Phase change problem with natural convection

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Overview

Simulation Tool: FreeFem++

Developed by: *F. Hecht. New development in freefem++. J. Numer. Math., 2012.*
Reference to: G. Sadaka et. al., Parallel finite-element codes for the simulation of two-dimensional and three-dimensional solid-liquid phase-change systems with natural convection, Comput. Phys. Comm. 257 (2020) 107492,

- **Mmg**: an open source software for simplicial remeshing, FreeFEM provide the interface for the Mmg. `https://www.mmgtools.org/`
- **ffddm**: a FreeFEM library for parallelization with domain decomposition methods.

Visualization: **Paraview**

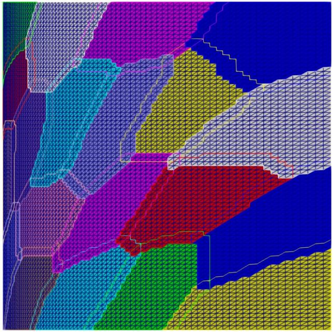

Figure: Domain decomposition on an adaptive mesh with multiple MPI processors

Overview

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The heat transfer equation

In the general heat conduction equation[M.M. Brahim thesis, 2016], the enthalpy H is defined as the sum of sensible and latent heat:

$$\partial_t H - \nabla \cdot (\kappa \nabla T) = 0,$$

$$H(T) = \int_0^T \rho c_p dT + \rho f(T) \Delta H,$$

where the liquid fractional function:

$$f(T) = \begin{cases} 0, & T(x,t) < T_m \\ 1, & T(x,t) \geq T_m \end{cases}$$

Re-write the equation:

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) - \rho_s \Delta H_m \frac{\partial f}{\partial t}.$$

Phase field function

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Definition

In a confined domain $\Omega \in R^d, (d = 2, 3)$, a phase variable (or a labelling function) $\phi(x, t)$ is introduced to label the liquid and solid phase, respectively:

$$\phi(\mathbf{x}, t) = \begin{cases} -1, & \text{phase 1} \\ 1, & \text{phase 2.} \end{cases}$$

with a thin smooth transition layer of thickness ε connecting the two phases.

Interface:

$$\{\mathbf{x} : \phi(\mathbf{x}, t) = 0\}.$$

Phase field method

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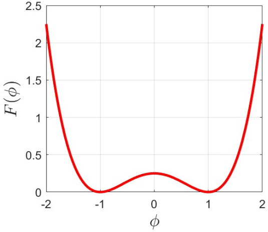
Define the free energy functional:

$$E(\phi) = \int_\Omega (\frac{\varepsilon^2}{2}|\nabla\phi|^2 + F(\phi))d\mathbf{x},$$

where $F(\phi) = \frac{1}{4}(1-\phi^2)^2$ is the Ginzburg-Landau double well potential.

$$F(-1) = F(1) = 0,$$

$$f(\phi) := F'(\phi) = \phi^3 - \phi, f'(-1) = f'(1) = 0.$$



The dynamics eqns can be determined by a gradient flow by taking the variational derivative in L^2:

$$\phi_t + (u\cdot\nabla)\phi = -\gamma\frac{\delta E}{\delta\phi},$$

$$\phi_t + (u\cdot\nabla)\phi = \gamma(\varepsilon^2\Delta\phi - f(\phi)).$$ Allen-Cahn eqn

Governing Equations on the phase field method

We consider the case with velocity equals to zero, and with the heat transfer equation, the governing dynamical equation can be approach as follows:

$$\alpha\varepsilon^2\phi_t = \varepsilon^2\Delta\phi - f(\phi) + \lambda\varepsilon(T - T_m)g(\phi),$$
$$\rho c_p T_t = \nabla\cdot(\kappa\nabla T) - \frac{\rho_s \Delta H_m}{2}\phi_t.$$

where

$$g(\phi) = G'(\phi) = (1-\phi^2)^2, \qquad \rho(\phi) = \frac{1-\phi}{2}\rho_s + \frac{1+\phi}{2}\rho_l,$$
$$c_p(\phi) = \frac{1-\phi}{2}c_{ps} + \frac{1+\phi}{2}c_{pl}, \qquad \kappa(\phi) = \frac{1-\phi}{2}\kappa_s + \frac{1+\phi}{2}\kappa_l.$$

