third dimension in the previous definitions (note that the expressions under the integrals **int2d** and **int3d** are identical):

```

macro grad(u) [dx(u),dy(u),dz(u)] //
macro Grad(u) [grad(u#1),grad(u#2),grad(u#3)] //
macro div(u) (dx(u#1)+dy(u#2)+dz(u#3)) //
macro ugrad(u,v) ([u#1,u#2,u#3] '*grad(v)) //
macro UgradV(u,v) [ugrad(u,v#1),ugrad(u,v#2),ugrad(u,v#3)] //
macro c(w,Z,v) (UgradV(w,Z) '*[v#1,v#2,v#3]) //

macro VarfStatNATCONV(varfName, meshName, VhName)
varf varfName([uw1,uw2,uw3,pw,Tw],[v1,v2,v3,q,TT])
= int3d(meshName,qforder=ord)( b(uw,q) - gamma*pw*q
+ c(uw,u,v) + c(u,uw,v) + IRe*a(uw,v) + b(v,pw)
- coef*dfB(T)*Tw*v3

```



```

        + ugrad(u,Tw)*TT + ugrad(uw,T)*TT + grad(Tw)'*
          grad(TT)*IPr )
    + bcu1 + bcu2 + bcu3 + bcT;
// EOM

macro VarfrhsStatNATCONV(varfName, meshName, VhName)
  varf varfName([uw1,uw2,uw3,pw,Tw],[v1,v2,v3,q,TT])
    = int3d(meshName,qforder=ord)( c(u,u,v) + ugrad(u,T)
      *TT - coef*dfB(T)*T*v3 + coef*fB(T)*v3 )
    + bcu1 + bcu2 + bcu3 + bcT;
// EOM

```

### 3.2. Domain decomposition method

The main time-consuming part in the algorithm (23) lies in the resolution of the sequence of linear systems of the form  $Ax = b$ . To reduce the computational time, we implement an overlapping Schwarz domain decomposition method to solve these linear systems in parallel. This task becomes an easy job by using the parallel framework `ffddm`, which was recently made available in FreeFem++ (Tournier et al., 2019). `ffddm` defines high-level functionalities for parallel data distribution among processors and facilitates the use of domain decomposition methods by providing several types of preconditioners (Dolean et al., 2015). We describe below the Restricted Additive Schwarz (RAS) preconditioner used in this study.

First, the triangular mesh  $\mathcal{T} := \mathcal{T}_h$  is partitioned into  $N_S$  non-overlapping meshes  $\{\mathcal{T}_i\}_{1 \leq i \leq N_S}$  (see Fig. 1b) using standard graph partitioners available in FreeFem++, such as `Scotch` (Pellegrini and Roman, 1996) or `Metis` (Karypis and Kumar, 1998). If  $\delta$  is a positive integer, the *overlapping* decomposition  $\{\mathcal{T}_i^\delta\}_{1 \leq i \leq N_S}$  is defined recursively as follows:  $\mathcal{T}_i^\delta$  is obtained by including all mesh elements of  $\mathcal{T}_i^{\delta-1}$  and adding recursively one layer of elements. For  $\delta = 0$ ,  $\mathcal{T}_i^\delta = \mathcal{T}_i$  and a non-overlapping decomposition is obtained. In practice we use  $\delta = 1$  which corresponds to an overlap of width 2.

Let  $W_h = \mathbf{V}_h \times Q_h \times V_h$  be the global finite element space for velocity, pressure and temperature variables, and let  $\{W_i^\delta\}_{1 \leq i \leq N_S}$  be the local finite element space defined on  $\{\mathcal{T}_i^\delta\}_{1 \leq i \leq N_S}$ . Consider the restrictions  $\{R_i\}_{1 \leq i \leq N_S}$  from  $W_h$  to  $\{W_i^\delta\}_{1 \leq i \leq N_S}$ , and a local partition of unity  $\{D_i\}_{1 \leq i \leq N_S}$  such that

$$\sum_{i=1}^{N_S} R_i^T D_i R_i = I_{n \times n}. \quad (26)$$

Algebraically speaking, if  $n$  is the global number of unknowns and  $\{n_i\}_{1 \leq i \leq N_S}$  are the numbers of unknowns for each local finite element space, then  $R_i$  is a Boolean matrix of size  $n_i \times n$ , and  $D_i$  is a diagonal matrix of size  $n_i \times n_i$ , for all  $1 \leq i \leq N_S$ . Note that  $R_i^T$ , the transpose of  $R_i$ , is a  $n \times n_i$  matrix that gives the extension by 0 from  $W_i^\delta$  to  $W_h$ .

Using these matrices, one can define the following preconditioner, called Restricted Additive Schwarz preconditioner (RAS):

$$M_{\text{RAS}}^{-1} = \sum_{i=1}^{N_S} R_i^T D_i A_i^{-1} R_i, \quad (27)$$

with local subdomain matrices  $\{A_i\}_{1 \leq i \leq N_S} = \{R_i A R_i^T\}_{1 \leq i \leq N_S}$ . The preconditioner (27) is naturally parallel since its assembly requires the concurrent factorization of each  $\{A_i\}_{1 \leq i \leq N_S}$ . In practice, this operation is performed locally on different processes in a distributed computing context, as one subdomain is assigned to each MPI process. Likewise, applying (27) to a distributed vector requires only peer-to-peer communications between neighboring subdomains, and a local forward elimination and backward substitution (see chapter 8 of Dolean et al. (2015), for a more detailed description). `ffddm` makes very easy the task to assemble the operators necessary to use the RAS preconditioner and solve the linear system with a parallel GMRES algorithm. More details can be found in the User's manual of `ffddm` (Tournier et al., 2019).

### 3.3. Mesh adaptivity

For 2D simulations, we use the standard mesh adaptivity function (`adaptmesh`) offered by FreeFem++ (Hecht, 2012). The key idea implemented in this function (see also Borouchaki et al. (1996); Castro-Diaz et al. (2000); Hecht and Mohammadi (1997); George and Borouchaki (1998); Frey and George (1999); Mohammadi and Pironneau (2000)) is to use the Delaunay algorithm to generate a *new* triangular mesh with edges close to the unit length in the metric  $\mathcal{M} = \frac{|\mathcal{H}|}{\mathcal{E}}$ , where  $|\mathcal{H}(x)|$  is the Hessian of the variable  $\chi$  at point  $x$  (after being made positive definite) and  $\mathcal{E}$  the interpolation error for  $\chi$ . This implies to modify the scalar product used in the automatic mesh generator to evaluate distance and volume by defining a scalar product based on the evaluation of the Hessian  $\mathcal{H}$  of the variables of the problem. Equilateral elements are thus constructed, with an equally distributed interpolation error  $\mathcal{E}$  over the edges of the mesh. The previous approach could be generalized for a vector variable  $\chi = [\chi_1, \chi_2]$ . After computing the metrics  $\mathcal{M}_1$  and  $\mathcal{M}_2$  for each variable, the retained metric is the intersection  $\mathcal{M} = \mathcal{M}_1 \cap \mathcal{M}_2$ , defined such that the unit ball of  $\mathcal{M}$  is included in the intersection of the two unit balls of metrics  $\mathcal{M}_2$  and  $\mathcal{M}_1$  (for details, see the procedure defined in Frey and George (1999)).

The use of the mesh adaptivity algorithm for 2D phase-change systems is described in detail in Rakotonrandisa et al. (2020). In 2D problems considered below, we took into account several metrics computed from different variables monitoring the evolution of the phase-change system. For the natural convection system, the mesh was adapted using the values of the two velocity components and the temperature. For phase-change systems, to accurately track the solid-liquid interface we added the variation of the enthalpy source term in the adaptivity criterion. For water systems (convection or freezing), we also added an extra function tracking the anomalous change of density around  $4^\circ\text{C}$ . To reduce the impact of the interpolation on the global accuracy for time-depending problems, we considered, for each variable used for adaptivity, the metrics computed at actual ( $t_{n+1}$ ) and previous ( $t_n$ ) time instants (see also Belhamadia et al. (2004a)). The capabilities of the mesh adaptivity algorithm in 2D are illustrated in §5.

For 3D simulations, the metric was first computed using `mshmet`, which is a FreeFem++ module, following the code:

```
load "mshmet"
real[int] hmetric(6*ThBackup.nv);
hmetric=mshmet(ThBackup,[u1Backup,u2Backup,u3Backup],
    normalization=1, aniso=1, nbregul=1, hmax=hmax, hmin=hmin, err
    =errh);
```

Several parameters of the mesh can be thus controlled ( $h_{min}$ ,  $h_{max}$ , anisotropy, etc). Then, the metric was regularized in order to avoid flat tetrahedra and saved in `m11[]` :

```
load "aniso"
boundaniso(6,hmetric,40);
fespace Wh6Backup(ThBackup,[P1,P1,P1,P1,P1,P1]);
Wh6Backup [m11,m21,m22,m31,m32,m33];
m11[]=hmetric;
```

The external software `mmg` (Dapogny et al., 2014) was finally loaded to read the saved metric and the old mesh to finally generate the adapted new mesh:

```
load "mmg"
ThBackup = mmg3d(ThBackup,metric=m11[],verbose=0,hmin=hmin,
    hmax=hmax,hgrad=adaptratio,mem=10000);
```

#### 4. Description of the programs

In this section, we first describe the architecture of the programs and the organization of the provided files. Then we focus on the list of input parameters and the structure of output files.

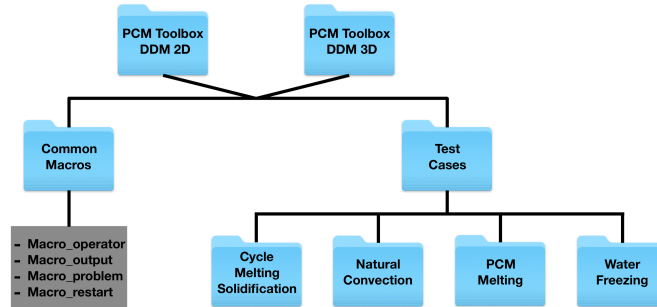


Figure 2: Folder tree structure of the PCM.Toolbox.DDM.2D and PCM.Toolbox.DDM.3D to solve solid-liquid phase-change problems.

##### 4.1. Program architecture

Figure 2 gives a schematic overview of the content of the Toolbox. To facilitate the reading and the assimilation of the programs, we separated the 2D and 3D Toolboxes in directories `PCM.Toolbox.DDM.2D` and `PCM.Toolbox.DDM.3D`. Many detailed comments were included in programs, with direct reference to the mathematical expressions used in this paper. The used FreeFem syntax was intentionally kept at a low level of technicality and supplemented with detailed comments when specific more technical syntax was used.

This directory is organized as follows:

1. The directory **Common\_Macros** contains five files:
  - *Macro\_operator.idp* includes macros and functions defining mathematical operators,
  - *Macro\_problem.idp*: macros defining the variational formulation of the problem,
  - *Macro\_restart.idp*: macros used to start a new simulation from a saved field,
  - *Macro\_output.idp*: macros used to save the solution with different formats.
2. The directory **Test\_Cases** contains four subdirectories, each of them defining one of the following applications:
  - natural convection of air or water in a differentially heated square/cubic cavity,
  - melting of a PCM stored in containers of different shapes,
  - melting followed by solidification of a rectangular/cubic PCM,
  - freezing of pure water in a square/cubic cavity.

