Modelling Evaporation and Combustion of Fuel Droplets

Using Basilisk

Edoardo Cipriano

BGUM 2023 – Basilisk (Gerris) Users' Meeting 5-7th July, Paris

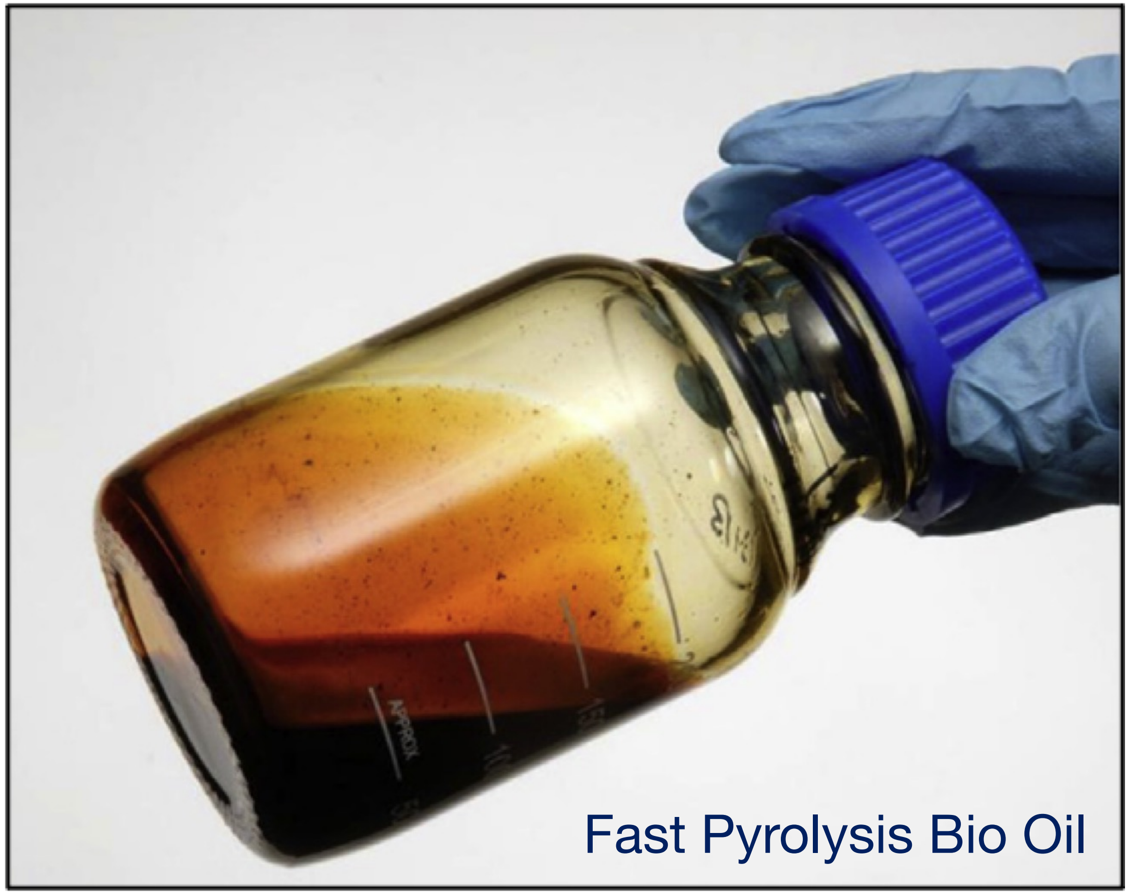
01

Motivation

Motivation and Aim of the Work

Alternative Liquid Fuels

Studied as possible alternatives to the use of fossil fuels



Broumand et al. *Progress in Energy and Combustion Science* (2020)

Fuel Produced From Waste

Is an interesting idea, but they **do not burn well** due to the high number of chemical species

Homogeneous Combustion

Of volatile components

Heterogeneous Combustion

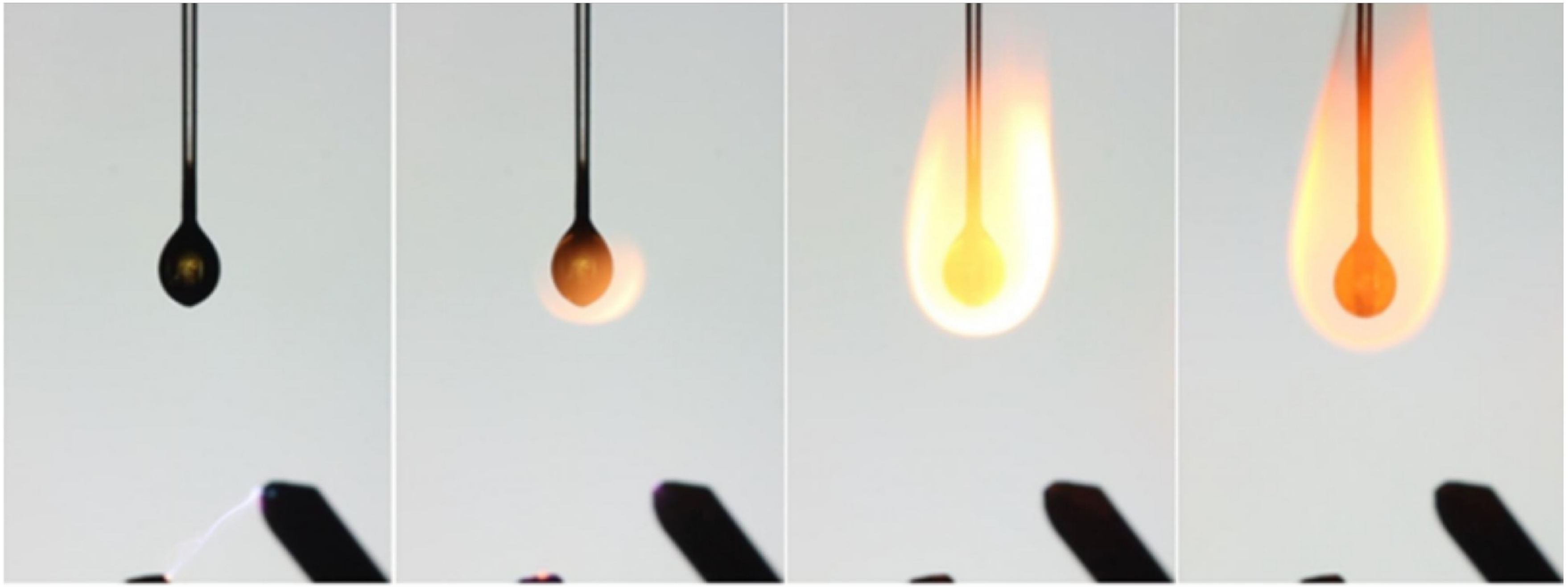
Of solid carbonaceous residuals

Albert-Green et al. *Biomass and Bioenergy* (2018)

Understanding the Behavior of Isolated Droplets

1. **Neglect Interactions**

Between the different droplets that compose the spray.

