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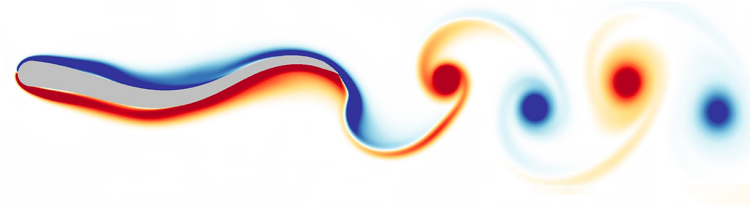

Computational Fluid Dynamics and Flow Physics Laboratory

A consistent, volume preserving, and adaptive mesh refinement-based framework for modeling phase changing non-isothermal gas-liquid-solid flows

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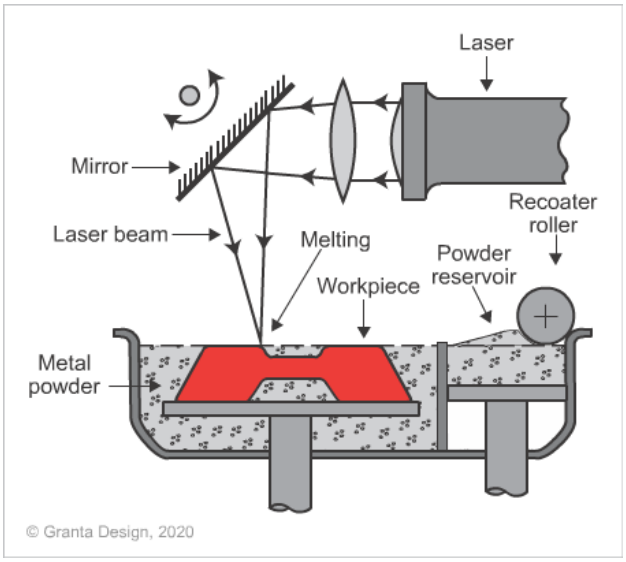
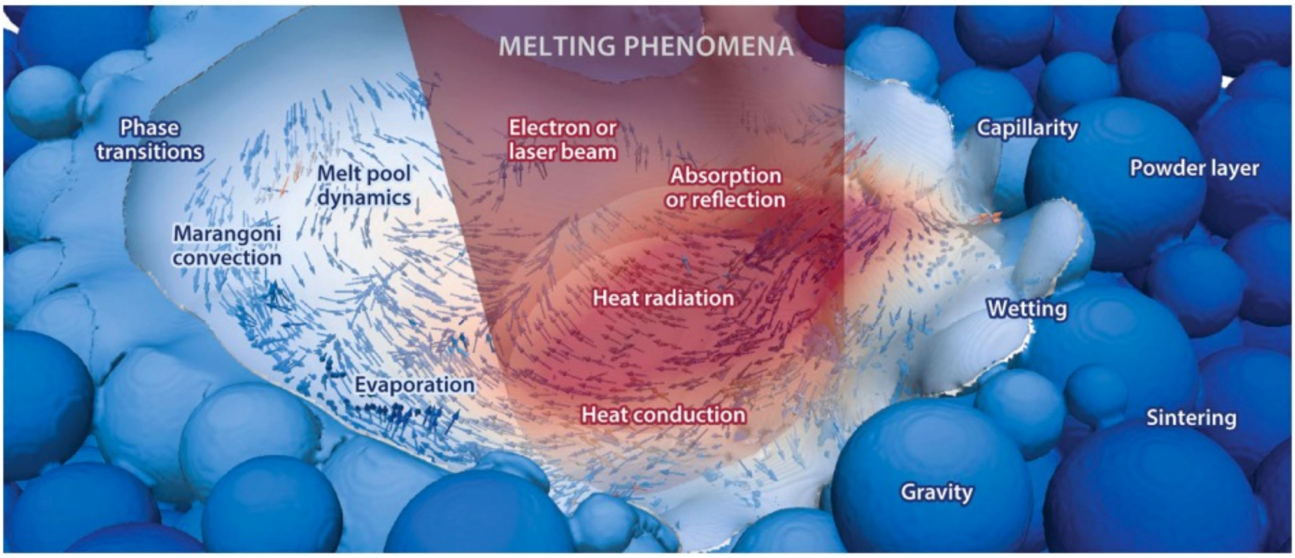
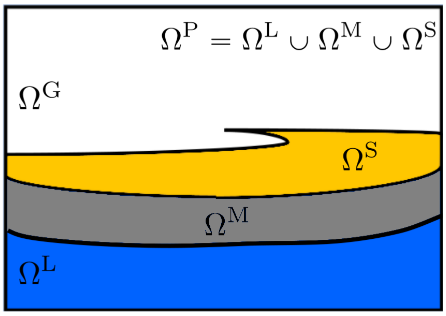
ICCFD 12, Kobe, Japan, 2024

Non-isothermal multiphase flows with phase change





A consistent Mathematical framework



Level set advection:

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \mathbf{u} \cdot \nabla \phi = 0$$

Heaviside advection:

$$H(\phi) = \begin{cases} 1 & \text{PCM} \\ 0 & \text{Gas} \end{cases}$$

$$\frac{H^{n+1} - H(\phi)^n}{\Delta t} + \nabla \cdot \phi \mathbf{u} = H \nabla \cdot \mathbf{u}$$

$$\varphi = \begin{cases} 1, & \text{Liquid} \\ 0, & \text{Solid} \end{cases}$$

Mass conservation:

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \nabla \cdot m_\rho = 0$$

Enthalpy equation:

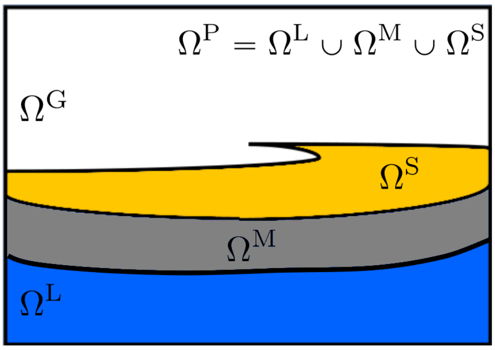
$$\frac{\rho^{n+1} h^{n+1} - (\rho h)^n}{\Delta t} + \nabla \cdot (m_\rho h) = \nabla \cdot (\kappa \nabla T) + Q_{\mathrm{src}}$$

