Accurate interface tracking for phase-change problems with natural convection

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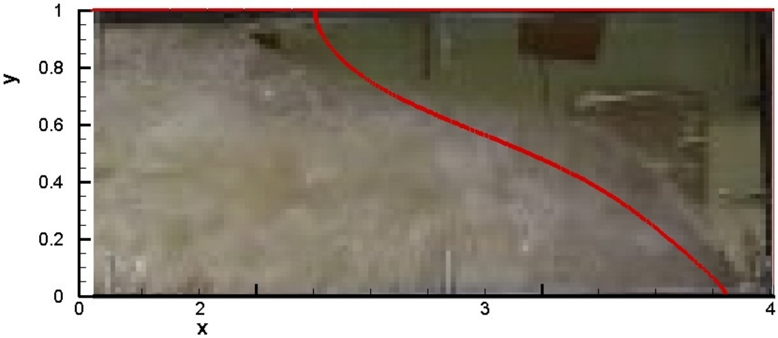
Outline

Motivation

Phase change materials (PCM)

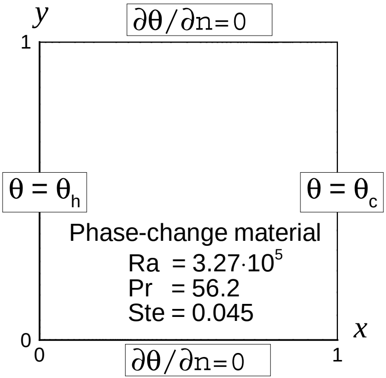


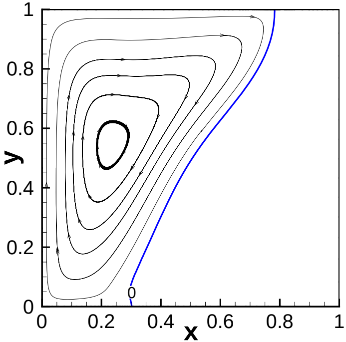
Melting of a PCM alcane. Experimental image.
Orange Labs (Lannion).

Outline

Mathematical model

- single domain approach [e.g. Ma & Zhang, IJNMHFF, 2006.]
- enthalpy methods [e.g. Voller & Prakash, IJHMT, 1987.]





Navier-Stokes-Boussinesq enthalpy based models

$$Re = \frac{\rho_{ref} V_{ref} L_{ref}}{\mu_l}, \quad Pr = \frac{\nu_l}{\alpha_l}, \quad Ra = \frac{g \beta L_{ref}^3 (T_h - T_c)}{\nu_l \alpha_l},$$

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

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} + \nabla p - \frac{1}{Re} \nabla \cdot \left(2 \mu_{sl}(\theta) \, \vec{D}(\vec{u}) \right) - f_B(\theta) \, \vec{e}_y = 0.$$

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

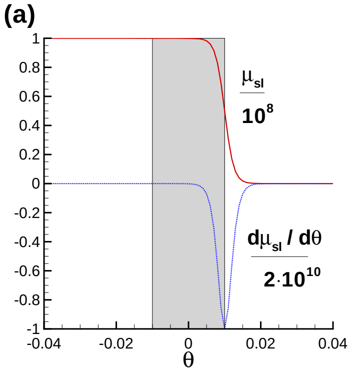
$$f_B(\theta) = \frac{Ra}{Pr \, Re^2} \theta, \quad f_B(\theta) = g(\rho_{ref} - \rho(\theta)/\rho_{ref} .$$