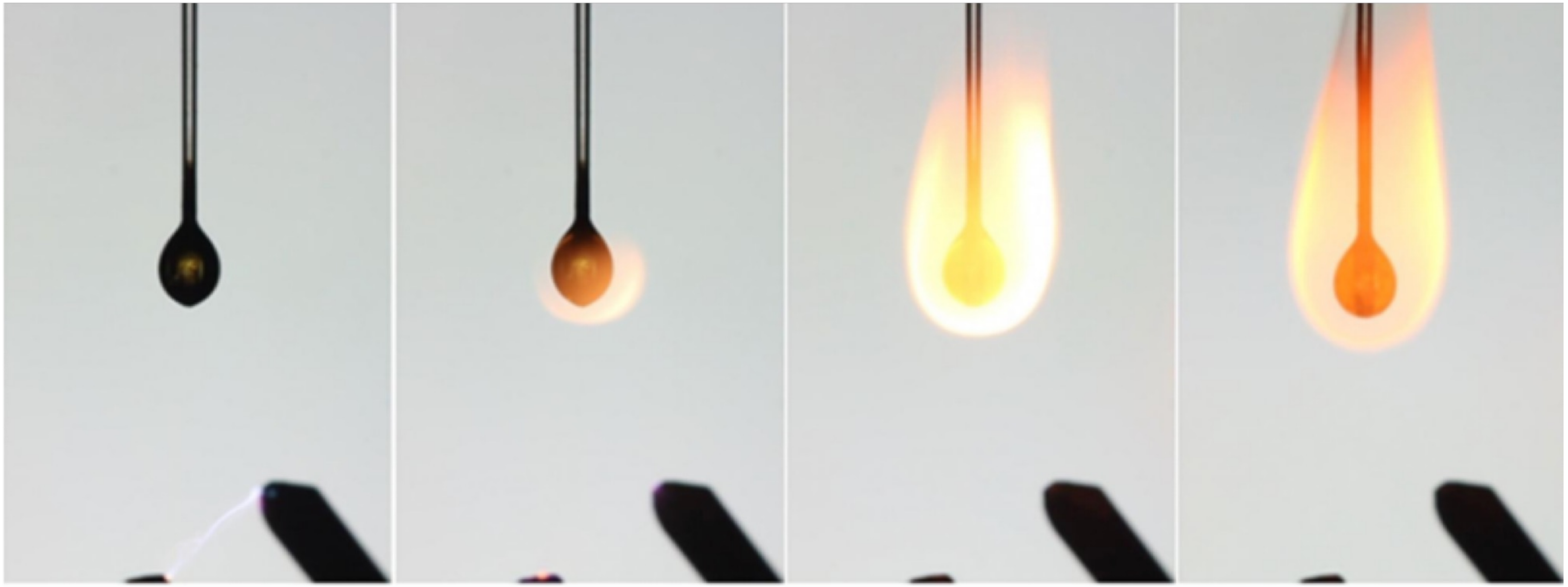


Sankaranarayanan et al. *Fuel* (2019)

Understanding the Behavior of Isolated Droplets

2. Refine Understanding

Of the evaporation and combustion processes.

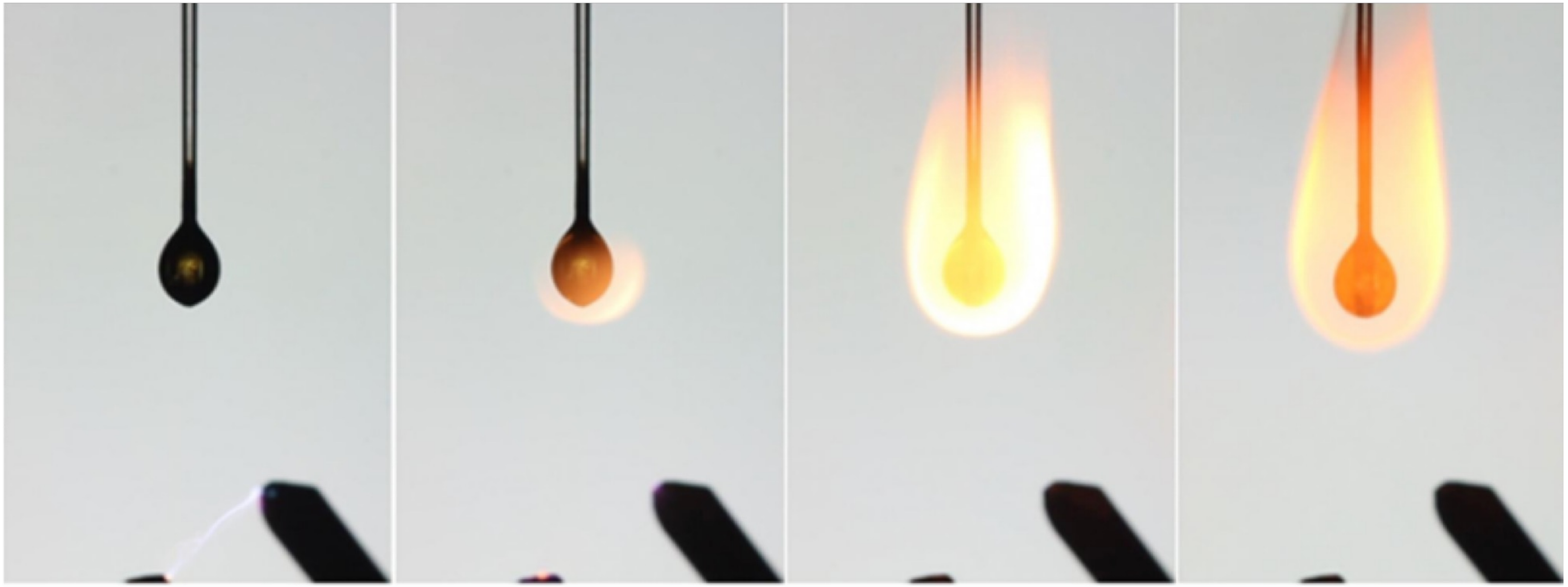


Sankaranarayanan et al. *Fuel* (2019)