Each subdirectory contains three files: *NEWTON\_\$case.edp* is the main FreeFem++ script file, *param\_phys.inc* defines the physical parameters and *param\_num.inc* the numerical parameters. The 3D Toolbox is supplemented with the script *Read\_3D\_data.edp*, which reads data from the RST folder and generates the files for visualization with Medit, Paraview or Tecplot. For example, to run the natural convection case of air in a square cavity, the user can use the following command in a terminal window: `mpirun -np 6 FreeFem++-mpi NEWTON_stat_natconv_ddm.edp -wg -v 0 -ns`.

The folder structure of each test case is illustrated in Figure 3. The obtained solutions are saved in the folder **OUTPUT/Data**. Depending on the output format selected by the user, data files are generated in specific folders for being visualized with Tecplot, Paraview, Gnuplot or Medit. We also provide in the folder **Figures** ready-made layouts for each visualization software. The user can thus obtain the figures from this paper using newly generated data. More details about the output structure are given below.

#### 4.2. Input parameters

Physical parameters and parameters related to the run are separated into two files.

- (1) The file *param\_phys.inc* contains the physical descriptions of the problem:

- **typeT**: is the finite-element type for the temperature, with possible values P2 or P1,
- **Torder**: is the order of accuracy of the time integration scheme, with possible values 1 (Euler scheme) or 2 (Gear scheme),
- **scalAdim**: defines the characteristic scales of the problem, see (4). Possible values 1, 2 or 3 correspond to the following choice of the characteristic scales (Danaila et al., 2014):

$$(1) : V_{ref}^{(1)} = \frac{\nu_l}{H} \implies t_{ref}^{(1)} = \frac{H^2}{\nu_l} \implies Re = 1, \quad (28)$$

$$(2) : V_{ref}^{(2)} = \frac{\alpha}{H} \implies t_{ref}^{(2)} = t_{ref}^{(1)} Pr \implies Re = 1/Pr, \quad (29)$$

$$(3) : V_{ref}^{(3)} = \frac{\nu_l}{H} \sqrt{\frac{Ra}{Pr}} \implies t_{ref}^{(3)} = t_{ref}^{(1)} \sqrt{\frac{Pr}{Ra}} \implies Re = \sqrt{\frac{Ra}{Pr}}, \quad (30)$$

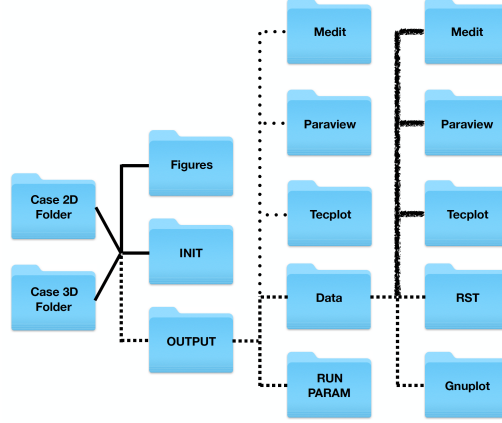


Figure 3: Structure of each Test-case folder. Solid lines in the diagram correspond to folders which come with the Toolbox, the dashed lines to folders generated after running the script *NEWTON.case.edp*, the hashed lines to folders generated after running the script *NEWTON.case.edp* in the 2D case. Finally, the dotted lines indicate folders generated after running the script *Read.3D.data.edp*, which reads data from the RST folder and generates the Medit, Paraview and Tecplot files for visualization.

- $\mathbf{x}_l, \mathbf{x}_r, \mathbf{y}_l, \mathbf{y}_r$ : are the values defining the dimensions of the cavity  $[x_l, x_r] \times [y_l, y_r]$ ,
- **Pr, Ra, Ste**: are the Prandtl, Rayleigh and Stefan numbers, see (6) and (5),
- $\mathbf{T}_{hot}, \mathbf{T}_{cold}$ : are dimensionless temperatures according to (4),
- **bcu<sub>1</sub>, bcu<sub>2</sub>, bcT**: are macros defining the velocity (u) and the temperature (T) boundary conditions,
- **epsi**: is the half width  $\varepsilon$  of the mushy region. Default value = 0.01,
- **dt**: is the dimensionless time step,
- **t<sub>max</sub>**: is the dimensionless final time,

- **Parameters for regularization functions:**

The parameters of the hyperbolic-tangent function (9) used to regularize discontinuous functions are set by default as follows:

	$f_s$	$f_l$	$a_s$	$\theta_s$	$R_s$	$C_{CK}$	b
<i>Enthalpy</i>	0	1/Ste	1	0.01	0.01	-	-
<i>Carman - Kozeny</i>	0	1	1	0.01	0.01	$10^6$	$10^{-7}$
<i>Conductivity (water)</i>	1	2.26/0.578	1	$\theta_f$	0.015	-	-

- **rho(T) and Drho(T)**: (water cases only) define the density and its derivative as functions of the temperature, following the model (Gebhart and Mollendorf, 1977):

$$\rho(T) = \rho_m(1 - \omega|T - T_m|^q),$$

$\rho_m$ [kg/m <sup>3</sup> ]	$\omega$ [°C <sup>-q</sup> ]	q	$T_m$ [°C]
999.972	$9.2793 \cdot 10^{-6}$	1.894816	4.0293

- **f<sub>B</sub>(T), df<sub>B</sub>(T)**: define the buoyancy force and its derivative.

(2) The file *param\_num.inc* contains the parameters controlling the run.

**Restart parameters:**

- **Nsave**: the solution is saved every *Nsave* time steps in the **Data** folder (see Figure 3). The temperature and the velocity fields are saved in **Tecplot** and **Medit** folders, while the liquid fraction, the Nusselt number, and the accumulated heat input are saved in the **Gnuplot** folder.
- **Nrestart**: restart files (mesh and solution) are saved every *Nrestart* time steps. Solutions at current and previous iterations, the CPU time, the accumulated heat input  $Q_0$ , and the time step  $dt$  are saved in the folder **RST**.
- **Ncondt**: allows the user to stop the run and save the solution properly. The file **OUTPUT/zz.condt** is read every *Ncondt* time steps: if the user replaces the value "0" in this file by "1" the run is stopped. This is a simple solution for a clean stop of the job by the user. Default value = 20.
- **Nremesh**: the mesh is adapted every *Nremesh* iterations. If this parameter is set to "1" the mesh is adapted every time step.
- **IFrestart**: is a Boolean controlling the set up of the initial field.  
*IFrestart* = 0, the initial condition is built in the code for each test case. For the PCM melting cases, the PCM is initially motionless at isothermal temperature. To set-up a smooth initial field, a few time steps (with very small  $\delta t$ ) are computed by increasing progressively the boundary temperature at the hot wall and the Rayleigh number (by continuation). Outputs are saved in **OUTPUT/Data-RST-0**.  
*IFrestart* > 0, (positive integer values) the solution field previously computed at iteration *IFrestart* is loaded from the folder **OUTPUT/Data-RST-filenameRST/RST**, with **filenameRST** a variable selecting the restart folder. Note that for 3D cases, the user has to copy manually the solution used as restart field to the folder **INIT**.  
*IFrestart* < 0, (negative integer values), the same principle for loading a solution is used, but from the folder **INIT** (see Figure 3). The solution fields stored in this folder could come from different previous calculations (*e.g.* a steady state solution or, for the water, the natural convection field before freezing).

**Newton parameters:**

- **epsconv**: is the value of the stopping criterion for steady cases,

- **gamma**: is the penalty parameter in (13). Default value =  $10^{-7}$ ,
- **tolNewton**: is the Newton tolerance  $\xi_N$  (see (23)). Default value =  $10^{-6}$ ,
- **newtonMax**: limits the maximum number of iterations in the Newton algorithm (23). Default value = 50.

**Mesh parameters:**

- **nbseg**: is the number of segments for the discretization along the  $x$  and  $y$  directions,
- **errh**: is the interpolation error level. Default value = 0.02,
- **hmin, hmax**: are the minimum and maximum edge size, respectively,
- **adaptratio**: is the ratio for a prescribed smoothing of the metric. For a value less than 1.1 no smoothing is done. Default value = 1.5,
- **nbvx**: is the maximum number of vertices allowed in the mesh generator. Default value = 50000.

**Output parameters:**

- **dircase**: is the name of the output folder,
- **fcase**: is the prefix-name for output files.
- **Paraview, Tecplot, Medit, Gnu**: correspond to the name of the visualization software to be used; the format of the outputs written in **OUTPUT/Data** (see Figure 3) is set accordingly.

#### 4.3. Outputs

When a computation starts, the **OUTPUT** directory is created (see Figure 3). It contains two folders storing the output data and the echo of the run parameters. The folder **Data** contains four subdirectories with different output format files of the computed solution. File names are created using the prefix defined by the parameter **fcase**, the current iteration and the current dimensionless time  $t$ . Solution files can be visualized using either Tecplot or any other CFD Visualization tools (Paraview, Visit, etc.). Moreover, *.gmsh* (mesh) and *.rst* (fields) files are generated in the folder **RST** to enable restarts of the computation. Note that the folder **FFglut** contains FreeFem++ scripts that read and visualize the RST-files to facilitate the selection of a restart field. An *.echo* file with a summary of the main parameters, information on the run and the names of the output files is saved in the folder **RUNPARAM**. This directory additionally contains a copy of the *.inc* parameter files, allowing an easy identification of each case and preparing an eventual rerun of the same case.

## 5. 2D parallel simulations

In this section we consider well defined 2D benchmarks used to validate numerical codes for natural convection and phase-change problems. All these cases were described in detail in [Rakotondrandisa et al. \(2020\)](#) and computed using sequential codes. We present below the results obtained for the same cases, but using parallel computations with the new Toolbox: (i) the natural convection of air (§5.1), (ii) the melting or solidification of a phase-change material (PCM) (§5.2) and (iii) the convection and the freezing of pure water (§5.3). This approach allows us to test the programs by adding progressively non-linearities in the Newton algorithm. In the following, we validate each case with respect to the physical reference data available in the literature. To have a quick overview of the benefits of using parallel computing, we compare in Table 1 computational times of sequential and parallel computations. To make the simulations accessible and testable by using a personal computer with a multi-thread processor, we use in this section only 6 MPI processes.

Case	1 thread	6 threads	speed-up	max of number of triangles	number of iterations	ratio CPU time adapt / iteration
Unsteady NC of air, $Ra = 10^6$	00:01:39	00:00:50	1.98	2,902	53	18%
PCM-Case #1	00:06:39	00:04:35	1.45	2,590	81	5%
PCM-Case #2	01:31:11	00:40:44	2.23	5,928	501	8%
PCM-Case #3: 1 tube	00:25:09	00:19:18	1.3	5,052	401	6%
PCM-Case #3: 4 tubes	00:28:57	00:16:13	1.78	13,507	151	6%
PCM-Case #3: 9 tubes	00:33:28	00:17:44	1.88	24,866	100	5%
PCM-Case #4	06:31:31	01:38:35	3.97	5,371	2,001	15%
PCM-Case #5	00:07:52	00:03:17	2.39	2,898	117	12%
Cycle of a PCM	00:13:58	00:08:49	1.58	3,160	383	17%
NC of water	00:00:36	00:00:21	1.71	2,686	20	14%
Unsteady NC of water	00:01:49	00:00:54	2.02	3,368	33	10%
Water freezing	00:22:49	00:13:38	1.67	3,743	296	10%

Table 1: Comparison of CPU times for 2D simulations. All computation were performed on a Macbook pro 2.2GHz Intel Core i7, 16GB of DDR4 2400 MHz RAM.