Navier Stokes system:

$$\frac{\rho^{n+1} \mathbf{u}^{n+1} - (\rho \mathbf{u})^n}{\Delta t} + \nabla \cdot (m_\rho \mathbf{u}) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)\right] + \rho \mathbf{g} - A_d \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = -\frac{1}{\rho} \frac{\mathrm{D}\rho}{\mathrm{D}t}$$

A Novel Low Mach Enthalpy Method



$$H = \begin{cases} 1, & \text{PCM} \\ 0, & \text{Gas} \end{cases}$$

$$\varphi = \begin{cases} 1, & \text{Liquid} \\ 0, & \text{Solid} \end{cases}$$

Enthalpy Equation:

$$\frac{\rho^{n+1} h^{n+1} - (\rho h)^n}{\Delta t} + \nabla \cdot (m_\rho h) = \nabla \cdot (\kappa \nabla T) + Q_{\mathrm{src}}$$

h − T Relation:

$$h = \begin{cases} C^{\mathrm{S}} T, & T < T^{\mathrm{sol}}, \\ \bar{C}(T - T^{\mathrm{sol}}) + h^{\mathrm{sol}} + \varphi \frac{\rho^{\mathrm{L}}}{\rho} L, & T^{\mathrm{sol}} \leqslant T \leqslant T^{\mathrm{liq}}, \\ C^{\mathrm{L}}(T - T^{\mathrm{liq}}) + h^{\mathrm{liq}}, & T > T^{\mathrm{liq}}, \end{cases}$$

φ − h Relation:

$$\varphi = \begin{cases} 0, & h < h^{\mathrm{sol}}, \\ \dfrac{\rho^{\mathrm{S}}(h^{\mathrm{sol}} - h)}{h(\rho^{\mathrm{L}} - \rho^{\mathrm{S}}) - \rho^{\mathrm{L}} h^{\mathrm{liq}} + \rho^{\mathrm{S}} h^{\mathrm{sol}}}, & h^{\mathrm{sol}} \leqslant h \leqslant h^{\mathrm{liq}}, \\ 1, & h > h^{\mathrm{liq}}. \end{cases}$$

Equation of State:

$$\rho = \rho^G + (\rho^S - \rho^G) H + (\rho^L - \rho^S) H \varphi$$

Low Mach Equation:

$$\nabla \cdot \mathbf{u} = -\frac{1}{\rho} \frac{\mathrm{D}\rho}{\mathrm{D}t}$$

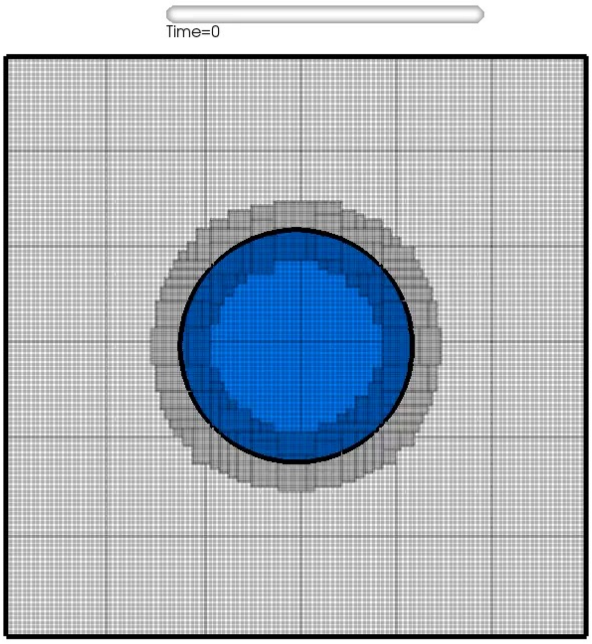
$$\nabla \cdot \mathbf{u} = -\frac{\rho^{\mathrm{S}} \rho^{\mathrm{L}}}{\rho^2} (\rho^{\mathrm{L}} - \rho^{\mathrm{S}}) H \frac{(h^{\mathrm{liq}} - h^{\mathrm{sol}})}{\left(h(\rho^{\mathrm{L}} - \rho^{\mathrm{S}}) - \rho^{\mathrm{L}} h^{\mathrm{liq}} + \rho^{\mathrm{S}} h^{\mathrm{sol}}\right)^2} (\nabla \cdot \kappa \nabla T)$$

Consistent time integrators

- The use of the same mass flux $\mathbf{m}_\rho$ in various transport equations ensures numerical stability for high density ratio flows

- Option 1: Use the same time integration scheme for mass, momentum and enthalpy equations.

- Option 2: Include additional stabilizing terms (shown in red below) in the momentum and energy equations.



Test problem: isothermal advection of a dense bubble in inviscid gas

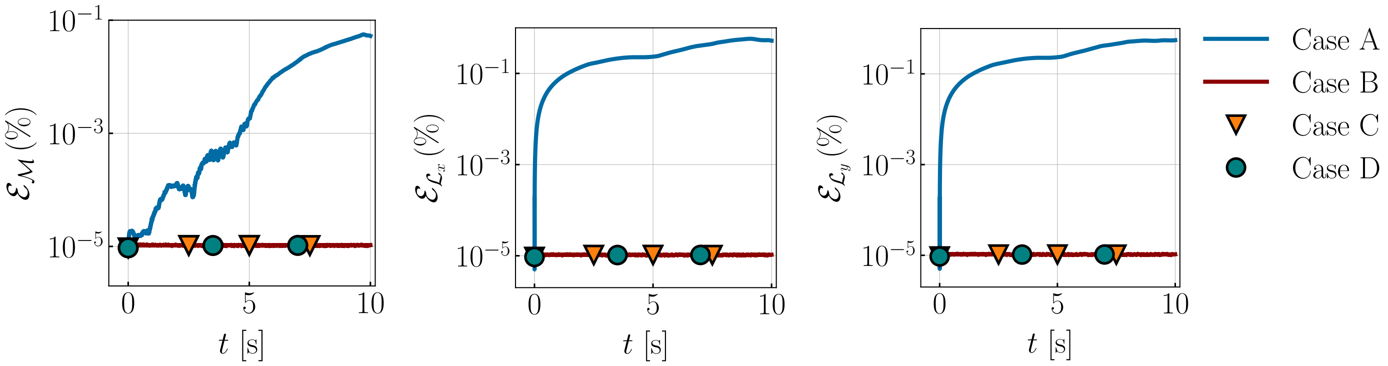
$\rho_i/\rho_o = 10000 \qquad (u, v) = (1, 1)$