Understanding the Behavior of Isolated Droplets

3. Sub-Grid-Scale Models

For Spray combustion simulations using less detailed models (i.e. Euler-Lagrange).



Sankaranarayanan et al. *Fuel* (2019)

POLITECNICO
MILANO 1863

Develop a Numerical Model For the Evaporation and Combustion Of Multicomponent Droplets

02

Numerical Model

VOF-Based CFD Model

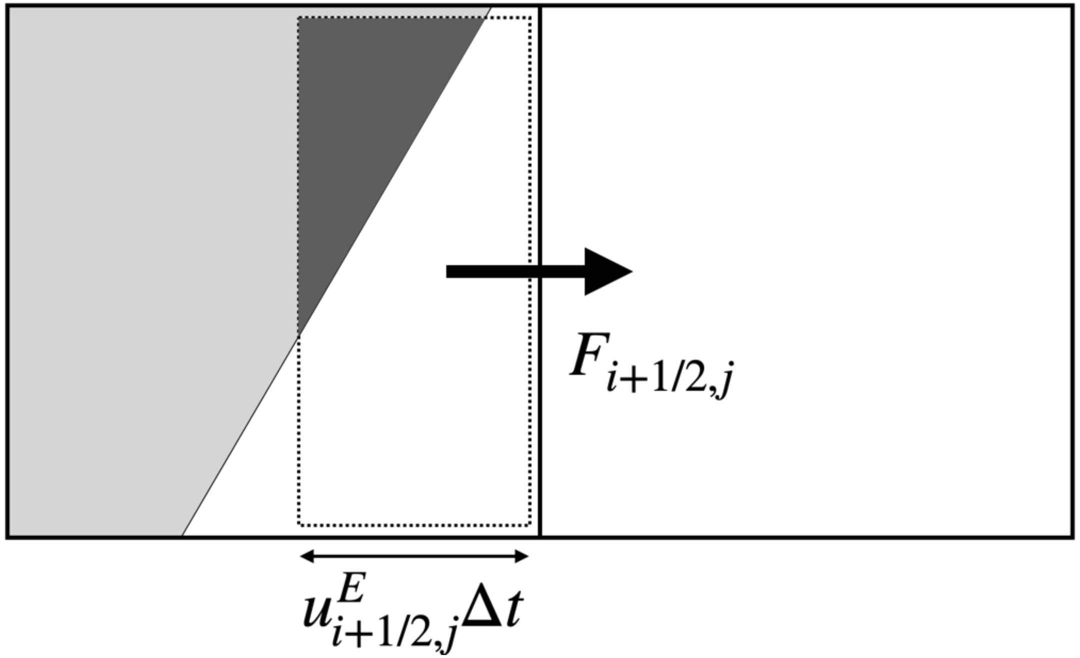
Numerical Model: Geometric Volume-Of-Fluid

Transport of the Interface

Solving an advection equation on the volume fraction field:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\underline{\mathbf{u}}) = -\frac{\dot{m}}{\rho_l}\delta_\Gamma$$

Evaporation Term Removes Liquid



Numerical Model: Geometric Volume-Of-Fluid

Transport of the Interface

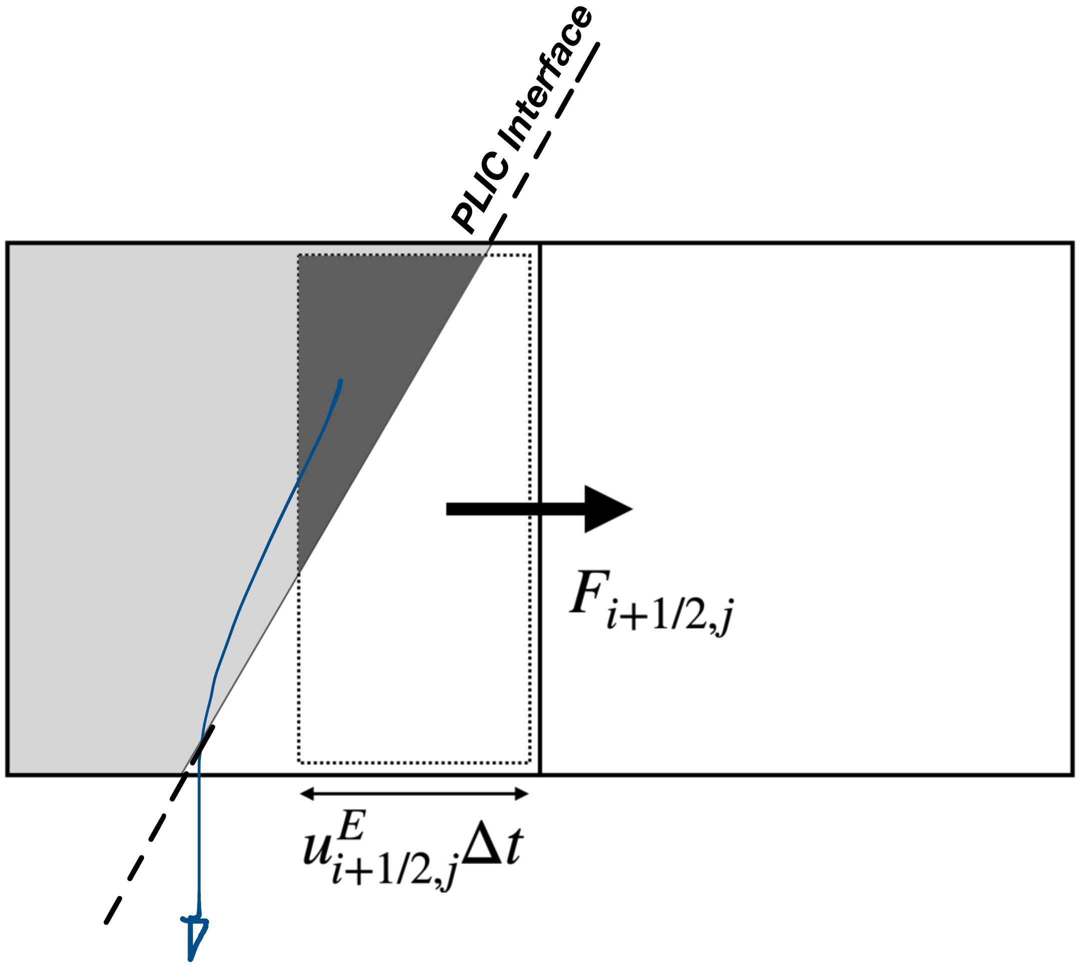
Solving an advection equation on the volume fraction field:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\underline{\boldsymbol{u}}) = -\frac{\dot{m}}{\rho_l}\delta_\Gamma$$