### 5.1. Natural convection of air

We start by testing the Newton algorithm (20)-(22) for the case of natural convection, *i. e.*  $C = K = 1$ ,  $A_{mushy}(\theta) = S(\theta) = 0$ . We consider the classical problem of the thermally driven square cavity  $[0, 1] \times [0, 1]$ , filled with air. The Boussinesq term  $f_B(\theta)$  is then linear and takes the form (5). Top and bottom walls are adiabatic, while the temperature is fixed on the left (hot) wall and the right (cold) wall. Natural convection flows are computed for three values of the Rayleigh number:  $Ra = 10^4, 10^5, 10^6$ . The Prandtl number is set to  $Pr = 0.71$ . For these values of the  $Ra$  number, the flow is known to be steady (Le Quéré, 1991) and therefore, we also solve the time-independent version of equations (20)-(22).

We provide programs for both steady (time-independent) and time-dependent cases. The steady case is performed using a continuation following the Rayleigh number: a smaller value for  $Ra$  is set initially and is then smoothly increased until reaching the wanted value. The time-dependent case is computed until a steady state with a single convection cell is reached.

The temperature is imposed at the right (cold) wall as  $\theta_c = -0.5$  and at the left (hot) wall as  $\theta_h = 0.5$ . Top and bottom walls are adiabatic. The initial condition models a cavity filled with motionless air ( $\mathbf{u} = 0$ ), with a linear distribution of the temperature. Both steady and time-dependent codes converge to the same flow state, with a single convection cell. For this final state, horizontal  $u(y)$  and vertical  $v(x)$  velocity profiles were extracted at mid-domain ( $y = 0.5$  and  $x = 0.5$ , respectively) and plotted in Figure 4. Our results are in very good agreement with reference numerical results obtained by Le Quéré (1991) with a spectral code.

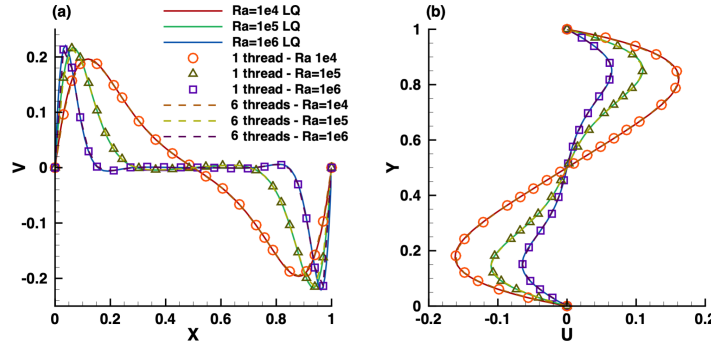


Figure 4: Natural convection of air in a differentially heated cavity for values of  $Ra$  ranging from  $10^4$  to  $10^6$ . (a) Vertical velocity profile  $v(x)$  along the horizontal symmetry line ( $y = 0.5$ ). (b) Longitudinal velocity profile  $u(y)$  along the vertical symmetry line ( $x = 0.5$ ). Results obtained using the present Toolbox, with a mesh resolution  $nbseg = 80$ . Comparison with the spectral simulations by Le Quéré (1991) (solid lines).

Table 2 offers a quantitative assessment of the accuracy of the present Newton method. The values of  $u_{max}$  and the location  $Y$  of this maximum are compared to reference values from Le Quéré (1991). The Newton method gives results identical to reference values, with a difference less than 0.1%.

Run		$u_{max}$ at $x=0.5$ (error)	$Y$ (error)
Reference values	spectral	0.0648344	0.850
Newton (Steady)	$nbseg = 80$	0.0648126 (0.03 %)	0.850394 (0.05 %)
Newton (Unsteady)	$nbseg = 80$	0.0647805 (0.08 %)	0.850394 (0.05 %)

Table 2: Natural convection of air in a differentially heated cavity. Maximum value  $u_{max}$  of the horizontal velocity profile at mid-domain ( $x = 0.5$ ) and location  $Y$  of this maximum. Comparison to reference values reported by [Le Quéré \(1991\)](#).

### 5.2. Melting or solidification of a phase-change material (PCM)

We continue our validation tests by considering the full system (20)-(22) for the case of the melting or solidification of a phase-change material. Two new non-linearities are now present in the system: the Carman-Kozeny penalty term  $A_{mushy}(\theta)$  and the enthalpy source term  $S(\theta)$ . The function  $S$  is regularized using (10). We also consider that the material properties in the liquid and solid are the same, *i. e.*  $C = K = 1$ . This is a frequent assumption ([Wang et al., 2010](#); [Ma and Zhang, 2006](#)). Five cases were computed (the exact values of the defining parameters are summarized in Table 3):

- PCM-Case #1 simulates the experimental study of [Okada \(1984\)](#). It consists of a differentially heated square cavity, filled with octadecane paraffin.
- PCM-Case #2 is extracted from the collective publication by [Bertrand et al. \(1999\)](#), compiling the results of different numerical approaches used for the simulation of the melting of a PCM at high Rayleigh numbers.
- PCM-Case #3 simulates the melting of a cylindrical PCM with heated inner tubes, as in [Luo et al. \(2015\)](#).
- PCM-Case #4 simulates the melting of Gallium in a rectangular cavity heated by the side-wall, as in [Hannoun et al. \(2003\)](#).
- PCM-Case #5 simulates the solid crust formation in a highly distorted PCM domain, as in [Nourgaliev et al. \(2016\)](#).

We summarize in Table 3 the values of physical parameters and the scales used to simulate these cases. The values of the CPU time necessary to run each case (with default parameters) are given in Table 1.

	case #1	case #2	case #3	case #4	case #5
$Ra$	$3.27 \cdot 10^5$	$10^8$	$5 \cdot 10^4$	$7 \cdot 10^5$	$10^6$
$Pr$	56.2	50	0.2	0.0216	0.1
$Ste$	0.045	0.1	0.02	0.046	4.854
$\delta t$	1	$10^{-2}$	$10^{-2}$	$10^{-5}$	1
$V_{ref}$	$\frac{\nu_l}{H}$	$\frac{\nu_l}{H}$	$\frac{\nu_l}{H}$	$\frac{\nu_l}{H}$	$\frac{\nu_l}{H} \sqrt{\frac{Ra}{Pr}}$

Table 3: Parameters for the cases simulating the melting of a phase-change material.

### 5.2.1. PCM-Case #1: Melting of an octadecane PCM in a square cavity

Okada (1984) studied experimentally the melting of an octadecane PCM in a square cavity of height  $H = 1.5$  cm. His results were often used to validate numerical methods (Okada, 1984; Wang et al., 2010; Ma and Zhang, 2006; Danaila et al., 2014). The material is initially solid ( $\theta_0 = -0.01$ ) and melts progressively starting from the left boundary, maintained at a hot temperature  $\theta_h = 1$ . The right boundary is also isothermal, with cold temperature  $\theta_c = -0.01$ . Horizontal boundaries are adiabatic. The other parameters of this case are reported in Table 3. The computation starts from a refined mesh near the hot boundary. Mesh adaptivity is applied every time step. Figure 5 shows in the left panel the adapted mesh at  $t = 80.1$  and the 6 subdomains of the domain decomposition used for the parallel computation. The velocity vectors in the liquid phase, represented in the middle panel, show the strong convection cell affecting the shape of the liquid-solid interface. To offer a quantitative validation of this computation, we compare in Fig. 5 (right panel) the position of the solid-liquid interface at  $t = 40.1$  and  $t = 80.1$  with the experimental data of Okada (1984) at time instants  $t = 39.9$  and  $t = 78.7$ . The obtained shape and position of the liquid-solid interface is very close to experimental results. We show in the same figure that the parallel computation (6 threads) gives the same results as the sequential simulation (1 thread).

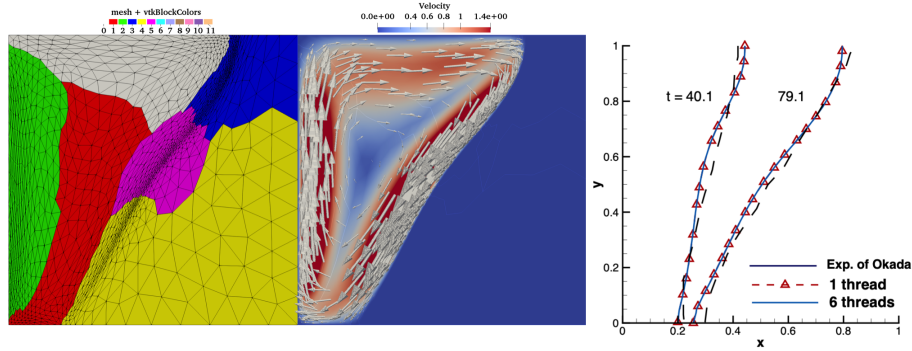


Figure 5: PCM-Case #1. Melted PCM at time instant  $t = 80.1$ . Adapted finite-element mesh and subdomains used for the domain decomposition and parallel computing with 6 threads (left panel). Velocity vectors in the liquid phase (central panel). Position of the solid-liquid interface and comparison with experimental data of Okada (1984) for two time instants (right panel).

### 5.2.2. PCM-Case #2: Melting of an octadecane PCM with high Rayleigh number

This case considers the same problem of the melting of a PCM, but with a very high value of the Rayleigh number,  $Ra = 10^8$  (see Table 3). This case is very challenging since the natural convection becomes important in the fluid flow, and enhances considerably the heat transfer. Bertrand et al. (1999) compiled results provided by five different authors (Lacroix, Le Qu  r  , Gobin-Vieira, Delannoy and Binet-Lacroix) who used different numerical methods to compute the basic configuration presented in this section. This benchmark is a very demanding numerical test. The high velocity, inducing a very narrow thermal boundary layer, can lead to unrealistic results if under-resolved. This explains why two investigators among the five failed to correctly predict the process.

We show in Fig. 6 an illustration of the flow configuration at dimensionless time  $t = 5$ . The adapted mesh and the domain decomposition for the parallel computation with 6 threads is presented in the left panel. The convection flow is depicted in the middle panel. Note the very narrow boundary layers, which impose a very refined mesh in these regions. This flow particularity explains why this case is rather costly in terms of computational time (see Table 1), when compared to the previous one. The right panel of Fig. 6 offers a quantitative validation of this computation. The position of melting front at  $t = 5$  is in good agreement with that reported by Gobin and Le Quéré. Details of their numerical method are presented in Gobin and Le Quéré (2000). Gobin used a front-tracking method based on a coordinate transformation with a finite volume method and a  $62 \times 42$  grid, while Le Quéré solved a single domain model using a second-order finite volume method with a  $192 \times 192$  grid. The interest of the mesh adaptation is clearly demonstrated for this case, since we initially used a coarse  $40 \times 40$  grid.