$$\frac{\breve{\boldsymbol{\rho}}^{n+1,k+1}\mathbf{u}^{n+1,k+1} - \breve{\boldsymbol{\rho}}^{n}\mathbf{u}^{n}}{\Delta t} + \mathbf{C}\left(\mathbf{u}_{\text{adv}}^{(2)}, \breve{\boldsymbol{\rho}}_{\text{lim}}^{(2)}\mathbf{u}_{\text{lim}}^{(2)}\right) = \boldsymbol{\mathcal{R}}\mathbf{u}^{n+1,k} + \text{ viscous} + \text{pressure} + \text{other forces}$$

$$\frac{\breve{\boldsymbol{\rho}}^{n+1,k+1}h^{n+1,k+1} - \breve{\boldsymbol{\rho}}^{n}h^{n}}{\Delta t} + A\left(h_{\text{lim}}^{(1)}, \breve{\boldsymbol{\rho}}_{\text{lim}}^{(1)}\mathbf{u}_{\text{adv}}^{(1)}\right) = \mathcal{R}h^{n+1,k} + (\nabla\cdot\kappa\nabla T)^{n+1,k+1} + Q_{\text{src}}^{n+1,k}$$

Bhalla et al., A robust incompressible Navier-Stokes solver for high density ratio multiphase flows, J. Comput. Phys. 390 (2019) .

Importance of Consistent Integrators



RK-2 integrator is employed for the momentum equation in all 4 cases

Case A: SSP-RK3 integrator for mass equation.

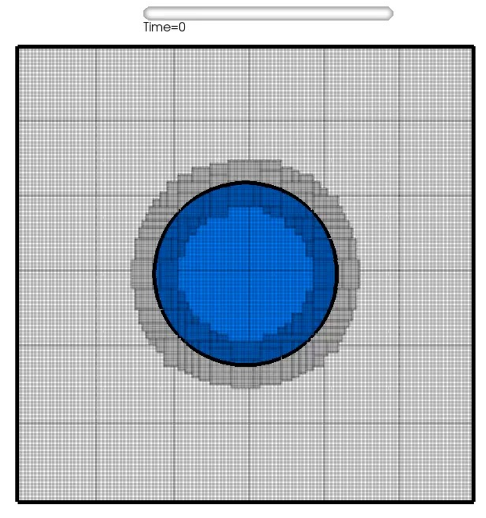
Case B: SSP-RK3 integrator for mass equation, and residual force in the momentum equation.

Case C: RK-2 integrator for mass equation.

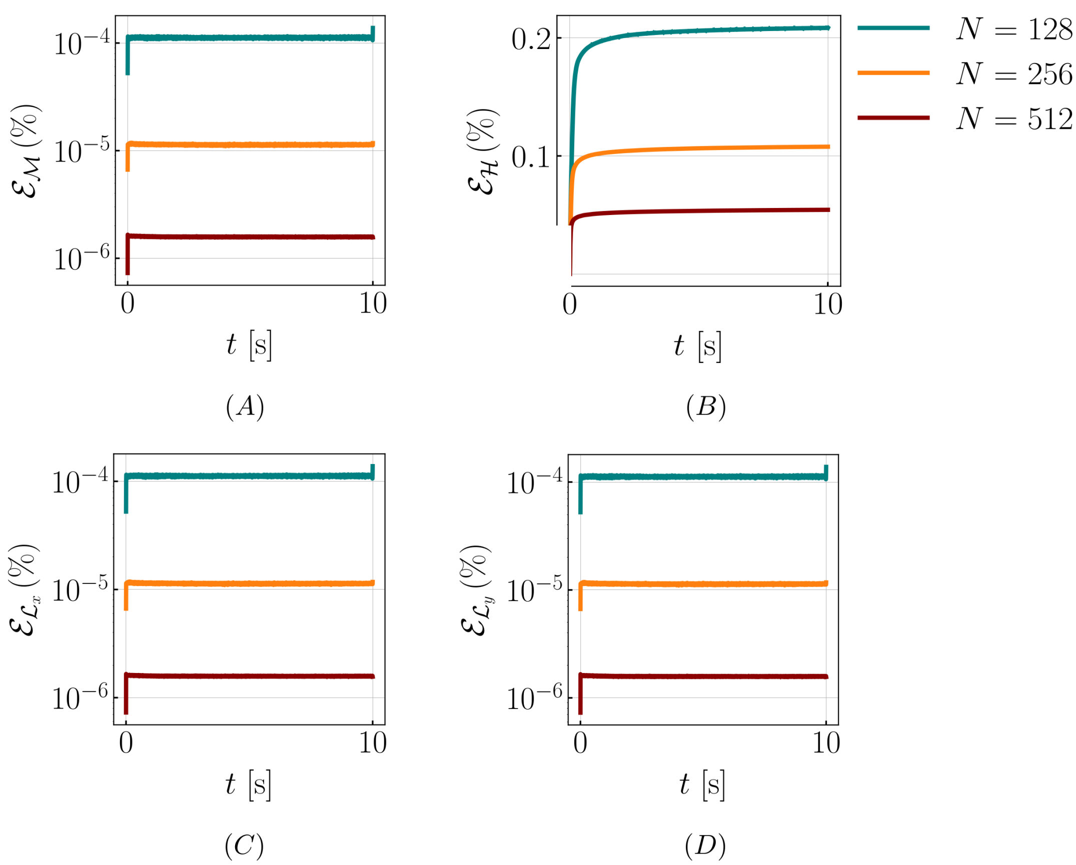
Case D: RK-2 integrator for mass equation, and residual force in the momentum equation

Cases B, C and D preserve momentum, enthalpy and phase of the system.