$$\Downarrow$$

$$\frac{\partial c}{\partial t} + \nabla \cdot [c(\boldsymbol{u} + \boldsymbol{u}_\Gamma)] = 0$$

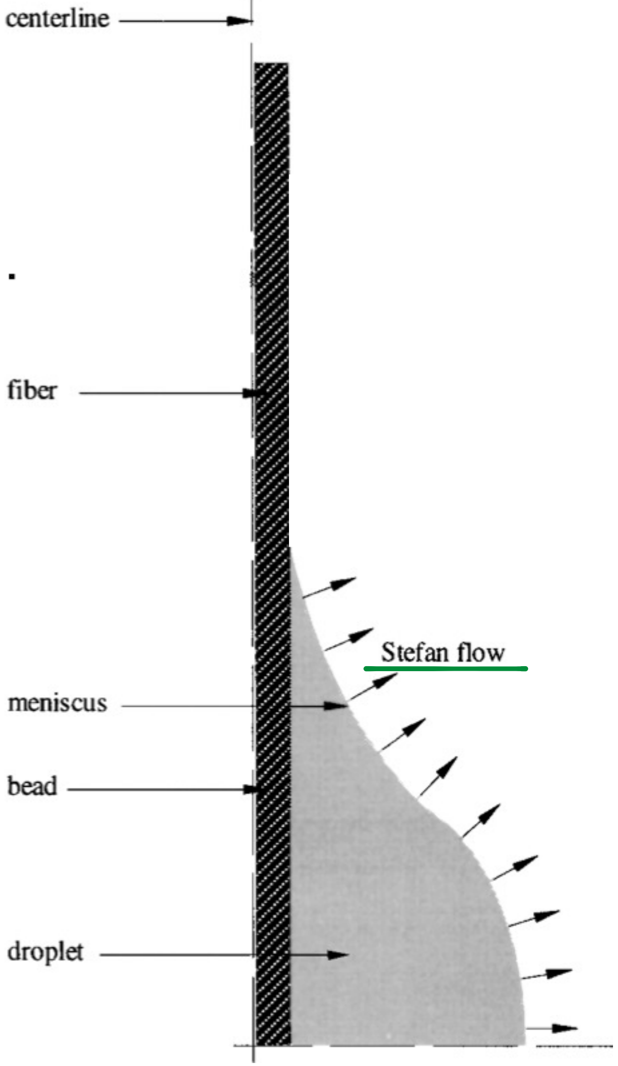
Interface Regression Velocity



Flux of liquid fraction (grey area)

Numerical Model: Pressure-Velocity Coupling

Avedisian C.T., et al, *Journal of Propulsion and Power* (2000)



Navier-Stokes Equations

For variable density incompressible flows with phase change:

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\nabla\cdot(\boldsymbol{u}\otimes\boldsymbol{u})\right)=\mu\nabla\cdot(\nabla\boldsymbol{u}+\nabla^{T}\boldsymbol{u})-\nabla p+\rho\boldsymbol{g}+\boxed{\sigma\kappa\boldsymbol{n}_{\boldsymbol{\Gamma}}\delta_{\Gamma}}$$

$$\nabla\cdot\boldsymbol{u}=\dot{m}\underline{\left(\frac{1}{\rho_l}-\frac{1}{\rho_g}\right)}\delta_{\Gamma}$$