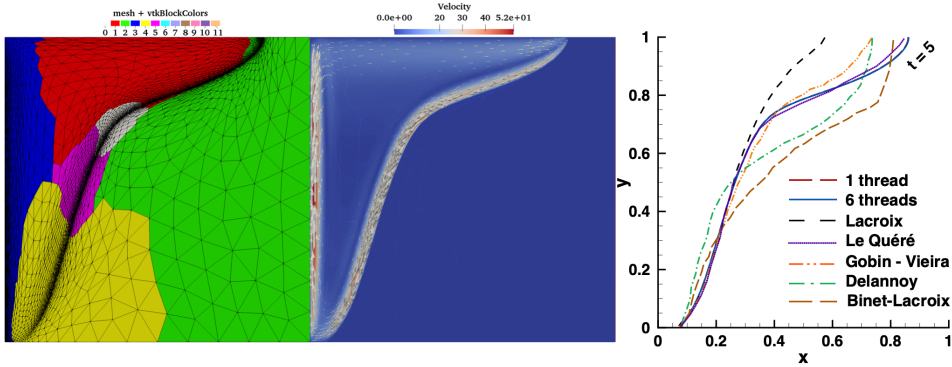


Figure 6: PCM-Case #2. Melting of the PCM with high Rayleigh number ( $Ra = 10^8$ ). Simulated configuration at time instant  $t = 5$ . Adapted finite-element mesh and subdomains used for the domain decomposition and parallel computing with 6 threads (left panel). Velocity vectors in the liquid phase (central panel). Position of the solid-liquid interface and comparison with five sets of results presented in Bertrand et al. (1999).

### 5.2.3. PCM-Case #3: Melting of cylindrical PCM with inner heated tubes

A more complex geometry, suggested by Luo et al. (2015), is simulated in this section. It consists of a cylindrical PCM of radius  $R = 1$  with heated tube inclusions of different arrangements. This configuration is also interesting from a practical point of view. Agyenim et al. (2010) pointed out that more than 70% of the PCM containers used for heat storage are using shell-tube systems. We simulate three configurations, with one, four and nine heated tubes (see Fig. 7). The size of the tubes is adjusted to have the same total tube area for all configurations. The radius  $R_i$  of the inner tube is  $R_i = R/4$  for the case with one tube,  $R_i = R/8$  for the four heated tubes case and  $R_i = R/12$  for the case with nine tubes. The inner tubes are heated at constant  $\theta = \theta_h$  (Dirichlet boundary condition). A Neumann boundary condition ( $\partial\theta/\partial n = 0$ ) is used for the outer boundary. For the velocity, all boundaries are considered as non-slip walls ( $\mathbf{u} = 0$ ).

For the three configurations, Fig. 7 shows the adapted mesh and the domain decomposition with 6 subdomains (left column), the velocity vectors (central column) and

the temperature field (right column). The time instants are chosen to have the same liquid fraction in the system,  $L_f = 80\%$ . Only half of the domain is simulated, since all configurations are symmetric with respect to the vertical axis. The mesh is refined initially around the inner tubes, and is dynamically adapted at each time step around the melting front and in the thermal boundary layer area.

To estimate the heat-storage efficiency of each configuration, we plot in Figure 8 the time evolution of the liquid fraction  $L_f$ . Including more heated tubes results in an enhanced heat transfer and a faster melting process. The nine-tube configuration melts 5 times faster than the reference configuration with one tube. Note also from Figure 8 the good agreement between our results and those reported by Luo et al. (2015), obtained using a completely different model based on the Lattice Boltzmann Method. We checked again that the results obtained with 6 threads are identical to those computed with the sequential code.

#### 5.2.4. PCM-Case #4: Melting of Gallium in a rectangular cavity

The melting of the Gallium in a rectangular cavity is a challenging case that generated an animated debate in the literature, since Dantzig (1989), Le Quéré and Gobin (1999) showed that the flow has to display a multi-cellular structure, resulting from the hydrodynamic instabilities during the conduction regime before the onset of convection. This multi-cellular flow configuration was also found numerically by Hannoun et al. (2003). These authors pointed out that coarse grids or inconsistencies in the mathematical model could generate unphysical flows, with a mono-cellular convection cell. Therefore, this case is a relevant exercise to test the accuracy of our method. The parameters of this case are reported in Table 3. To capture the very small convection cells during the first step of the melting, Hannoun et al. (2003) used a  $800 \times 1,120$  fixed grid. With our adaptive method, a maximum of 4820 triangles are necessary to reproduce the numerical result of Hannoun et al. (2003). The grid size is thus reduced with our method by a factor of 100. We illustrate in Fig. 9 the configuration of the phase-change system at dimensionless time  $t = 0.02$ . Note in the left panel the refined mesh at the liquid-solid interface and also at the borders of each convection cell. The multi-cellular structure of the flow is illustrated by the velocity field presented in the middle panel. The structure of the temperature field in the right panel shows that the rolls of the convection cells are well resolved. The number of cells decreases later through a process of roll merging, as it was also reported by Hannoun et al. (2003). Our numerical results are in good agreement with the observations of Hannoun et al. (2003), Cerimele et al. (2002) and Giangi and Stella (2000).

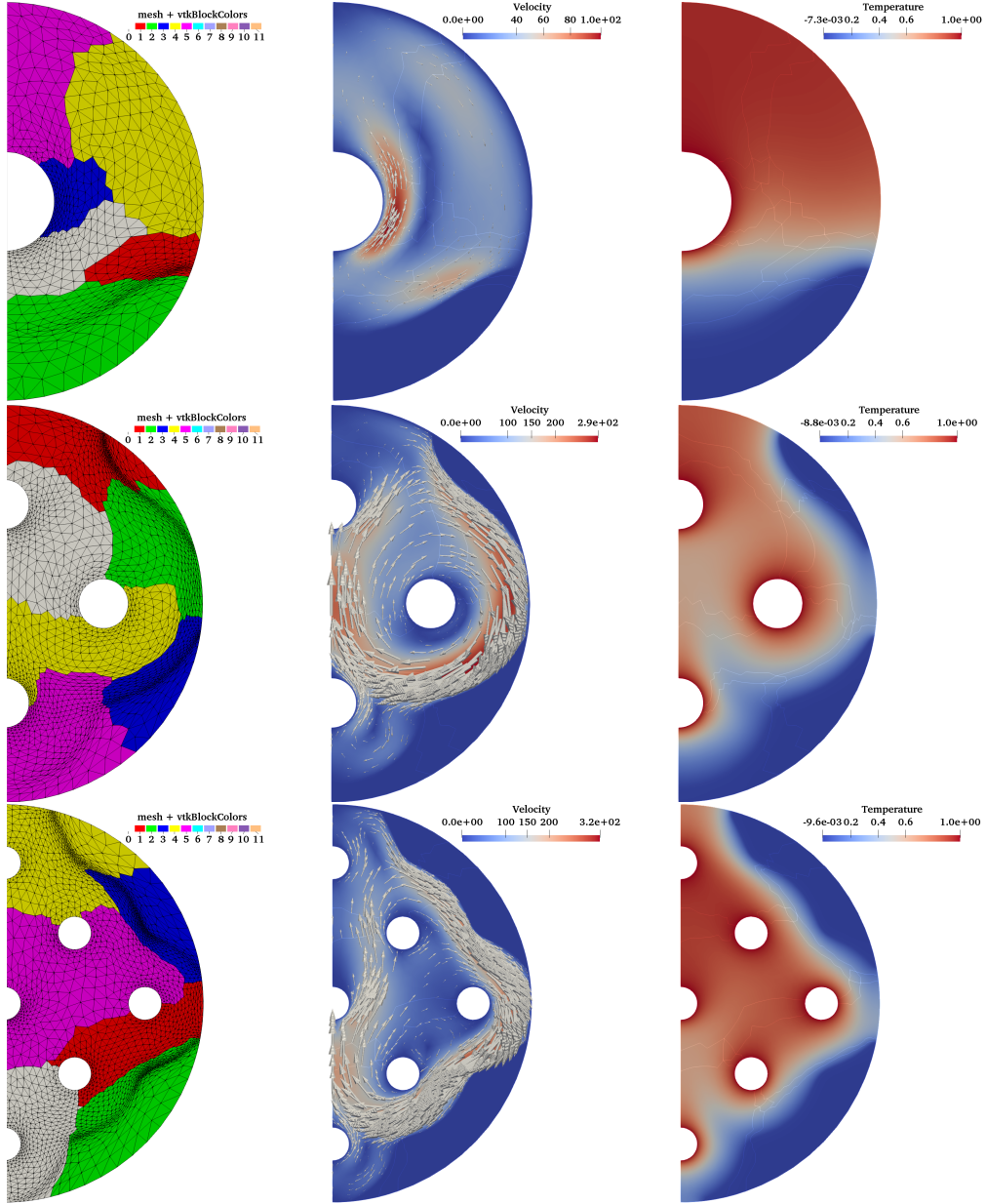


Figure 7: PCM-Case #3. Melting of a cylindrical PCM with heated inner tubes. Flow configuration for one tube at  $t = 2.491$  (first row), four tubes at  $t = 0.981$  (middle row) and nine tubes at  $t = 0.411$  (last row). Time instants correspond to the same liquid fraction in the system,  $L_f = 80\%$ . Adapted mesh and domain decomposition with 6 subdomains (left column), velocity vectors with background color representing the velocity intensity (central column) and temperature field (right column).



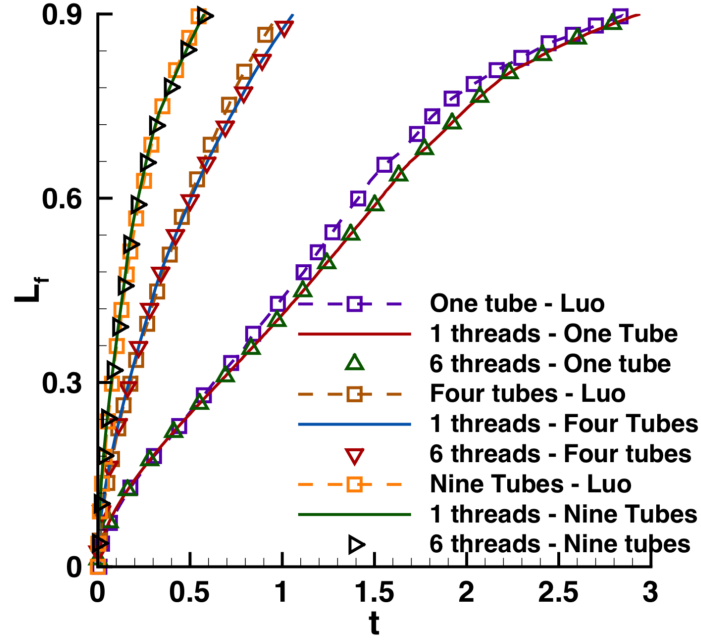


Figure 8: PCM-Case #3. Melting of a cylindrical PCM with heated inner tubes. Time evolution of the liquid fraction for configurations with one, four, and nine heated tubes. Comparison with numerical results of Luo et al. (2015).

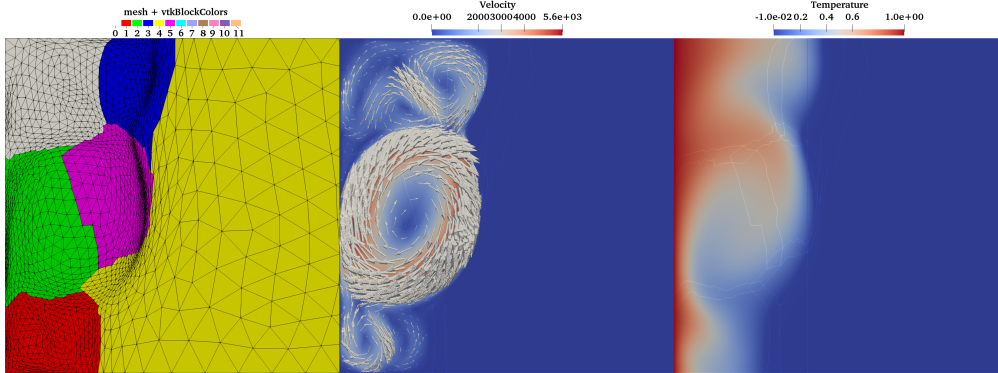


Figure 9: PCM-Case #4. Melting of Gallium. Simulated configuration at  $t = 0.02$ . Adapted finite-element mesh and subdomains used for the domain decomposition and parallel computing with 6 threads (left panel). Velocity vectors in the liquid phase (central panel). Temperature field (right panel).