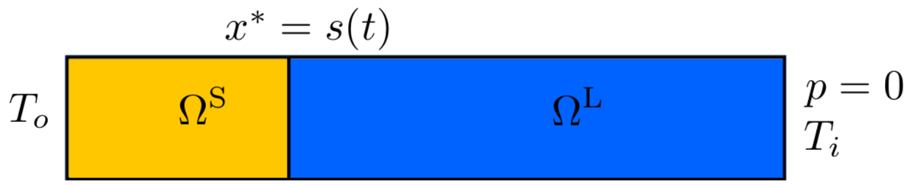
Grid convergence study



Test problem: isothermal advection of a dense bubble in inviscid gas



Solving two phase Stefan Problem with density jump



SOLIDIFICATION PROBLEM

Heat equations

$$\rho^{\mathrm{S}} C^{\mathrm{S}} \frac{\partial T^{\mathrm{S}}}{\partial t} = \kappa^{\mathrm{S}} \frac{\partial^2 T^{\mathrm{S}}}{\partial x^2} \in \Omega^{\mathrm{S}}(t),$$

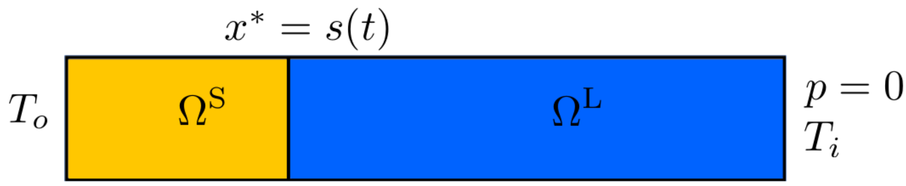
$$\rho^{\mathrm{L}} C^{\mathrm{L}} \left(\frac{\partial T^{\mathrm{L}}}{\partial t} + u^{\mathrm{L}} \frac{\partial T^{\mathrm{L}}}{\partial x} \right) = \kappa^{\mathrm{L}} \frac{\partial^2 T^{\mathrm{L}}}{\partial x^2} \in \Omega^{\mathrm{L}}(t)$$

Stefan condition

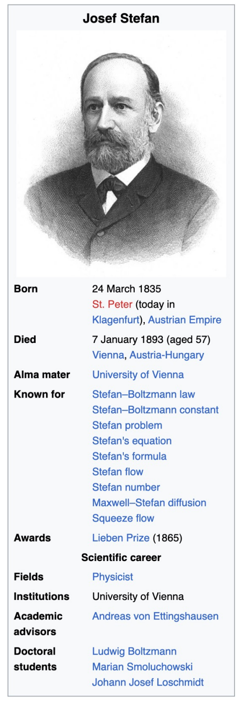
$$\rho^{\mathrm{S}} \left[(C^{\mathrm{L}} - C^{\mathrm{S}})(T_m - T_r) + L - \frac{1}{2}(1 - R_\rho^2) \left(\frac{\mathrm{d}s}{\mathrm{d}t} \right)^2 \right] \frac{\mathrm{d}s}{\mathrm{d}t} = \left(\kappa^{\mathrm{S}} \frac{\partial T^{\mathrm{S}}}{\partial x} - \kappa^{\mathrm{L}} \frac{\partial T^{\mathrm{L}}}{\partial x} \right)_{x^*}.$$

$$R_\rho = \rho^{\mathrm{S}} / \rho^{\mathrm{L}}$$

Solving two phase Stefan Problem with density jump



SOLIDIFICATION PROBLEM



$$\rho^{\mathrm{S}} C^{\mathrm{S}} \frac{\partial T^{\mathrm{S}}}{\partial t} = \kappa^{\mathrm{S}} \frac{\partial^2 T^{\mathrm{S}}}{\partial x^2} \in \Omega^{\mathrm{S}}(t),$$

$$\rho^{\mathrm{L}} C^{\mathrm{L}} \left(\frac{\partial T^{\mathrm{L}}}{\partial t} \boxed{+ u^{\mathrm{L}} \frac{\partial T^{\mathrm{L}}}{\partial x}} \right) = \kappa^{\mathrm{L}} \frac{\partial^2 T^{\mathrm{L}}}{\partial x^2} \in \Omega^{\mathrm{L}}(t)$$

Heat equations

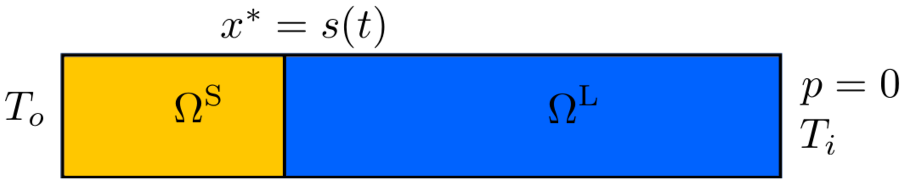
$$\rho^{\mathrm{S}} \left[\boxed{(C^{\mathrm{L}} - C^{\mathrm{S}})(T_m - T_r)} + L \boxed{- \frac{1}{2}(1 - R_\rho^2) \left(\frac{\mathrm{d}s}{\mathrm{d}t} \right)^2} \right] \frac{\mathrm{d}s}{\mathrm{d}t} = \left(\kappa^{\mathrm{S}} \frac{\partial T^{\mathrm{S}}}{\partial x} - \kappa^{\mathrm{L}} \frac{\partial T^{\mathrm{L}}}{\partial x} \right)_{x^*}.$$

Stefan condition

$$R_\rho = \rho^{\mathrm{S}} / \rho^{\mathrm{L}}$$

Terms in red boxes pertain to density jumps.
These are ignored in the literature.
We consider them.