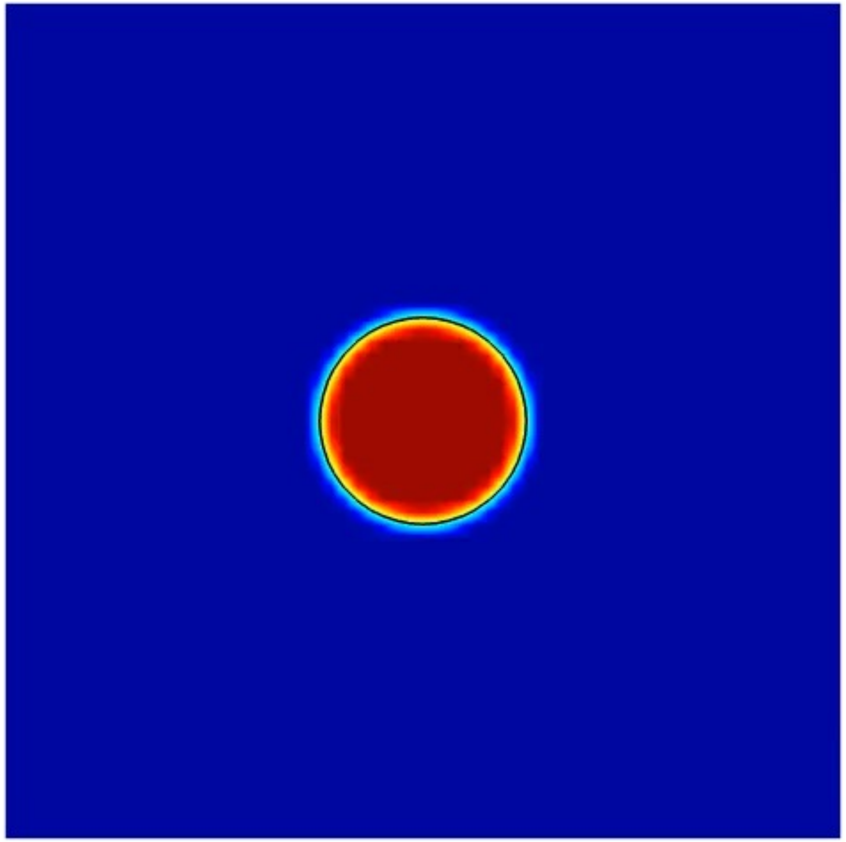
Surface Tension Force

Expansion Due to the Phase Change
(Responsible for the Stefan flow)

↓

Discontinuity in the Velocity Field

Numerical Model: Pressure-Velocity Coupling



Navier-Stokes Equations

For variable density incompressible flows with phase change:

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+\nabla\cdot(\boldsymbol{u}\otimes\boldsymbol{u})\right)=\mu\nabla\cdot\left(\nabla\boldsymbol{u}+\nabla^{T}\boldsymbol{u}\right)-\nabla p+\rho\boldsymbol{g}+\boxed{\sigma\kappa\boldsymbol{n}_{\boldsymbol{\Gamma}}\delta_{\Gamma}}$$

$$\nabla\cdot\boldsymbol{u}=\dot{m}\underline{\left(\frac{1}{\rho_l}-\frac{1}{\rho_g}\right)}\delta_{\Gamma}$$

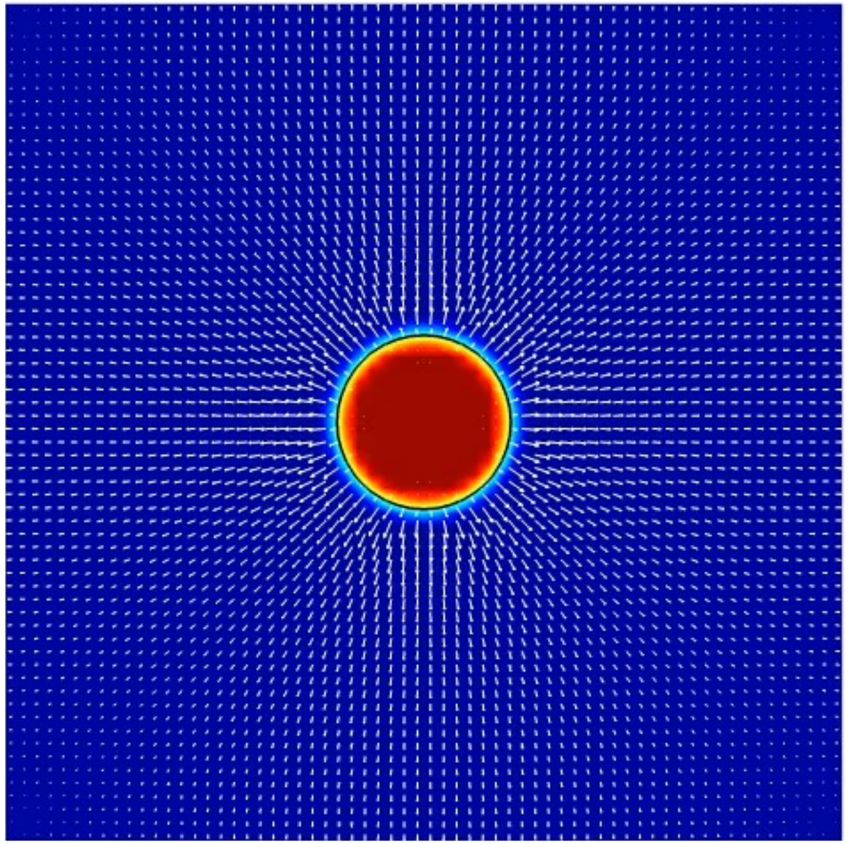
Surface Tension Force

Expansion Due to the Phase Change
(Responsible for the Stefan flow)