### 5.2.5. PCM-Case #5: Solid crust formation in a highly distorted domain

This final PCM case considers the solidification of a PCM in a domain with a more complicated shape (Fig. 10). This case was simulated by [Nourgaliev et al. \(2016\)](#), using a discontinuous Galerkin finite element method. The fluid is initially motionless, with an initial dimensionless temperature  $\theta_0 = 2$ . The temperature of fusion is set to  $\theta_f = 1.4$ , according to [Nourgaliev et al. \(2016\)](#) (see Table 3 for the values of all parameters). The left side boundary is maintained at a cold temperature  $\theta_c = 1.39$  in the initial stage. The right wall is isothermal, with hot temperature  $\theta_h = 2$ . A nearly steady-state natural circulation is induced in the early time evolution of the flow. Then, the cold temperature at the left wall is decreased to  $\theta_c = 1$ , below the temperature of solidification. At this point, the formation of a solid crust layer starts at the left boundary. Figure 10 depicts the configuration of the solid-liquid system at dimensionless time  $t = 30$ . Mesh adaptivity used metrics computed from the two components of the velocity and from the phase-change variables (enthalpy and temperature). Consequently, it is shown in the left panel that the mesh is well adapted near the solid-liquid front and following the distorted shape of the convection cell in the liquid phase. In the middle panel, we notice the high velocity values defining the convection cell, waving in the liquid phase. The final panel of Fig. 10 shows the temperature field, with the solid phase well identified in blue. This structure of the flow is in a very good agreement with that reported by [Nourgaliev et al. \(2016\)](#).

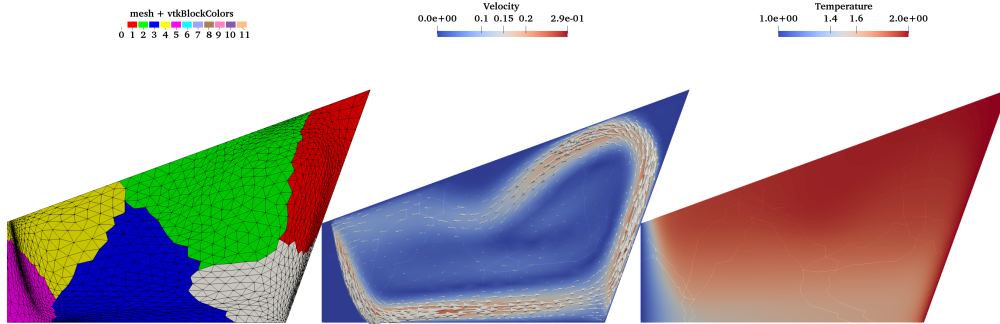


Figure 10: PCM-Case #5. Solid crust formation in a distorted domain. Simulated configuration at  $t = 29.33$ . Adapted finite-element mesh and subdomains used for the domain decomposition and parallel computing with 6 threads (left panel). Velocity vectors in the liquid phase (central panel). Temperature field (right panel).

### 5.3. Natural convection of water and water freezing

In this section we consider phase-change systems using water. Since pure water exhibits non-linear density variation for  $T < 10.2^\circ\text{C}$ , with a maximum at  $T_m = 4.0293^\circ\text{C}$ , the Boussinesq force becomes non-linear. Convection or freezing of water are therefore interesting cases to test the flexibility of our Toolbox to deal with additional non-linear terms. We used the following density-temperature formula suggested by [Gebhart and Mollendorf \(1977\)](#):

$$\rho(T) = \rho_m (1 - w |T - T_m|^q), \quad (31)$$



with  $\rho_m = 999.972 \text{ [kg/m}^3]$ ,  $w = 9.2793 \cdot 10^{-6} [(\text{°C})^{-q}]$ , and  $q = 1.894816$ .

Hence, the buoyancy term  $f_B = g(\rho_{ref} - \rho)/\rho_{ref}$  in (1) is not any more linear and becomes after scaling:

$$f_B(\theta) = \frac{Ra}{Pr Re^2} \frac{1}{\beta \delta T} \frac{\rho(\theta_f) - \rho(\theta)}{\rho(\theta_f)}, \quad (32)$$

where  $\beta = (1/\rho_m)(d\rho/dT)$  is the thermal expansion coefficient taking the value  $\beta = 6.91 \cdot 10^{-5} \text{ [(K)}^{-1}]$  (Scanlon and Stickland, 2004).

We simulate a differentially heated square cavity filled with liquid pure distilled water. This problem was investigated experimentally and numerically by [Giangi et al. \(2000\)](#); [Kowalewski and Rebow \(1999\)](#); [Michalek and Kowalewski \(2003\)](#). The non-dimensional parameters describing the problem are (see [Michalek and Kowalewski \(2003\)](#) for physical details):  $Ra = 2.518084 \cdot 10^6$ ,  $Pr = 6.99$  and  $Ste = 0.125$ .

### 5.3.1. Natural convection of water

The initial temperature is linearly distributed in the square cavity, with a hot temperature  $T_h = 10 \text{ °C}$  at the left wall and a cold temperature  $T_c = T_f = 0 \text{ °C}$  at the right wall. The temperature field and the streamlines of the steady state are presented in Figure 11a. The isoline  $\theta = \theta_m$ , corresponding to the line of maximum density is represented by a dashed line. Due to the anomalous thermal variation of water density, two recirculating zones are formed in the flow: a lower (abnormal) recirculation in the vicinity of the cold wall where  $\theta < \theta_m$  and an upper (normal) one where the density decreases with temperature ( $\theta > \theta_m$ ).

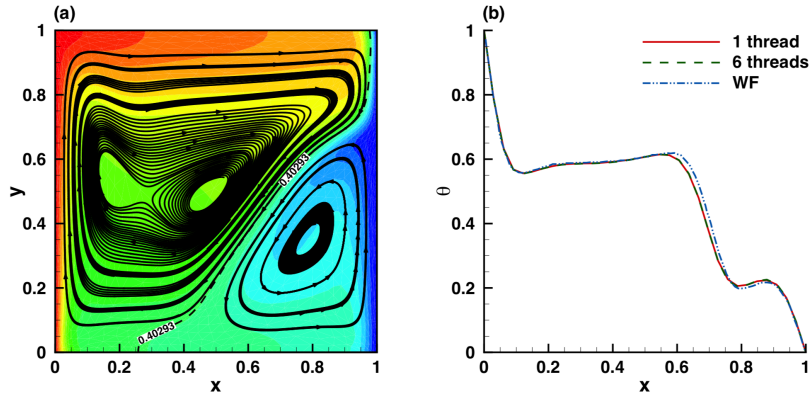


Figure 11: Natural convection of water in a differentially heated cavity. Non-dimensional temperature  $\theta$  at steady state. (a) Two-dimensional temperature field and streamlines showing the two recirculating zones. (b) Temperature profile along the horizontal central line. Comparison with the numerical results of [Michalek and Kowalewski \(2003\)](#).

A more precise comparison with previously published results is shown in Figure 11b. The obtained temperature profile  $\theta(x)$  along the horizontal central line of the cavity ( $y = 0.5$ ) is in good agreement with the numerical results of [Michalek and Kowalewski \(2003\)](#). Their results were obtained with finite-volume and finite-difference codes (FLUENT and FRECONV3V).

### 5.3.2. Water freezing

We finally consider the difficult case of water freezing in a square cavity. The initial state for this computation is the convection steady pattern in the cavity presented in Figure 11. The freezing starts by dropping smoothly the temperature of the cold right wall from  $T_c = 0^\circ\text{C}$  to  $T_c = -10^\circ\text{C}$ . The new boundary condition on the right cold wall is imposed by setting a very thin layer of  $\delta x = 0.01$ , with constant temperature  $T = T_c$  and zero velocity.

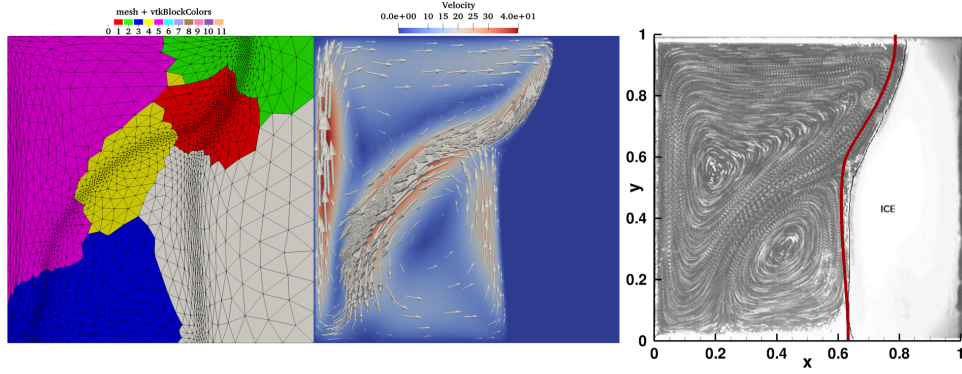


Figure 12: Freezing of pure water. Simulated configuration at  $t = 1.61$ . Adapted finite-element mesh and subdomains used for the domain decomposition and parallel computing with 6 threads (left panel). Velocity vectors in the liquid phase (central panel). Comparison with the experimental image from [Kowalewski and Rebow \(1999\)](#); the thick red line represents the solid-liquid interface computed with the present method (right panel).

Figure 12 shows the flow configuration at dimensionless time  $t = 1.61$ . The left panel depicts the domain composition and the adapted mesh following two lines of interest: the solid-liquid interface  $T = 0$  and the line  $T = T_m$  separating the two recirculating zones (see the middle panel of the same figure). The metrics used for adaptivity were computed from the two components of the velocity, the temperature and a  $P_1$  tanh-function  $\phi(T)$  "tracking" the value  $T_m$ . To reduce the impact of the interpolation on the global accuracy we used both  $\phi(T^n)$  and  $\phi(T^{n+1})$  in the adaptivity procedure (see also [Belhamadia et al. \(2004a\)](#)). This adaptivity strategy allowed us to accurately capture the structure and the extent of the two recirculating zones, features that are difficult to obtain with fixed meshes (discrepancies in numerical results are described in [Giangi et al. \(2000\)](#); [Kowalewski and Rebow \(1999\)](#); [Michalek and Kowalewski \(2003\)](#)). In the right panel of Fig. 12 we superimpose the experimental image from [Kowalewski and Rebow \(1999\)](#) with our numerical results for the same physical time  $t_\varphi = 2340[s]$ . The position of the solid-liquid interface and the flow pattern in the liquid phase correspond very well qualitatively to the experimental image. The simulation was performed with a small time step ( $\delta t = 10^{-2} \approx 15[s]$ ). Note from Table 1 that the computational time for this case is more than reasonable (23 minutes using 1 thread and only 13 minutes with 6 threads).