Solving two phase Stefan problem



SOLIDIFICATION PROBLEM

Analytical solution:

$$T^{\mathrm{S}} = T_o + (T_m - T_o)\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha^{\mathrm{S}} t}}\right) \Big/ \operatorname{erf}\left(\lambda(t)\sqrt{\frac{\alpha^{\mathrm{L}}}{\alpha^{\mathrm{S}}}}\right)$$

$$T^{\mathrm{L}} = T_i + (T_m - T_i)\frac{\operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha^{\mathrm{L}} t}} - \lambda(t)\left(1 - R_\rho\right)\right)}{\operatorname{erfc}\left(\lambda(t) R_\rho\right)}$$

Transcendental equation for λ :

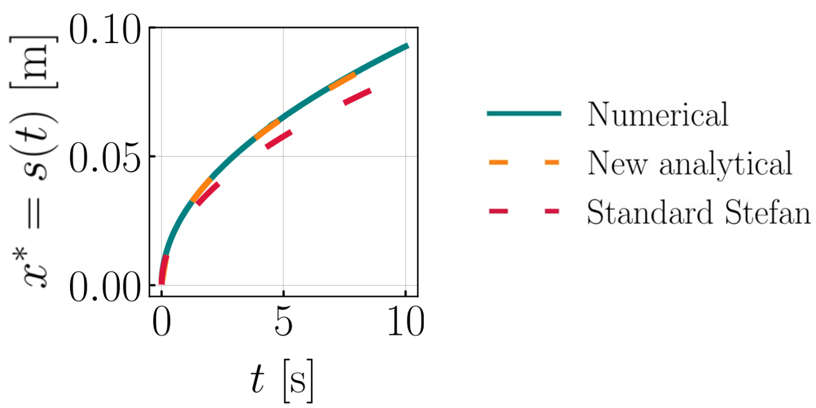
$$\rho^{\mathrm{S}}\left[L^{\mathrm{eff}} - \frac{(1 - R_\rho^2)}{2}\left(\frac{\lambda^2 \alpha^{\mathrm{L}}}{t}\right)\right]\lambda\sqrt{\alpha^{\mathrm{L}}} =$$

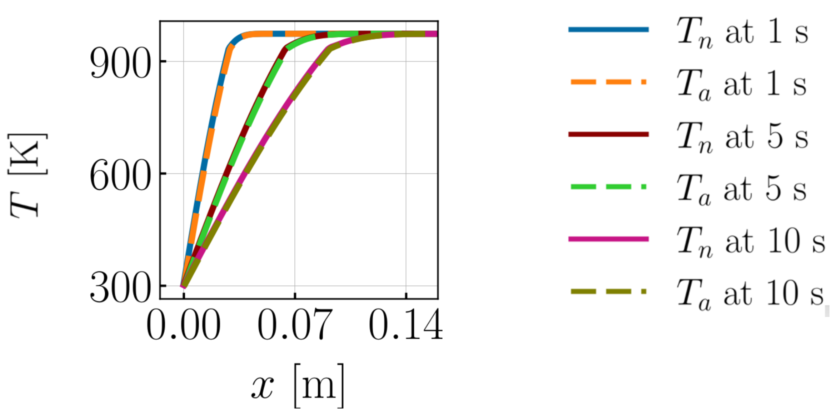
$$\kappa^{\mathrm{S}}\frac{T_m - T_o}{\operatorname{erf}\left(\lambda\sqrt{\frac{\alpha^{\mathrm{L}}}{\alpha^{\mathrm{S}}}}\right)}\frac{e^{-\lambda^2 \alpha^{\mathrm{L}}/\alpha^{\mathrm{S}}}}{\sqrt{\pi \alpha^{\mathrm{S}}}} + \kappa^{\mathrm{L}}\frac{T_m - T_i}{\operatorname{erfc}\left(\lambda R_\rho\right)}\frac{e^{-\lambda^2 R_\rho^2}}{\sqrt{\pi \alpha^{\mathrm{L}}}}$$

- R. Thirumalaisamy, **A. P. S. Bhalla**, 2023, A low Mach enthalpy method to model non-isothermal gas-liquid-solid flows with melting and solidification, *International Journal of Multiphase Flow*, vol. 169, 104605.

Stefan problem with density difference

Expansion $\rho^{\mathrm{S}}/\rho^{\mathrm{L}} < 1$





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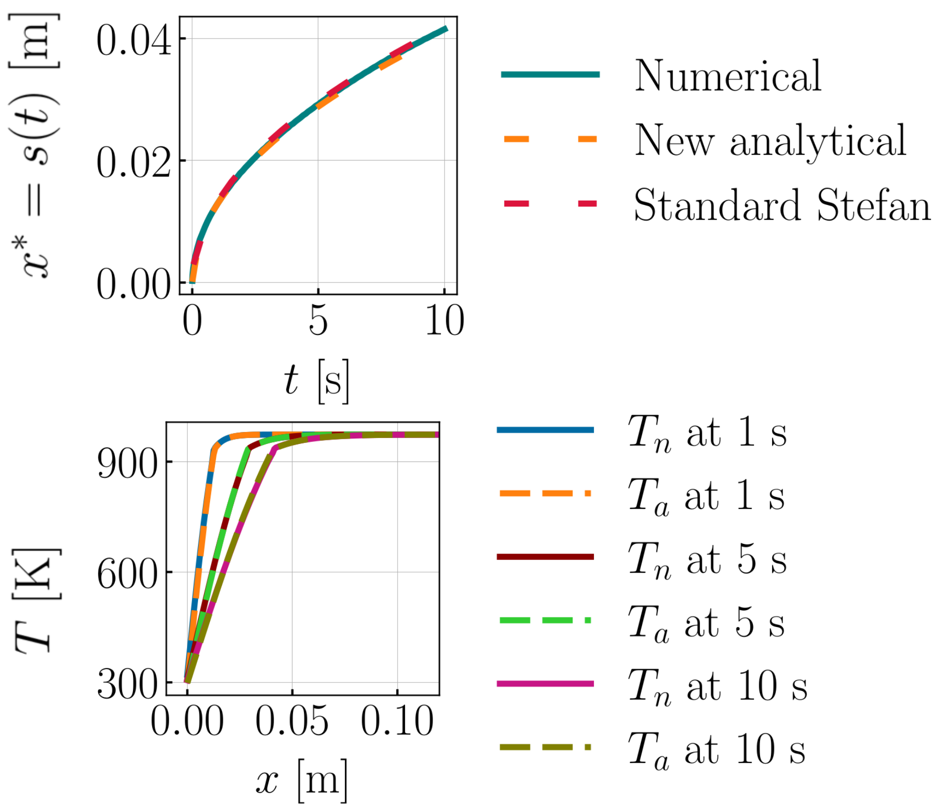
Stefan problem with density difference