Mushy region for phase change

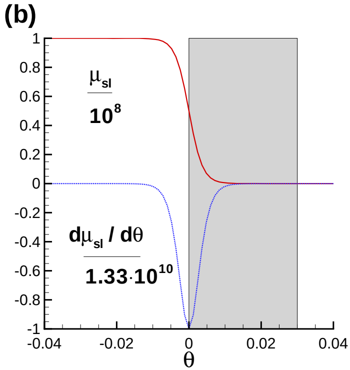
- compute huge gradients for

$\mu_{sl}(\theta), C = c_s/c_l, K = k_s/k_l, S = s/(T_h - T_c)$

- regularize these functions in the mushy region



PCM melting



water solidification

Outline

Finite element discretization: penalization method

$$
\begin{aligned}
b\left(\vec{u}^{n+1}, q\right) - \gamma(p^{n+1}, q) &= 0, \forall\, q \in Q \\
\frac{1}{\delta t}\left(\vec{u}^{n+1}, \vec{v}\right) + c\left(\vec{u}^{n+1}; \vec{u}^{n+1}, \vec{v}\right) + a\left(\mu_l; \vec{u}^{n+1}, \vec{v}\right) & \\
+b\left(\vec{v}, p^{n+1}\right) - \left(f_B(\theta^{n+1})\, \vec{e}_y, \vec{v}\right) &= \frac{1}{\delta t}\left(\vec{u}^{n}, \vec{v}\right), \forall\, \vec{v} \in \vec{V} \\
\frac{1}{\delta t}\left(\theta^{n+1}, \phi\right) - \left(\vec{u}^{n+1} \cdot \nabla\phi, \theta^{n+1}\right) + \left(\frac{K}{Pr}\nabla\theta^{n+1}, \nabla\phi\right) &= \frac{1}{\delta t}\left(\theta^{n}, \phi\right), \forall\, \phi \in V,
\end{aligned}
$$

$$a : \vec{V} \times \vec{V} \to \mathbb{R}, \qquad a(\mu; \vec{u}, \vec{v}) = \int_\Omega 2\mu\, \vec{D}(\vec{u}) : \vec{D}(\vec{v}),$$

$$b : \vec{V} \times Q \to \mathbb{R}, \qquad b(\vec{u}, q) = -\int_\Omega \nabla \cdot \vec{u}\, q = -\sum_{i=1}^{2} \int_\Omega \partial_i u_i \cdot q$$

$$c : \vec{V} \times \vec{V} \times \vec{V} \to \mathbb{R}, \qquad c(\vec{w}; \vec{z}, \vec{v}) = \int_\Omega \left[(\vec{w} \cdot \nabla)\, \vec{z}\right] \cdot \vec{v} = \sum_{i,j=1}^{2} \int_\Omega w_j(\partial_j z_i) v_i.$$

Newton method

- fully-implicit formulation for the viscosity,
- mesh adaptivity with Taylor-Hood finite elements.

$$
\begin{aligned}
b\left(\vec{u}_w, q\right) - \gamma(p_w, q) &= b\left(\vec{u}^k, q\right) - \gamma(p^k, q), \\
\frac{1}{\delta t}\left(\vec{u}_w, \vec{v}\right) + c\left(\vec{u}_w; \vec{u}^k, \vec{v}\right) + c\left(\vec{u}^k; \vec{u}_w, \vec{v}\right) &+ a\left(\mu_l; \vec{u}_w, \vec{v}\right) + b\left(\vec{v}, p_w\right) \\
-\left(\frac{df_B}{d\theta}(\theta^k)\,\theta_w\,\vec{e}_y, \vec{v}\right) &= \frac{1}{\delta t}\left(\vec{u}^k - \vec{u}^n, \vec{v}\right) + c\left(\vec{u}^k; \vec{u}^k, \vec{v}\right) \\
&+ a\left(\mu_l; \vec{u}^k, \vec{v}\right) + b\left(\vec{v}, p^k\right) - \left(f_B(\theta^k)\,\vec{e}_y, \vec{v}\right) \\
\frac{1}{\delta t}\left(\theta_w, \phi\right) - \left(\vec{u}^k \cdot \nabla\phi, \theta_w\right) - \left(\vec{u}_w \cdot \nabla\phi, \theta^k\right) &+ \left(\frac{K}{Pr}\nabla\theta_w, \nabla\phi\right) = \\
\frac{1}{\delta t}\left(\theta^k - \theta^n, \phi\right) &- \left(\vec{u}^k \cdot \nabla\phi, \theta^k\right) + \left(\frac{K}{Pr}\nabla\theta^k, \nabla\phi\right).
\end{aligned}
$$