## 6. 3D parallel numerical results

All the 2D benchmarks presented in the previous section could be simulated in 3D using the second provided Toolbox `PCM_Toolbox_DDM_3D`. To avoid an excessively long paper, we shortly present in this section only the following selection of 3D cases: (i) the steady natural convection of air in a cubic cavity with  $Ra = 10^6$  (§6.1), (ii) the melting of a phase-change material (§6.2), within a cubic (§6.2.1) or cylindrical domain (§6.2.2), and (iv) the convection and the freezing of pure water in a cube (§6.3). Running parameters (the maximum number of degrees of freedom and the CPU times) for these cases are summarized in Table 4 and Table 5, for computations using  $P_1$  and  $P_2$  finite elements, respectively. Again, to make these simulations accessible with fast-running jobs in a batch-queuing system, we gave priority to jobs with a reasonable number of MPI processes (less than 400). We used 4GB memory for each CPU node for all simulations, excepting for the case PCM-Case #3 with 9 heated tubes, when 9GB of memory per node were necessary. In the subsequent sections, we present the results obtained with  $P_2$  finite elements for the temperature, since these simulations are more challenging. The results using  $P_1$  elements for the temperature are provided in the Supplemental Material <http://lmrs-num.math.cnrs.fr/2020CPCP2.html> containing images and animations of the cases presented in this section.

Case	CPU time	max of dof	processes	number of iterations	max mmg CPU time	ratio CPU time adapt / iteration
Unsteady NC of air, $Ra = 10^4$	00:55:21	249 625	6	23	9 sec.	6%
Unsteady NC of air, $Ra = 10^6$	01:14:49	725 097	56	50	20 sec.	19%
PCM-Case #1	07:42:32	3,299 661	224	80	53 sec.	16%
PCM-Case #3: 1 tube	16:02:31	3,809 760	224	401	65 sec.	17%
PCM-Case #3: 4 tubes	13:29:23	8,813 510	280	151	150 sec.	20%
PCM-Case #3: 9 tubes	10:37:44	14,860 117	364	71	262 sec.	24%
Cycle of a PCM	13:06:26	2,150 052	224	382	36 sec.	32%
NC of water	00:59:26	3,701 916	112	20	62 sec.	20%
Unsteady NC of water	06:39:40	5,492 302	112	37	76 sec.	14%
Water freezing	1-10:11:55	4,448 031	224	296	53 sec.	21%

Table 4: Running parameters for 3D simulations: the maximum number of degrees of freedom (dof) after mesh adaptivity, number of MPI processes for parallel computing and CPU time. All computations were performed using  $P_1$  finite elements for the temperature. All computation were performed using a parallel computer (CRIANN Computing Center and MATRICS platform) based on Intel Broadwell E5-2680 v4 @ 2.40GHz (14 cores per socket) architecture with two sockets per node and 128 GB of DDR4 2400 MHz RAM. An Intel Omnipath 100Gb/s low latency network was used for communications.

Case	CPU time	max of dof	processes	number of iterations	max mmg CPU time	ratio CPU time adapt / iteration
Unsteady NC of air, $Ra = 10^4$	01:12:38	313 769	6	23	9 sec.	5%
Unsteady NC of air, $Ra = 10^6$	01:22:33	913 057	56	50	20 sec.	18%
PCM-Case #1	08:05:24	4,871 640	224	80	66 sec.	13%
PCM-Case #3: 1 tube	21:49:27	3,919 350	224	401	49 sec.	12%
PCM-Case #3: 4 tubes	15:49:16	9,224 708	280	151	128 sec.	17%
PCM-Case #3: 9 tubes	13:23:43	14,981 519	364	71	210 sec.	17%
Cycle of a PCM	11:28:47	2,709 371	224	382	32 sec.	27%
NC of water	01:10:08	4,700 233	112	20	63 sec.	17%
Unsteady NC of water	07:14:19	6,049 784	112	35	82 sec.	12%
Water freezing	1-16:14:44	5,107 229	224	296	58 sec.	17%

Table 5: Same caption as for Table 5, but with all computations performed using  $P_2$  finite elements for the temperature.

### 6.1. Natural convection of air in a cubic cavity

We go back to the benchmark of natural convection of air described in §5.1 and add the third dimension in space. We thus simulate the thermally driven cubic cavity  $[0, 1]^3$ , filled with air. The temperature is now fixed on the left (cold) wall surface and the right (hot) wall surface. All the other lateral surfaces are adiabatic ( $\partial T / \partial n = 0$ ). No-slip walls are applied for the velocity on all boundary surfaces. We show in Fig. 13 the final (steady) flow configuration for  $Ra = 10^6$  obtained using the time-dependent solver with  $P_2$  finite-elements for the temperature. The mesh is mainly adapted following the boundary layers of the ascending and descending flows (Fig. 13a), which are clearly visible when representing the 3D velocity vectors (Fig. 13b). A quantitative assessment of the quality of the simulation is offered in Fig. 13c and Fig. 13d, comparing our results with those reported by Wakashima and Saitoh (2004). These authors solved the vorticity-stream function formulation of the Navier-Stokes equations using a fourth-order finite difference scheme and a uniform mesh of  $120^3$  grid nodes.

### 6.2. Melting of 3D phase-change materials

We simulate in this section 3D configurations of PCMs, in cubic or cylindrical geometries.

#### 6.2.1. Melting of a cubic octadecane PCM

We extend the 2D simulations presented in §5.2.1 to a 3D cubic domain  $\Omega = [0, 1]^3$ . We impose cold dimensionless temperature  $\theta_c = -0.01$  at  $x = 1$  (right wall), hot temperature  $\theta_h = 1$  at  $x = 0$  (left wall), and a homogeneous Neumann boundary condition at the remaining walls. A Dirichlet boundary condition  $\mathbf{u} = 0$  is prescribed for all surfaces defining  $\partial\Omega$ . The temperature distribution and the corresponding adapted mesh at  $t = 80.1$  is shown in Fig. 14a. The blue region denotes the solid phase. A zoom of

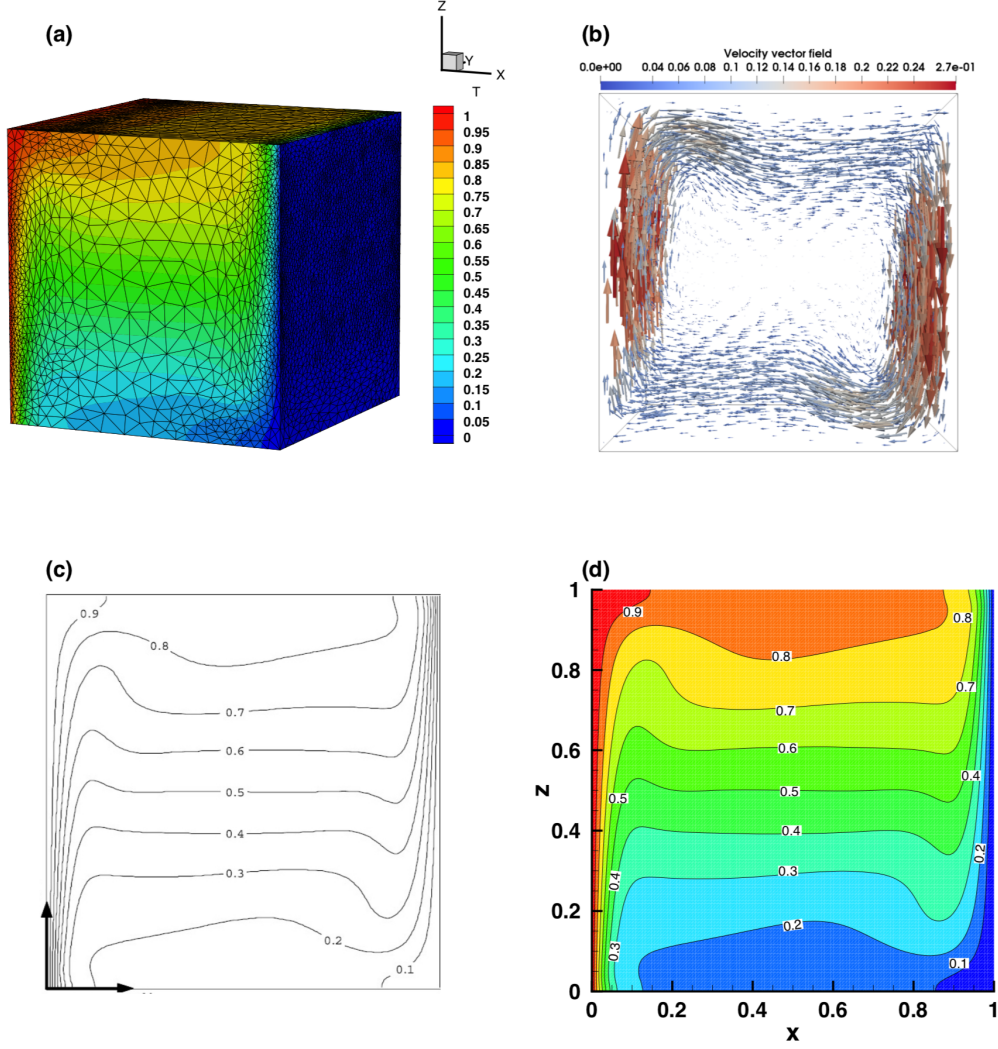


Figure 13: Natural convection of air in a cubic differentially heated cavity ( $Ra = 10^6$ ) computed with  $P_2$  finite elements for the temperature. (a) Adapted mesh with a maximum number of degrees of freedom of 913 057. (b) 3D velocity vector field in the final (steady) state. Temperature contour-lines in the central section of the cube ( $y = 0.5$ ): results of [Wakashima and Saitoh \(2004\)](#) (c) and present results (d). Parallel computation with 56 MPI processes.

the mesh in the mid-plane, at  $t = 80.1$ , refined along the iso-surface  $\theta = 0$ , is shown in Fig. 14b. As the heating progresses, the natural convection intensifies enough to have a pronounced influence on the shape of the interface. The temperature difference between the hot wall and the solid PCM induces a clockwise recirculation of the flow in the melted PCM (Fig. 14c). The shape of the liquid-solid interface at  $t = 80.1$  is also displayed in Fig. 14c, showing a non-uniform melting front receding from the top to the bottom



of the domain. The position of the solid-liquid interface at the mid-plane for 2D and 3D configurations is plotted in Fig. 14d. Differences between 2D and 3D results are visible. These are caused by the increase of the velocity in the liquid flow, induced by three-dimensional effects, as explained in Nikrityuk (2012).