Shrinkage $\rho^{\mathrm{S}}/\rho^{\mathrm{L}} > 1$



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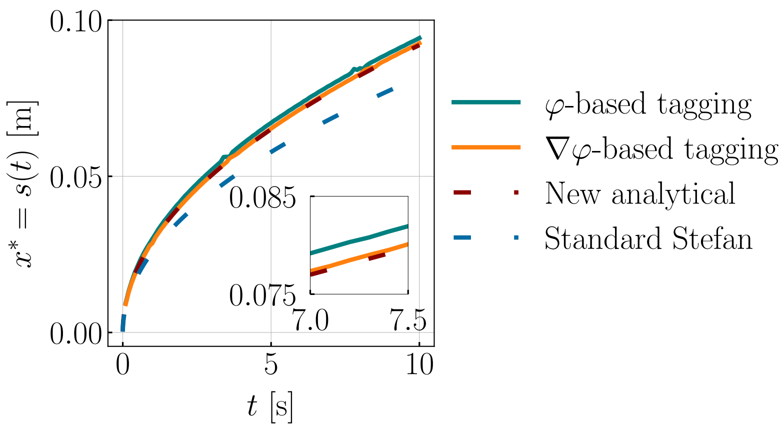
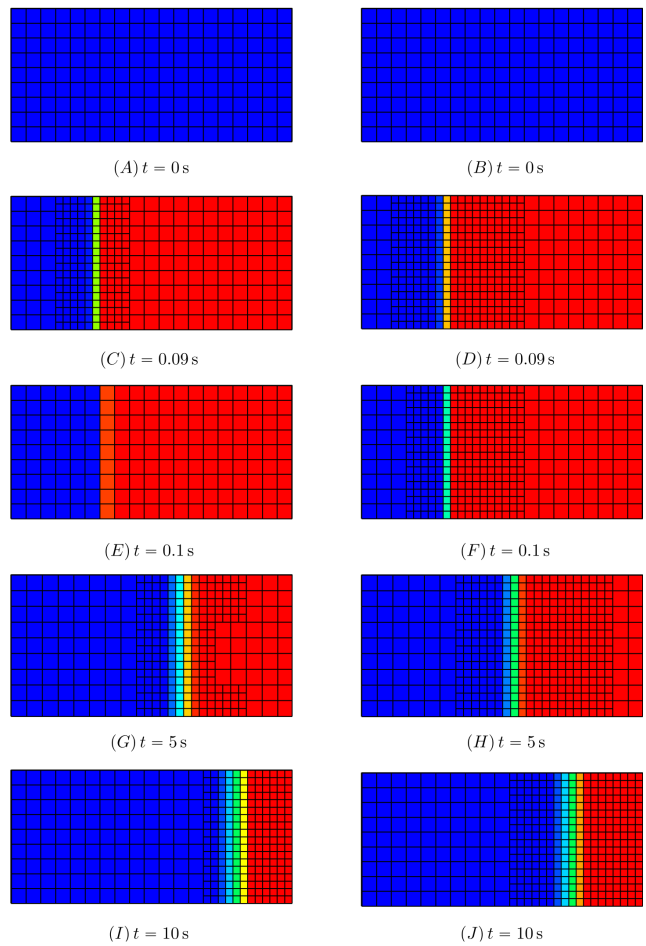
Adaptive mesh refinement

PCM-gas interface: Tagging cells based on the signed distance function

Liquid-solid interface:
1. φ-based tagging
2. $\nabla\varphi$-based tagging

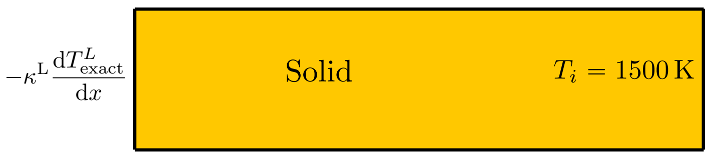


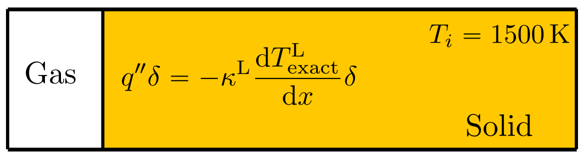


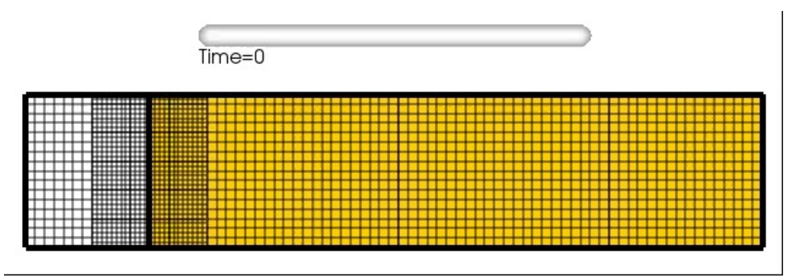
Laser-induced melting of metals with volume change

Numerical studies have relied on experimental data to validate heat source (e.g., laser beams) induced melting of metals and alloys.

We use two phase Stefan analytical solution to validate heat source-induced melting of metals in presence of gas.