Overview

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A model for convective melting problem

To solve $(\phi, T, \mathbf{u}, p)$:

$$
\begin{aligned}
&\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} - \nabla\cdot\nu\nabla\mathbf{u} + \nabla p + A(\phi)\mathbf{u} = \beta(T - T_m)\mathbf{e}_d,\\
&\nabla\cdot\mathbf{u} = 0,\\
&\alpha\varepsilon^2(\phi_t + \mathbf{u}\cdot\nabla\phi) = \varepsilon^2\Delta\phi - f(\phi) + \lambda\varepsilon(T - T_m)g(\phi),\\
&\rho c_p(T_t + \mathbf{u}\cdot\nabla T) = \nabla\cdot(\kappa\nabla T) - \frac{\rho_s\Delta H_m}{2}\phi_t.
\end{aligned}
$$

with

$$
A(\phi) = -\frac{C_{CK}(1-\phi)^2}{(1+\phi)^3 + b},\qquad \rho = \frac{1-\phi}{2}\rho_s + \frac{1+\phi}{2}\rho_l,
$$

$$
f(\phi) = F'(\phi) = \frac{1}{2}\phi(\phi^2 - 1),\qquad c_p = \frac{1-\phi}{2}c_{ps} + \frac{1+\phi}{2}c_{pl},
$$

$$
g(\phi) = G'(\phi) = (1-\phi^2)^2,\qquad \kappa = \frac{1-\phi}{2}\kappa_s + \frac{1+\phi}{2}\kappa_l.
$$

Drop the convective term $\mathbf{u} \cdot \nabla \phi$?

The term $\mathbf{u} \cdot \nabla \phi$ may not be necessary in the phase field equation:

$$\alpha \varepsilon^2 (\phi_t + \cancel{\mathbf{u} \cdot \nabla \phi}) = \varepsilon^2 \Delta \phi - f(\phi) + \lambda \varepsilon (T - T_m) g(\phi).$$

Drop the convective term $\mathbf{u} \cdot \nabla\phi$?

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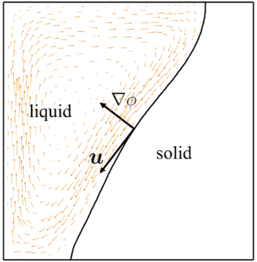
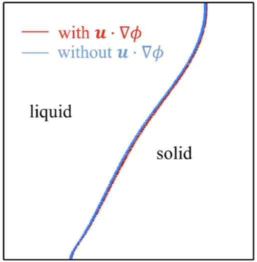
$$\alpha\varepsilon^2(\phi_t + \cancel{\mathbf{u} \cdot \nabla\phi}) = \varepsilon^2\Delta\phi - f(\phi) + \lambda\varepsilon(T - T_m)g(\phi).$$

- Flow and thermal convection from $\mathbf{u} \cdot \nabla\mathbf{u}$ and $\mathbf{u} \cdot \nabla T$
- Temperature-driven : $\lambda\varepsilon(T - T_m)g(\phi)$
- $\mathbf{u} \cdot \nabla\phi$ works only on the interface
- Orthogonality on interface: $\mathbf{u} \perp \nabla\phi$





A model for convective melting problem

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To solve $(\phi, T, \mathbf{u}, p)$:

$$\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} - \nabla\cdot\nu\nabla\mathbf{u} + \nabla p + A(\phi)\mathbf{u} = \beta(T - T_m)\mathbf{e}_d,$$
$$\nabla\cdot\mathbf{u} = 0,$$
$$\alpha\varepsilon^2\phi_t = \varepsilon^2\Delta\phi - f(\phi) + \lambda\varepsilon(T - T_m)g(\phi),$$
$$\rho c_p(T_t + \mathbf{u}\cdot\nabla T) = \nabla\cdot(\kappa\nabla T) - \frac{\rho_s\Delta H_m}{2}\phi_t.$$

with

$$A(\phi) = -\frac{C_{CK}(1-\phi)^2}{(1+\phi)^3 + b}, \qquad \rho = \frac{1-\phi}{2}\rho_s + \frac{1+\phi}{2}\rho_l,$$
$$f(\phi) = F'(\phi) = \frac{1}{2}\phi(\phi^2 - 1), \qquad c_p = \frac{1-\phi}{2}c_{ps} + \frac{1+\phi}{2}c_{pl},$$
$$g(\phi) = G'(\phi) = (1-\phi^2)^2, \qquad \kappa = \frac{1-\phi}{2}\kappa_s + \frac{1+\phi}{2}\kappa_l.$$