↓

Discontinuity in the Velocity Field

Numerical Model: Pressure-Velocity Coupling



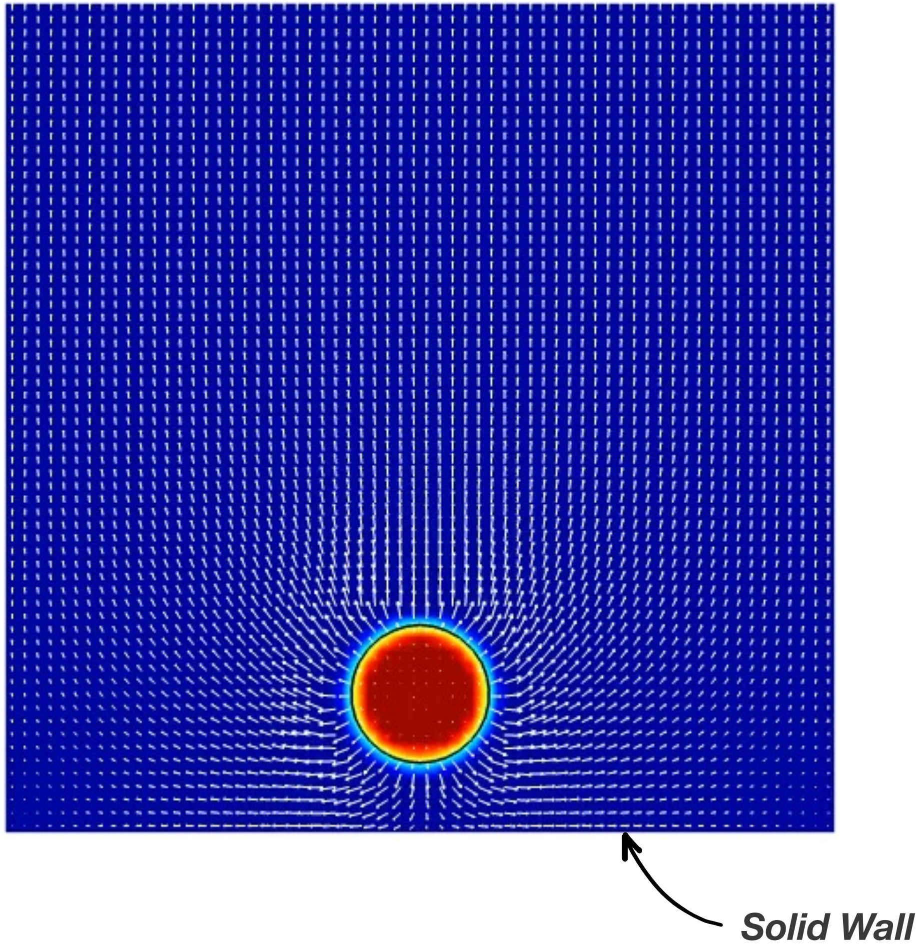
Double Pressure-Velocity Coupling

Solve another set of Navier-Stokes Equations that do not contain the volume expansion contribution

$$\rho\left(\frac{\partial \boldsymbol{u}^{\boldsymbol{E}}}{\partial t} + \nabla \cdot \left(\boldsymbol{u}^{\boldsymbol{E}} \otimes \boldsymbol{u}^{\boldsymbol{E}}\right)\right) = \mu\nabla \cdot \left(\nabla \boldsymbol{u}^{\boldsymbol{E}} + \nabla^{T} \boldsymbol{u}^{\boldsymbol{E}}\right) - \nabla p^{E} + \rho \boldsymbol{g} + \sigma\kappa \boldsymbol{n}_{\boldsymbol{\Gamma}} \delta_{\Gamma}$$

$$\nabla \cdot \boldsymbol{u}^{\boldsymbol{E}} \underbrace{= 0}_{\text{Divergence-free “extended” velocity } \boldsymbol{u}^{E}}$$

Numerical Model: Pressure-Velocity Coupling



Velocity-Potential Approach

Construct a velocity field u^S whose divergence is the expansion term.

$$\begin{cases} \nabla^2 \phi = \dot{m} \left(\frac{1}{\rho_g} - \frac{1}{\rho_l} \right) \delta_\Gamma \\ u^S = -\nabla \phi \end{cases}$$

We subtract this term from the field velocity:

$$\boldsymbol{u}^{\boldsymbol{E}} = \boldsymbol{u} - \boldsymbol{u}^{\boldsymbol{S}}$$

Numerical Model: Solution of Scalar Fields

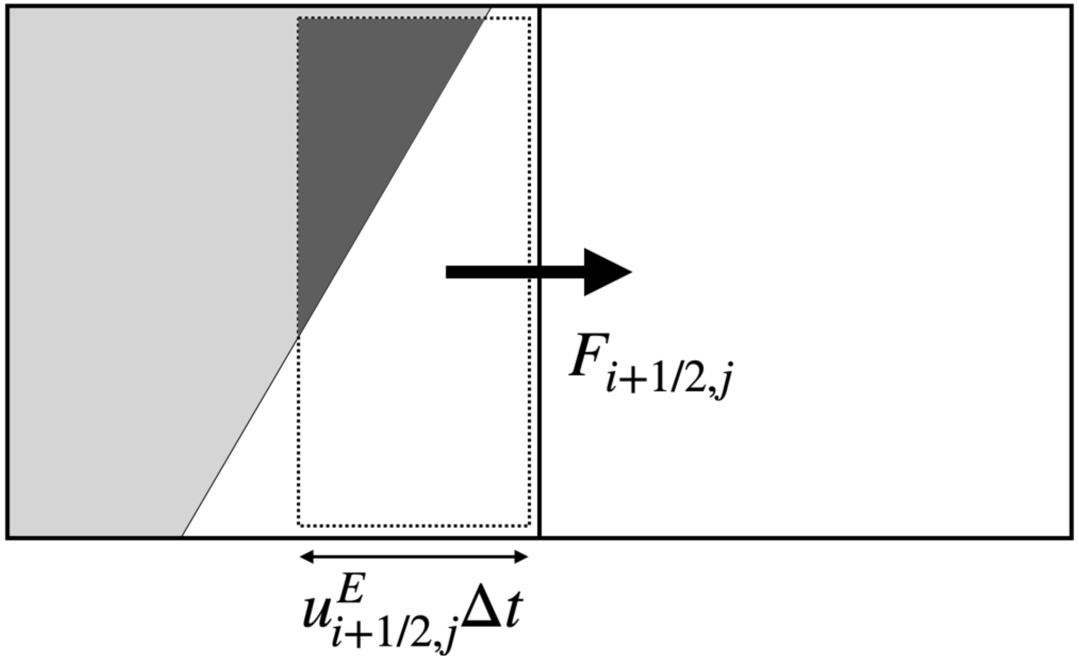
Temperature and Chemical Species Mass Fractions are considered as VOF-tracers ($t_i = c\omega_i$). We solve them using a **two-field approach**, splitting advection, diffusion, and reaction terms.

$$\frac{\partial \omega_{i,l}}{\partial t} + \underbrace{u \cdot \nabla \omega_i}_{\text{Advection}} = \underbrace{\nabla \cdot \left(\rho_l c D \nabla \omega_{i,l}\right) + \frac{\dot{m}_i}{\rho_l}\delta_\Gamma - \frac{\dot{m}_{tot}}{\rho_l}\delta_\Gamma \omega_{i,l}}_{\text{Diffusion and Phase Change}} + \underbrace{\sum_{j=1}^{NR} R_j \nu_{ij}}_{\text{Reactions}}$$

Numerical Model: Solution of Scalar Fields

Temperature and Chemical Species Mass Fractions are considered as VOF-tracers ($t_i = c\omega_i$). We solve them using a **two-field approach**, splitting advection, diffusion, and reaction terms.