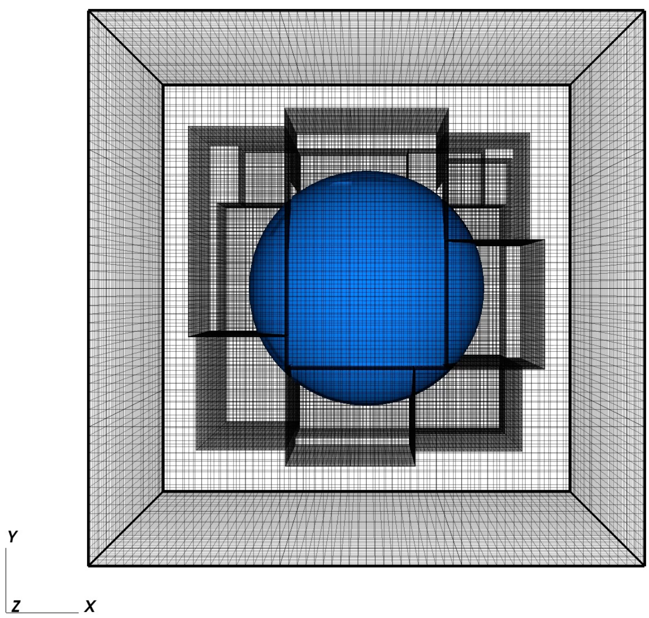




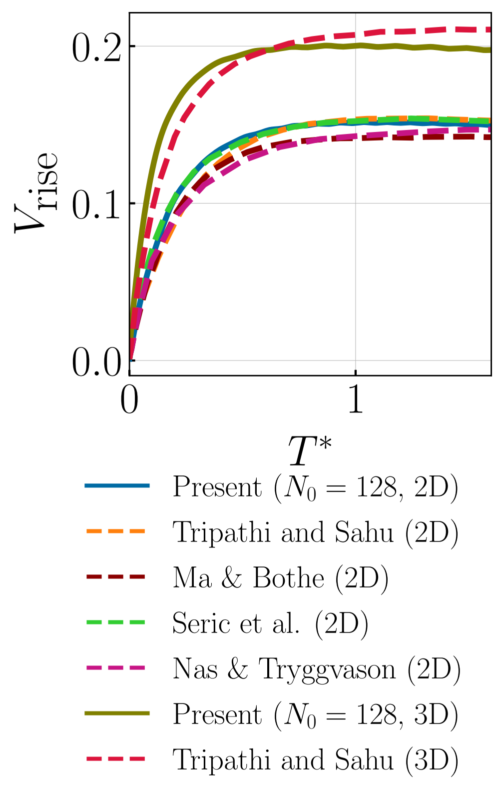
Thermocapillary Flows With Low Mach Enthalpy Method

$$\mathbf{f}_{\mathrm{st}} = \sigma\kappa\mathbf{n}\delta + \nabla_{||}\sigma\delta$$

$$\sigma = \sigma_0 + \left.\frac{\mathrm{d}\sigma}{\mathrm{dT}}\right|_0 (T - T_0)$$



We solve the enthalpy equation (not temperature)

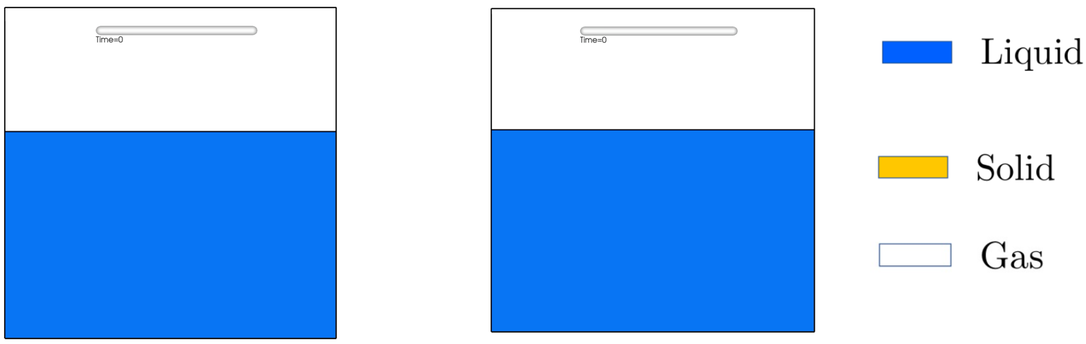


$$Re = Ma = 0.72,\ Ca = 0.0576$$

Simulating Metal Casting Defects

Pipe shrinkage

$\rho^{\mathrm{S}} > \rho^{\mathrm{L}}$ $\rho^{\mathrm{S}} < \rho^{\mathrm{L}}$

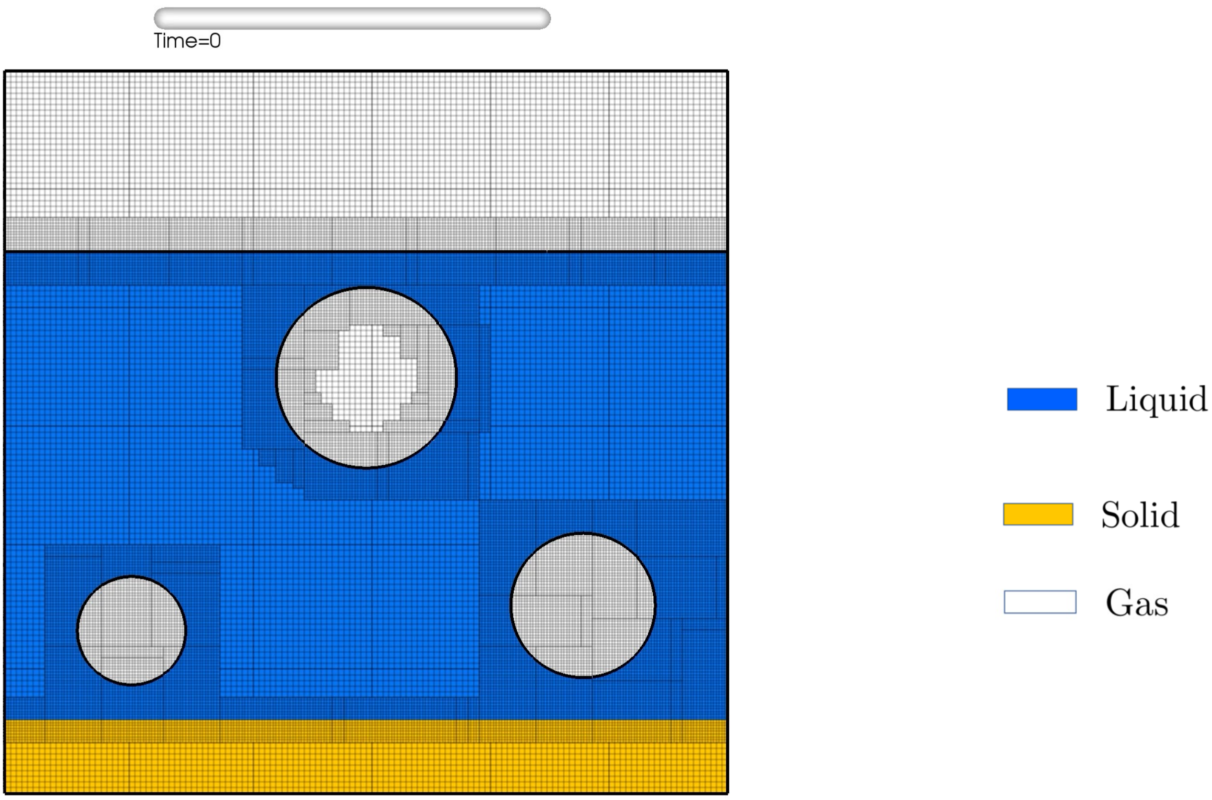


Shrinkage defect

Protrusion defect

Ludwig, A., Wu, M. and Kharicha, A., 2016. Simulation in metallurgical processing: Recent developments and future perspectives. *JOM*, *68*, pp.2191-2197.