LMRS

Implementation of the new method

FreeFem++ (www.freefem.org)

Free Generic PDE solver using finite elements (2D and 3D)

- powerful mesh generator,
- easy to implement weak formulations,
- use combined P1, P2 and P4 elements,
- complex matrices available,
- mesh interpolation and adaptivity.

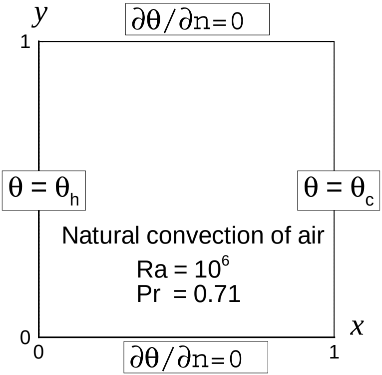
You are welcome to participate in the:

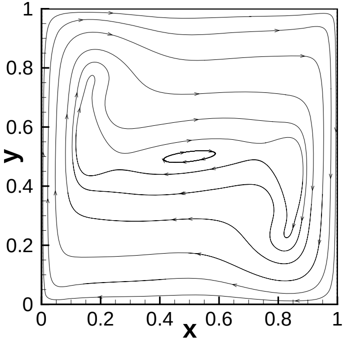
Workshop on FreeFem++ and Applications
Paris, December, every year.

Outline

(step 1) Natural convection of air

- only fluid phase,
- linear Boussinesq force.

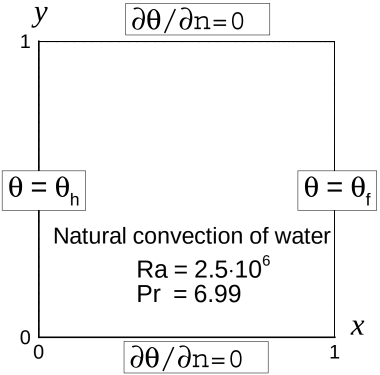


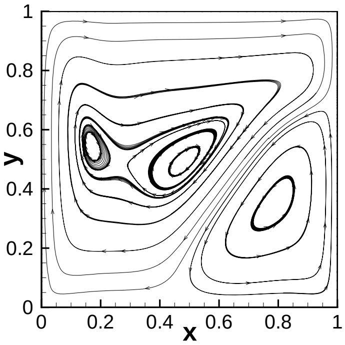


very good agreement with Le Quéré, Comput. Fluids, 1991.

(step 2) Natural convection of water (a)

- only fluid phase,
- non-linear Boussinesq force ($T_h = 10\,°C$, $T_c = 0\,°C$).





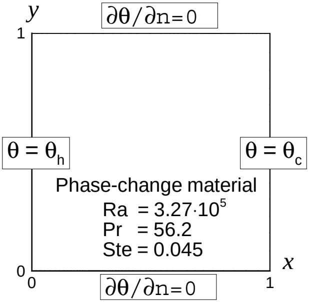
very good agreement with Michalek, Kowalewski, Task Q., 2003.

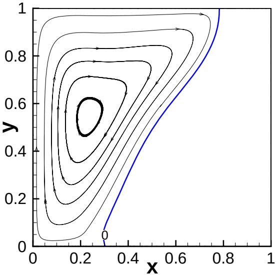
(step 2) Natural convection of water (b)

- only fluid phase,
- non-linear Boussinesq force.

(step 3) Melting of a PCM (a)

- fluid and solid phases,
- linear Boussinesq force.