Numerical Method

$$\frac{\mathbf{u}^{n+1}-\mathbf{u}^{n}}{\Delta t}+\mathbf{u}^{n}\cdot\nabla\mathbf{u}^{n+1}-\nu\Delta\mathbf{u}^{n+1}-A(\phi^{n})\mathbf{u}^{n+1}+\nabla p^{n+1}=\beta(T^{n}-T_{m})\mathbf{e}_{d},$$

$$\nabla\cdot\mathbf{u}^{n+1}=0,$$

$$\alpha\varepsilon^{2}\frac{\phi^{n+1}-\phi^{n}}{\Delta t}=\varepsilon^{2}\Delta\phi^{n+1}-f(\phi^{n})+\lambda\varepsilon(T^{n+1}-T_{m})g(\phi^{n}),$$

$$\rho c_{p}\left(\frac{T^{n+1}-T^{n}}{\Delta t}+\mathbf{u}^{n+1}\cdot\nabla T^{n+1}\right)=\nabla\cdot(\kappa\nabla T^{n+1})-\frac{\rho\Delta H_{m}}{2\Delta t}(\phi^{n+1}-\phi^{n}).$$

Maximum bound principle for phase field

$$(1 - \Delta t \alpha^{-1} \Delta)\phi^{n+1} = \phi^n - \Delta t \alpha^{-1} \varepsilon^{-2} (f(\phi^n) - \lambda \varepsilon (T^{n+1} - T_m) g(\phi^n)). \qquad (5)$$

Theorem (Maximum bound principle)

Assume that the initial value $\|\phi^0\|_\infty \leq 1$, if the time step size Δt satisfies the condition:

$$\frac{1}{\Delta t} \geq \alpha^{-1} \varepsilon^{-2} \max_y \max_{|x| \leq 1} \frac{\partial^2 D}{\partial x^2}, \qquad (6)$$

with $D(x, y) := F(x) - \lambda\varepsilon(y - T_m)G(x), \quad x \in [-1, 1], y \in [T_c, T_h]$,
then the scheme (5) *preserves the maximum bound principle:*

$$\|\phi^n\|_\infty \leq 1, \quad \forall n \geq 0.$$

We have an estimate of Δt by (6):

$$\frac{1}{\Delta t} \geq \alpha^{-1} \varepsilon^{-2} (1.5391 \lambda \varepsilon |y_{\max} - T_m| + 0.0344).$$

Validation on tolerable time step size

In the case of melting Octadecane in a unit square cavity, we set the parameters:
$\rho = \rho_s = 1, c_p = 1, \kappa = 0.0178, \nu = 1, C_{ck} = 10^6, b = 10^{-7}, \Delta H_m = 22.22, \varepsilon = 0.01, T_m = 0, \beta = 125.77, \lambda = 10^3, t_{\max} = 79.1$ and $h \in [0.002, 0.07]$.

If $y_{\max}$ is taken from the heating temperature as 1, then the estimate $\Delta t = 0.0166$. This condition is too strong, because the term $\lambda\varepsilon(T - T_m)g(\phi)$ is only active on the interface, and T nearing the interface is lower than the heating temperature.

Δt	0.01	0.0166	0.0174	0.02	
$\lvert\max_n \lVert\phi^n\rVert_\infty - 1\rvert$	1e-5	2e-5	2e-5	2e-5	
Δt	0.066	0.08	0.1	0.15	0.2
$\lvert\max_n \lVert\phi^n\rVert_\infty - 1\rvert$	8e-5	9e-5	0.01825	0.10139	0.18748

Table: The bound of phase field solution with different time step size in case of melting of Octacane.