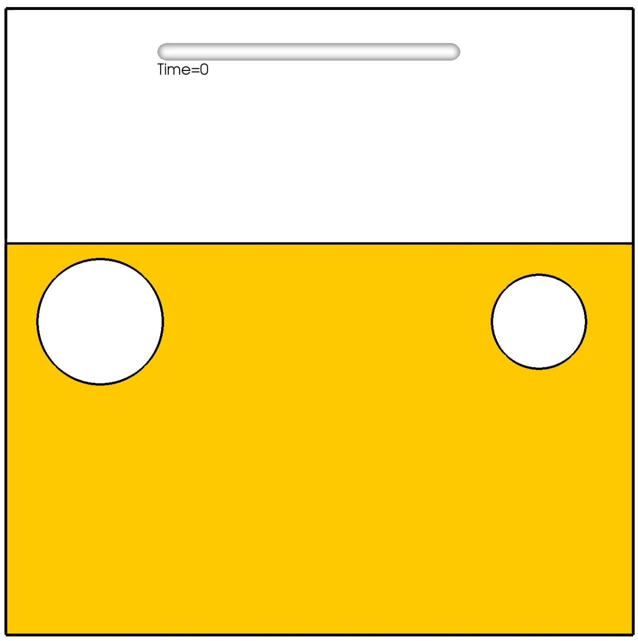
Simulating Porosity Defects



Melting and Re-solidification of Aluminum (Surface Tension Effects)

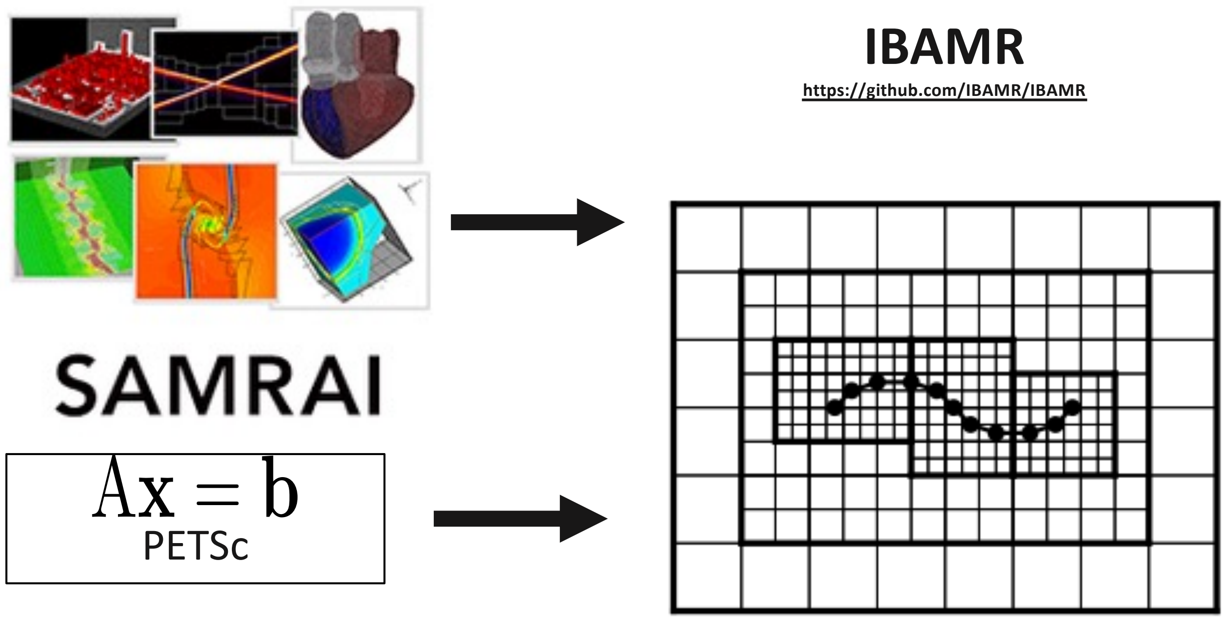
Solid Aluminum
Liquid Aluminum

$T > T_M \quad t \leq 0.2$
$T = T_M \quad t > 0.2$



$T > T_M \quad t \leq 0.2$
$T = T_M \quad t > 0.2$

Implementation



IBAMR is a distributed-memory (MPI) parallel implementation of the immersed boundary (IB) method with support for Cartesian grid adaptive mesh refinement (AMR). Written in C++ and Fortran.

References

1. R. Thirumalaisamy, K. Khedkar, P. Ghysels, **A. P. S. Bhalla**, 2023, An effective preconditioning strategy for volume penalized incompressible multiphase flow solvers, *Journal of Computational Physics,* Vol. 490, 112325.

2. R. Thirumalaisamy, **A. P. S. Bhalla**, 2023, A low Mach enthalpy method to model non-isothermal gas-liquid-solid flows with melting and solidification, *International Journal of Multiphase Flow*, vol. 169, 104605.

3. N. Nangia, B. E. Griffith, N. A. Patankar, and **A. P. S. Bhalla**. "A robust incompressible Navier-Stokes solver for high density ratio multiphase flows." *Journal of Computational Physics* 390 (2019): 548-594.

4. R. Thirumalaisamy, **A. P. S. Bhalla**, 2024, A consistent, volume preserving, and adaptive mesh refinement-based framework for modeling non-isothermal gas-liquid-solid flows with phase change (submitted).

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Questions / Comments?