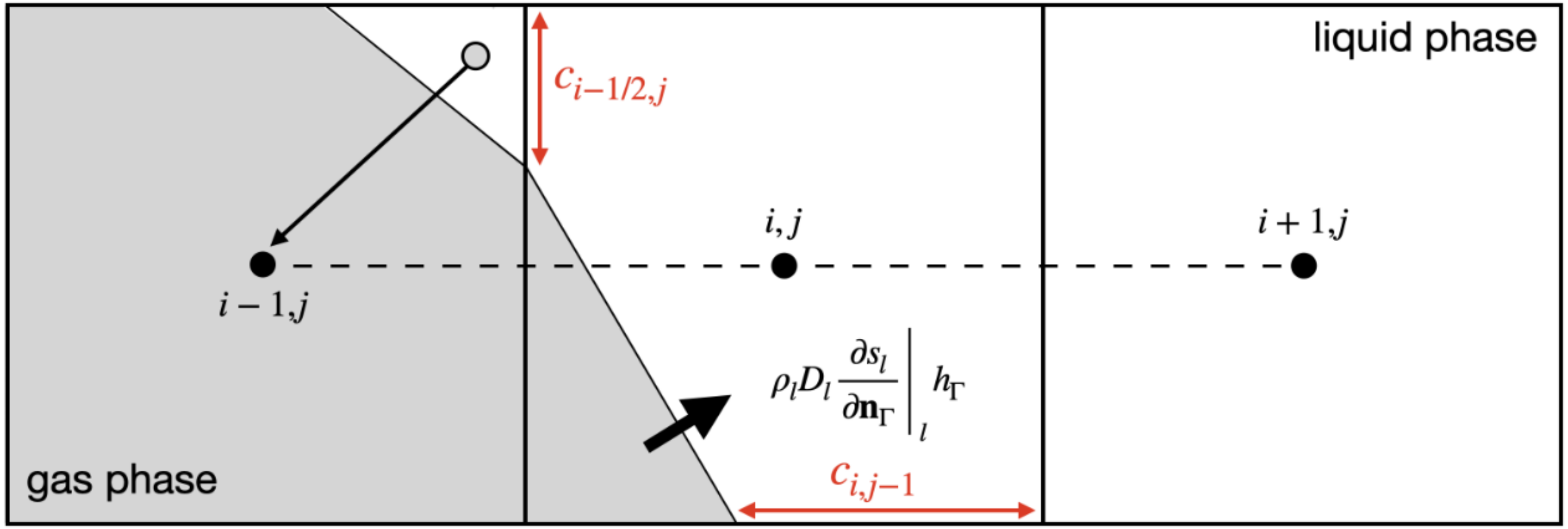
$$\frac{\partial \omega_{i,l}}{\partial t} + \underbrace{u \cdot \nabla \omega_i}_{\textit{Advection}} = \nabla \cdot \left(\rho_l c D \nabla \omega_{i,l}\right) + \frac{\dot{m}_i}{\rho_l}\delta_\Gamma - \frac{\dot{m}_{tot}}{\rho_l}\delta_\Gamma \omega_{i,l} + \sum_{j=1}^{NR} R_j \nu_{ij}$$



Numerical Model: Solution of Scalar Fields

Temperature and Chemical Species Mass Fractions are considered as VOF-tracers ($t_i = c\omega_i$). We solve them using a **two-field approach**, splitting advection, diffusion, and reaction terms.

$$\frac{\partial \omega_{i,l}}{\partial t} + u \cdot \nabla \omega_i = \underbrace{\nabla \cdot \left(\rho_l c D \nabla \omega_{i,l}\right) + \frac{\dot{m}_i}{\rho_l}\delta_\Gamma - \frac{\dot{m}_{tot}}{\rho_l}\delta_\Gamma \omega_{i,l}}_{\textit{Diffusion and Phase Change}} + \sum_{j=1}^{NR} R_j \nu_{ij}$$

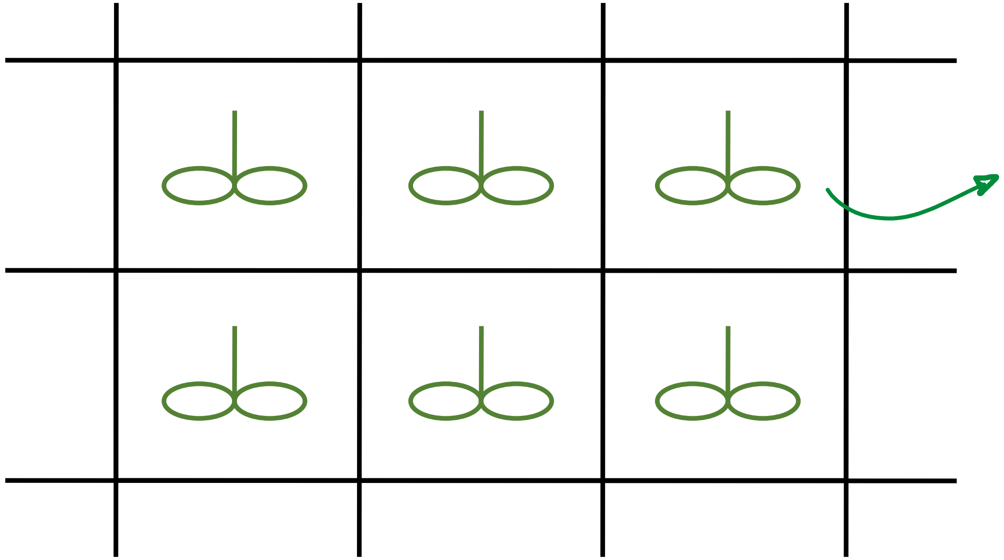


fracface.h from Lopez’ sandbox (Gennari 3D extension)