Melting of Octadecane

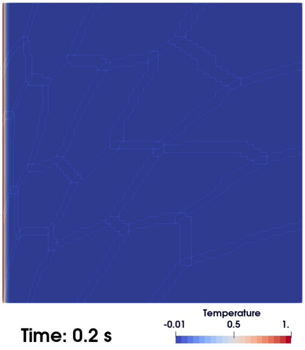


Figure: (a) Temperature

Figure: (b) Streamlines and phase field

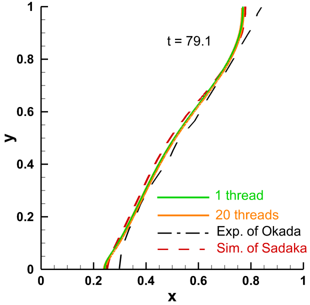
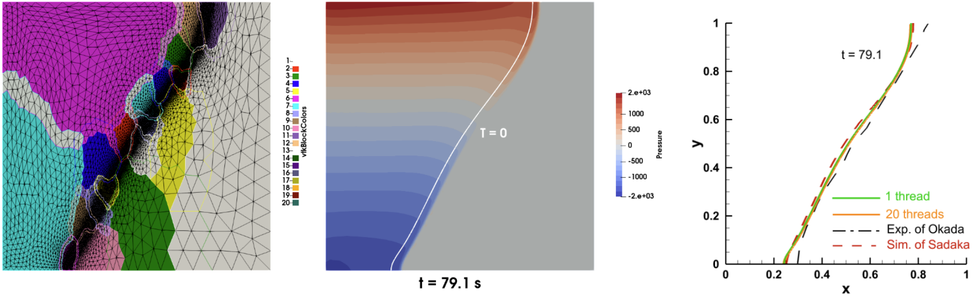


Figure: (c) Experimental Results

Melting of Octadecane



(a) (b) (c)

Figure: Melting of Octadecane at $t = 79.1$: (a) Domain decomposition with 20 MPI processors. (b) Pressure contours. (c) Comparison of interface positions: Our numerical results, results from the experiment by Okada et al. 1984, and numerical results from Sadaka et al. 2020.

Water Freezing

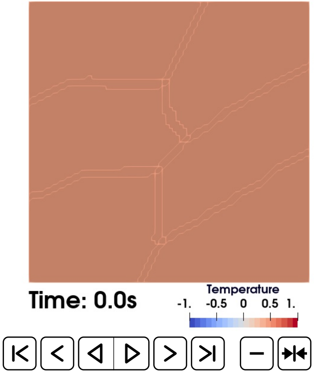


Figure: (a) Temperature

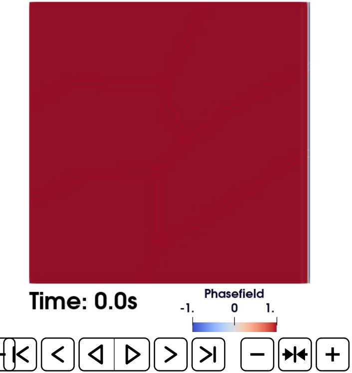


Figure: (b) Streamlines and phase field

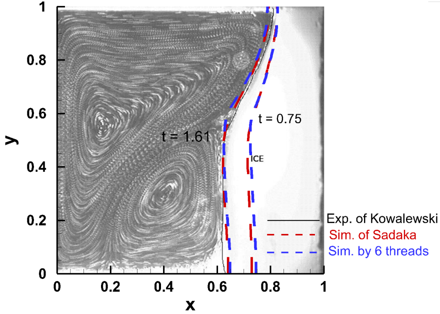
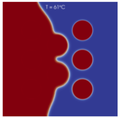


Figure: (c) Experimental photo

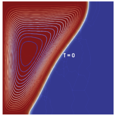
Summary

The classical system

$$\alpha\varepsilon^2\phi_t = \varepsilon^2\Delta\phi - f(\phi) + \lambda\varepsilon(T - T_m)g(\phi),$$
$$\rho c_p T_t = \nabla\cdot(\kappa\nabla T) - \frac{\rho_s \Delta H_m}{2}\phi_t.$$



PCM + enhancers,
without convection,
by:
Penalty on phase field



Pure PCM + convection,
by:
CK Penalty on velocity

1. **H. Yao***, M. Azaiez, A monolithic model for solid-liquid phase change problem, *Computer Methods in Applied Mechanics and Engineering*, 421,116794 , 2024.
2. **H. Yao***, A phase field method for convectional phase change problem preserving maximum bound principle, *Applied Numerical Mathematics*, 204, 232-248, 2024.

Merci
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