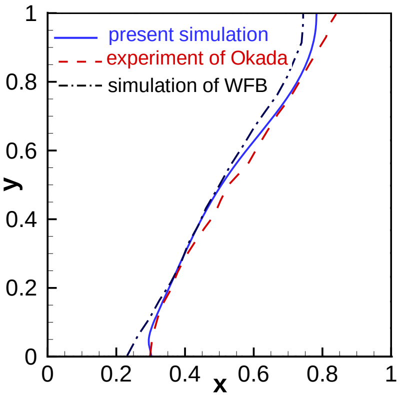




very good agreement with
(simulations) Wang, Faghri & Bergman, IJHMT, 2010
(experiments) Okada, IJHMT, 1984

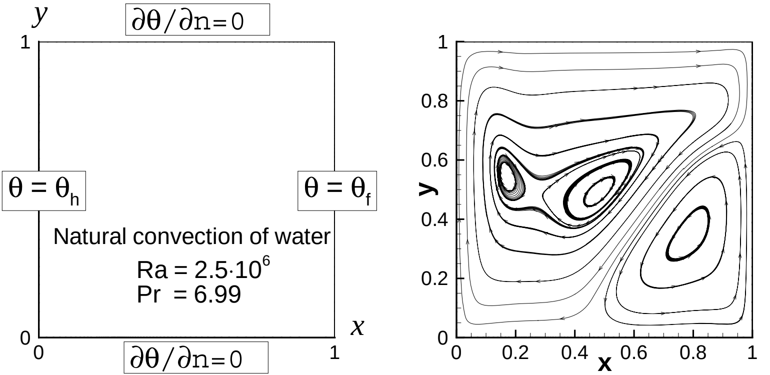
(step 3) Melting of a PCM (b)

- fluid and solid phases,
- linear Boussinesq force.



(step 4) Ice formation (a)

- fluid and solid phases,
- non-linear Boussinesq force ($T_h = 10\,°\mathrm{C}$, $T_c = -10\,°\mathrm{C}$).



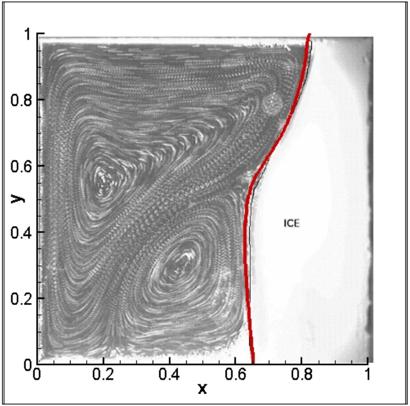
very good agreement with Kowalewski & Rebow, IJCFD, 1999.

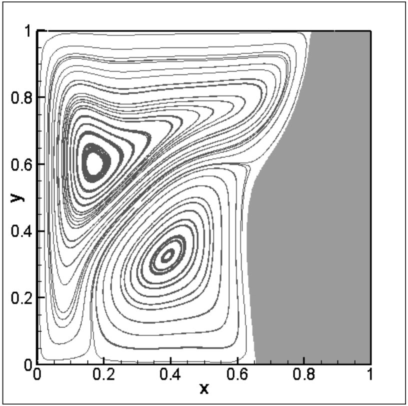
(step 4) Ice formation (b)

- fluid and solid phases,
- non-linear Boussinesq force.

Phase change system: ice formation (2)

Comparison with experiments.





Kowalewski & Rebow, Int. J. of Comput. Fluid Dynamics, 1999.

Conclusion

All the details are in the paper

I. Danaila, R. Moglan, F. Hecht, S. le Masson, J. Computational Physics, 2014.

Message 1: The new numerical method is effective for

- natural convection of air,
- natural convection of water,
- melting of a phase-change material,
- water freezing.

Message 2: You can freely test and use this method

- FreeFem++ is a free software,
- we can provide corresponding FreeFem++ scripts.