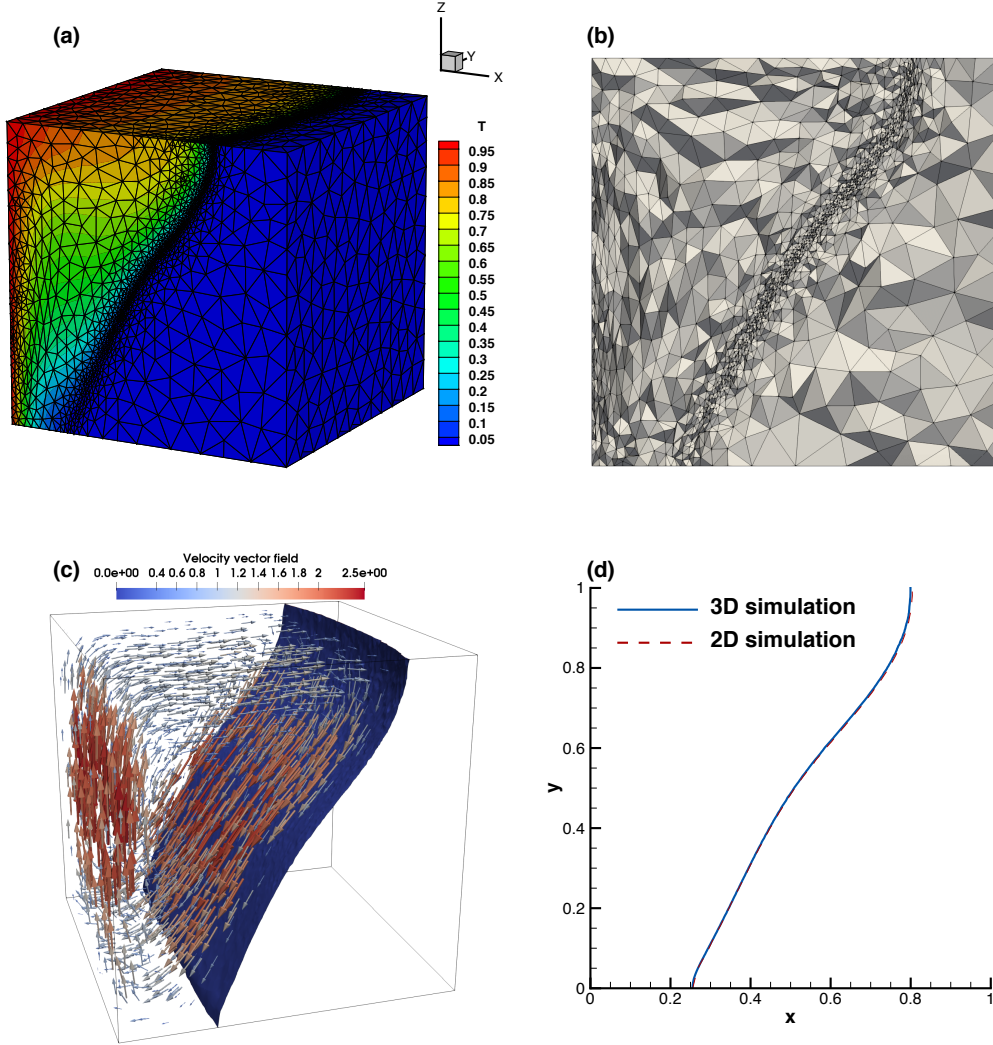


Figure 14: Melting of a cubic PCM (Okada, 1984) computed with  $P_2$  finite elements for the temperature. Configuration at  $t = 80.1$ , computed using 224 MPI processes with  $P_2$  finite elements for the temperature. (a) Adapted finite-element mesh with a maximum number of degrees of freedom  $\text{ndof} = 4,871\,640$ . (b) Illustration of the adapted mesh in the centre of the domain. (c) 3D velocity vectors and isosurface  $\theta = 0$  representing the liquid-solid interface. (d) 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).

### 6.2.2. Melting of a cylindrical PCM with inner heated tubes

We simulate the melting of a cylindrical PCM with inner heated tubes, as in §5.2.3. The 3D domain is now a horizontal cylinder of radius  $R = 1$  and length  $L = 0.25$ . In addition to the 2D configuration, we impose the following boundary conditions. For the temperature, a Dirichlet boundary condition ( $\theta = \theta_h = 1$ ) is applied at the inner tubes and a Neumann boundary condition ( $\frac{\partial \theta}{\partial n} = 0$ ) at the outer sections of the cylinder. For the velocity, a homogeneous Dirichlet boundary condition ( $\mathbf{u} = 0$ ) is prescribed on the lateral surfaces of external and inner cylinders and a symmetry boundary condition is imposed on the ending sections of the cylinder. The PCM is initially solid and when the melting process starts, a liquid layer grows around the heated tubes and expands toward the lateral boundary. A slice in the adapted mesh, the velocity vector field, and temperature iso-surfaces are illustrated in Fig. 15 for configurations with one, four, and nine heated tubes. The mesh is adapted along the melting front and in the boundary

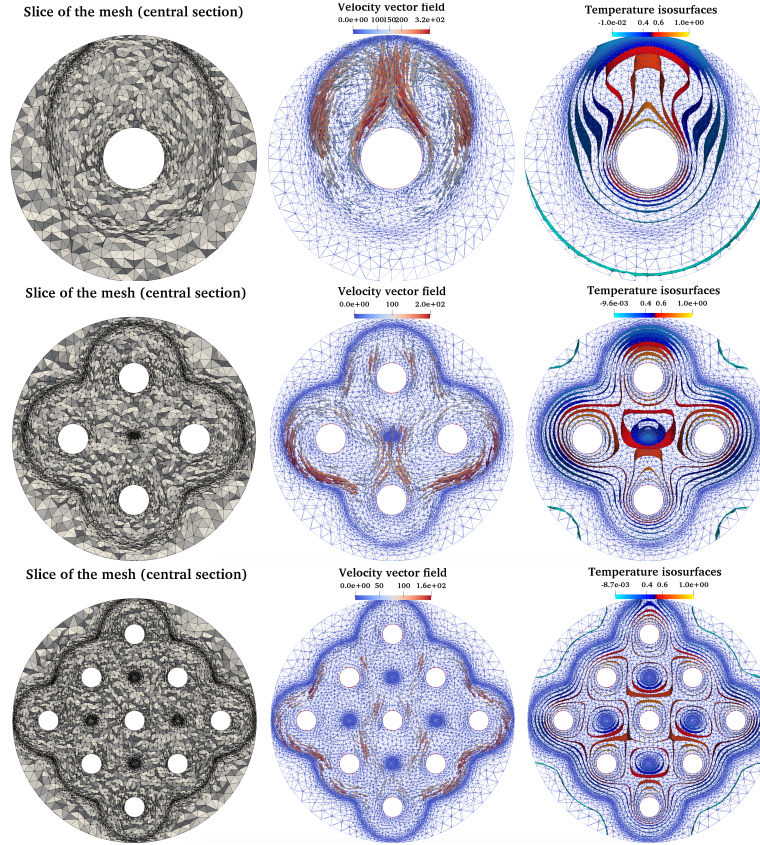


Figure 15: Melting of cylindrical PCM computed with  $P_2$  finite elements for the temperature. Adapted finite-element mesh (left panels), 3D velocity vector field (middle) and temperature iso-surfaces (right). Configurations with one inner heated tube (time instant  $t = 1.591$ , simulation with 224 MPI processes and a maximum number of degrees of freedom  $\text{ndof} = 3,919,350$ ), four tubes ( $t = 0.621$ , 280 processes and  $\text{max ndof} = 9,224,708$ ) and nine tubes ( $t = 0.331$ , 364 processes and  $\text{max ndof} = 14,981,519$ ).

layers around the heated tubes. Adaptivity is efficient even when the solid-liquid interface touches the outer wall (see left panels). Counter rotating flows are observed at the left and right parts of the cylindrical domain (middle panels). Iso-surfaces of temperature shown in the right panels also confirm that the evolution of the liquid flows keeps the symmetry of the configuration.

### 6.3. Natural convection of water and water freezing

We simulate in this final section the challenging case of the natural convection of water and the ice formation inside a differentially heated cubic cavity. The dimensionless parameters are the same that those used in §5.3.2. For the natural convection of water, the vertical walls at  $x = 0$  and  $x = 1$  are isothermal and have different temperatures  $\theta_h = 1$  and  $\theta_c = 0$ , respectively. The remaining walls are adiabatic. A homogeneous Dirichlet boundary condition  $\mathbf{u} = 0$  is applied on all walls. The fluid is initially at rest and the temperature is linearly distributed from the cold to the hot wall (see Fig. 16).

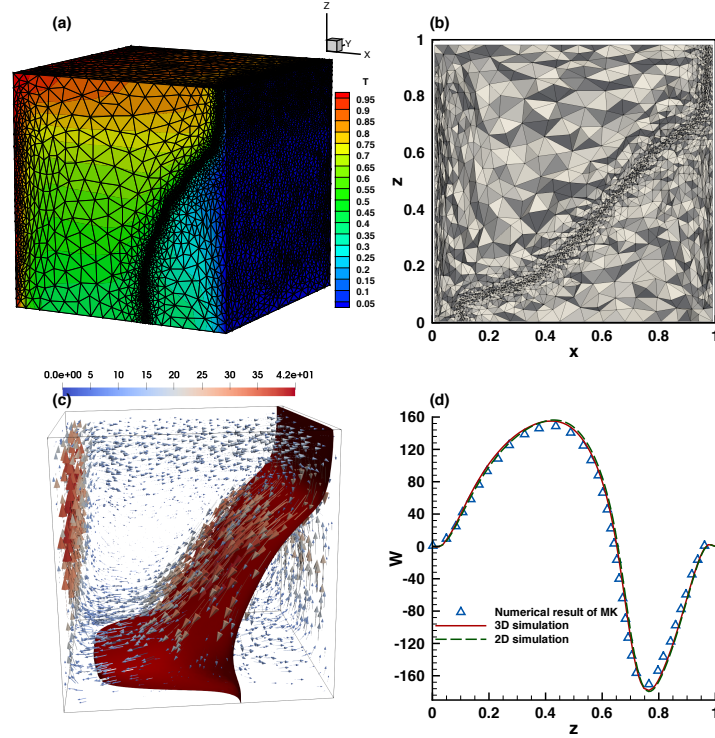


Figure 16: Natural convection of water in a differentially heated cubic cavity computed with  $P_2$  finite elements for the temperature. (a) Temperature distribution and 3D adapted finite element mesh at the steady state. (b) Illustration of the adapted mesh in the center of the domain. (c) Velocity vector field and temperature iso-surface  $\theta = 0.4$ . (d) Profile of the vertical velocity along the  $z$ -direction at the mid-plane ( $y = 0.5$ ) and  $x = 0.93$ . Comparison with the numerical benchmark suggested by [Kowalewski and Rebow \(1999\)](#) (symbols). Simulations using 112 MPI processes with  $P_2$  for the temperature and a maximum number of degrees of freedom  $\text{ndof}=4,700,233$ .



Given the anomalous thermal variation of water density, we also adapted the 3D mesh along  $\theta = 0.4$  to capture correctly the flow structure. The temperature distribution and the corresponding adapted mesh for the steady (time-independent) state computation is shown in Fig. 16a. The blue region identifies the cold water trapped by the abnormal fluid recirculation and the red region the hot fluid driven by the upper clockwise circulation. A cut in the mesh following the mid-plane (Fig. 16b) shows the internal structure of the mesh. Smaller tetrahedra are clearly observed in the vicinity of the walls and between the two counter-rotating circulation patterns. Figure 16c shows that the three-dimensional evolution of the flow (spiral movement of the fluid along the walls) affects the topology of the iso-surface  $\theta = 0.4$ .

Giangi et al. (2000) analyzed three-dimensional effects in both convection and freezing of water and they noted that only the flow in the symmetry plane is similar to the two-dimensional flow. They pointed out that no-slip velocity and adiabatic thermal boundary conditions at the side walls enhance three-dimensional effects near the walls. To validate this observation, we plot in Fig. 16d the profile of the vertical velocity along the  $z$  direction, at  $x = 0.93$  and passing through the velocity saddle point, where normal and abnormal convection streams collide in the vicinity of the cold wall. We compare both 2D and 3D simulations with 3D results of Michalek and Kowalewski (2003) (symbols), obtained with a finite-difference code. 3D (red solid line) profile agrees well with the benchmark solution with a maximum difference of 3%. As expected, the 2D (green dashed line) solution exhibits higher differences in the vicinity of the anomalous density variation, where the three-dimensional effect is maximum.

For the water freezing case, the simulation starts from the steady solution shown in Fig. 16. The cold temperature at the right wall is suddenly dropped from  $\theta_c = 0$  to  $\theta_c = -1$  (corresponding to physical temperature  $T_c = -10^\circ\text{C}$ ). Ice starts to form at the cold wall and expands towards the left wall. The temperature distribution and the adapted mesh at the final time  $t_\varphi = 2340[\text{s}]$  ( $t = 1.61$ ) are displayed in Figs. 17a and 17b.

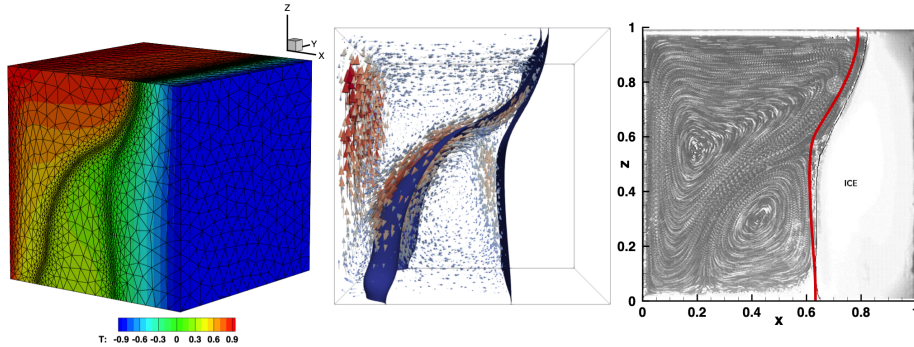


Figure 17: Freezing of pure water in a 3D cubical cavity computed with  $P_2$  finite elements for the temperature. (a) Temperature distribution and adapted mesh at time instant  $t = 1.61$ . (b) Cut through the adapted mesh at mid-plane. (c) 3D velocity vectors in the liquid phase and temperature iso-surfaces  $\theta = 0.4$  and  $\theta = 0$ . (d) Superimposition of the interface obtained in the present simulation (red line) on the experimental image of Kowalewski and Rebow (1999). Simulations using 224 MPI processes with  $P_2$  for the temperature and a max of degrees of freedom 5,107,229.

When compared to the natural convection case (Fig. 16), the mesh is also adapted along a second moving front represented by the solid-liquid interface (iso-surface  $\theta = 0$  shown in Fig. 17c). For the identification of flow structures during the ice formation, Fig. 17c shows the 3D velocity vectors, the iso-surface  $\theta = 0.4$  along the anomalous density variation, and the phase-change front at time instant  $t = 1.61$ . The effect of the secondary flow (see Nikrityuk (2012)) is visible from the curved shape of the iso-surface  $\theta = \theta_m$  in the transverse  $y$  direction. We note, however, that the shape of the solidification front is almost 2D. The buoyancy-induced fluid motion in the abnormal recirculation region is too weak to influence the solid front. Finally, the superimposition of the experimental image of Kowalewski and Rebow (1999) and the current simulation gives a good agreement for the location of the solid-liquid interface. Differences come mainly from the fact that the undercooling phenomenon during the solidification stage is not taken into account in our physical model.

#### 6.4. Scalability test for 3D parallel computations

We present the results for both strong and weak scalability tests. We simulate the 3D unsteady natural convection of air with  $Ra = 10^6$  presented in §6.1. Mesh adaptation is used only for the strong scalability test.

The CPU are Intel Broadwell E5-2680 v4 @ 2.40GHz (14 cores per socket). Each node has two sockets and 128 GB of DDR4 2400 MHz RAM. They communicate through Intel Omnipath 100Gb/s low latency network. First, we report the simulation time, the efficiency and speed-up for the weak (Fig. 18) and strong scalability tests (Fig. 19). Assuming a perfect speed-up for 8 cores, we obtained for 256 cores a speed-up of approximately 122.56 (weak) and 70.6 (strong), resulting in an efficiency of 47.9%(weak) and 27.6%(strong).

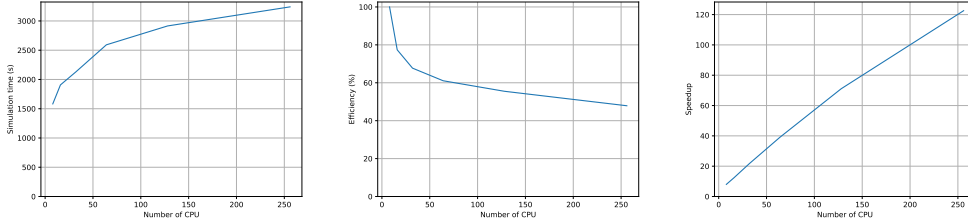


Figure 18: Weak scalability test for 3D simulations: simulation time (left), efficiency (center) and speed-up (right) for a number of processes ranging from 8 to 256.

In Figs. 20 (weak) and 21 (strong), we report the computational time for the main steps of the computational algorithm, namely the mesh adaptation, the matrix construction and the resolution of the linear system. For 8 cores, the mesh adaptation takes 221.9s (strong), the construction of the matrix 83.5s (strong) and 0.96s (weak) and the resolution of the linear system 4866.9s (strong) and 552.1s (weak). For 256 cores, the mesh adaptation takes 223.0s (strong), the construction of the matrix 76.4s (strong) and 6.91s (weak) and the resolution of the linear system 422.2s (strong) and 893.5s (weak). It results from this analysis that the only step that benefits from the parallelization is the resolution of the

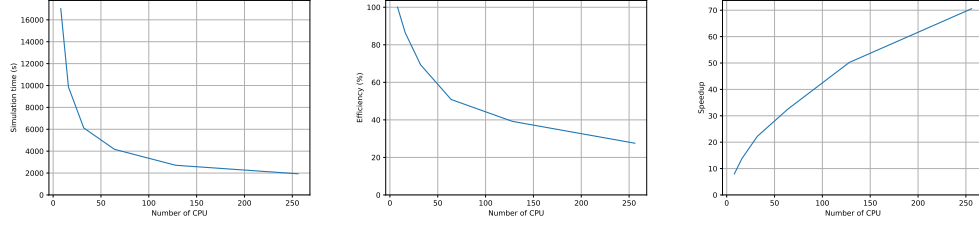


Figure 19: Strong scalability test for 3D simulations: simulation time (left), efficiency (center) and speed-up (right) for a number of processes ranging from 8 to 256.

linear system. The speed-up of the resolution of the linear system is 78.9 (strong) and 158.2 (weak), resulting in an efficiency of 36.0% (strong) and 61,8% (weak).

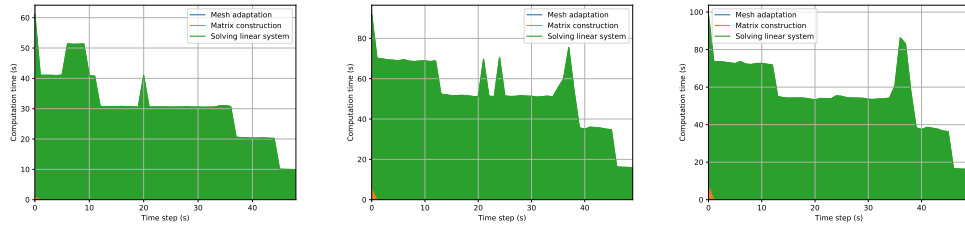


Figure 20: Weak scalability test: stacked timings of the main steps of the computation using 8 (left), 24 (center) and 112 (right) processes.

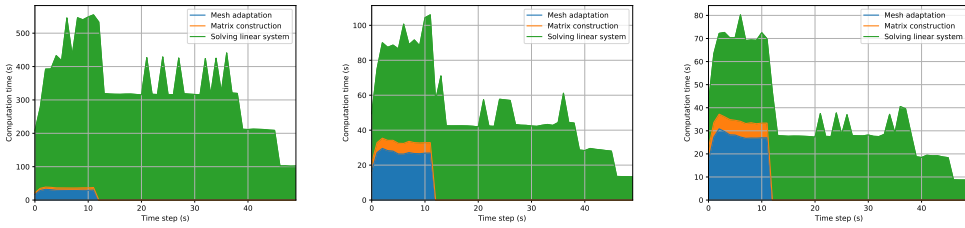


Figure 21: Strong scalability test: stacked timings of the main steps of the computation using 8 (left), 24 (center) and 112 (right) processes.

## 7. Summary and conclusions

The main advantage of the new toolbox distributed with this paper is to enable parallel computing of liquid-solid phase-change systems in 2D or 3D complex geometries. The physical model implemented in the software is one of the most accurate existing for such systems: the enthalpy-porosity model, based on the incompressible Navier-Stokes equations with Boussinesq approximation for thermal effects. This model captures all the characteristics of the flow developing in the liquid phase, dominated by convection. Using a Carman-Kozeny-type penalty term, added to the momentum equations to bring progressively the velocity to zero into the solid, results in a single-domain formulation of equations for both liquid and solid phases. We proved that this single-domain enthalpy-porosity model is well adapted to the use of Schwarz domain decomposition methods (DDM), and, consequently, to parallel computing.

The numerical method was implemented using FreeFem++ , a free software offering multiple advantages to easily implement a finite-element algorithm. The key ingredients of the implemented method are: (i) a second order accuracy in space ( $P_2$  finite elements for velocity and temperature,  $P_1$  for the pressure) and time (Gear scheme); (ii) the use of an adaptive finite element method with regularized functions representing the variation of thermodynamic properties at the solid-liquid interface, (iii) a fully implicit discretization with a Newton algorithm for solving the non-linear system of equations, and (iv) a parallel final algorithm using automatic partitioners (*Scotch* or *Metis*) and the recent library *ffdm* that makes available in FreeFem++ state-of-the-art scalable Schwarz domain decomposition methods. Mesh adaptivity is an essential ingredient of the toolbox and a new algorithm was implemented using external remeshing tools (*mmg*) for 3D configurations.

We presented careful validations of the toolbox by considering parallel 2D and 3D computations of well-known benchmark cases of increasing difficulty: natural convection of air, natural convection of water, melting or solidification of a phase-change material, and, finally, a water freezing case. For 2D configurations, parallel computations with the present toolbox using modest resources (6 MPI processes) can bring a CPU gain factor between 2 and 3, when compared to previous sequential algorithms ([Rakotonrandisa et al., 2020](#)). But the most significant progress brought by the new toolbox is to make affordable well-resolved 3D computations with mesh adaptivity, which are hardly accessible with sequential algorithms. The efficiency of the toolbox in 3D was demonstrated by simulating difficult cases (melting of a PCM, water freezing) in simple (cubic) or complex geometries (cylindrical with inner tubes).

Supplementary images and movies depicting the dynamics of some cases simulated in this paper are provided as Supplemental Material at <http://lmrs-num.math.cnrs.fr/2020CPCP2.html>.

To facilitate its use, the toolbox is provided with separate folders containing all the necessary files (parameters, restart files) necessary to run all the cases described in the paper. Ready-made scripts and layouts allow the user to generate the figures presented in this paper with newly generated data after running the programs. Validation data sets from experiments or previous publications are included in these layouts. As a consequence, the present parallel approach can be easily tested and eventually adapted to simulate other related phase-change problems. The modular programming and the syntax close to the mathematical formulation offer the possibility to address other computational

challenges related to different physical or mathematical models in this field. In particular, the possibility to enrich the physical model for the solidification will be considered in a future version of the toolbox.

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