Numerical Model: Solution of Scalar Fields

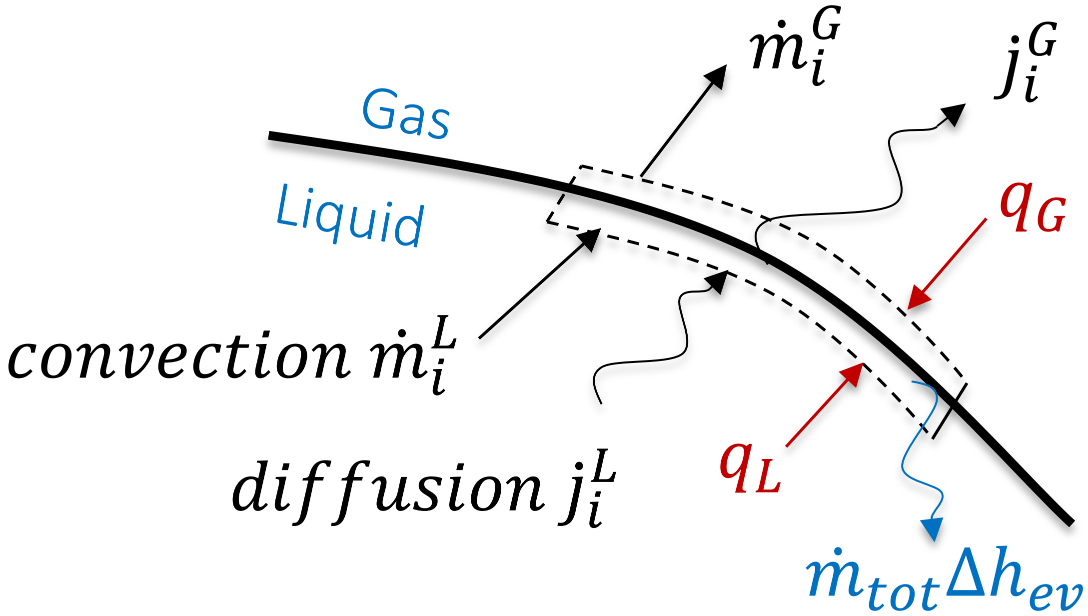
Temperature and Chemical Species Mass Fractions are considered as VOF-tracers ($t_i = c\omega_i$). We solve them using a **two-field approach**, splitting advection, diffusion, and reaction terms.

$$\frac{\partial \omega_{i,l}}{\partial t} + u \cdot \nabla \omega_i = \nabla \cdot \left(\rho_l c D \nabla \omega_{i,l}\right) + \frac{\dot{m}_i}{\rho_l}\delta_\Gamma - \frac{\dot{m}_{tot}}{\rho_l}\delta_\Gamma \omega_{i,l} + \underbrace{\sum_{j=1}^{NR} R_j \nu_{ij}}_{\textit{Reactions}}$$



Batch Reactor
(unsteady perfectly stirred vessel with reactions)

Numerical Model: Interface Jump Condition

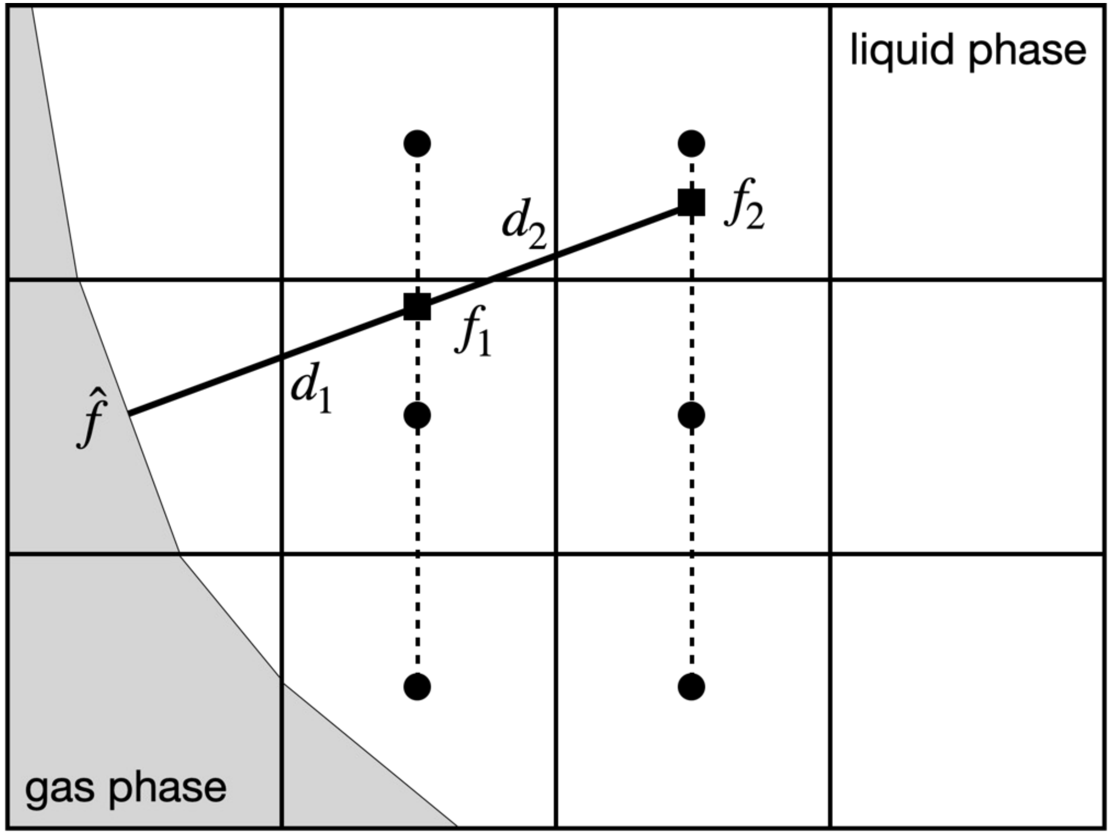


Non-Linear System

Of equations in every interfacial cell:
Computes the vaporization rate of every chemical species:

○ Mass Balance
○ Energy Balance
○ Thermodynamic Equilibrium

Numerical Model: Interface Jump Condition



Bothe, D., & Fleckenstein, S. *Chemical Engineering Science* (2013)

Interface Gradients Calculation

For the diffusive fluxes (Fick and Fourier Laws), we exploit a 6-points scheme adapted from the Embedded Boundary Method. Fundamental for the correct solution of the system:

$$\left(\frac{\partial f}{\partial \boldsymbol{n}_\Gamma}\right) = \left(c\,\frac{f_\Gamma - f_0}{d_0} + (1-c)\,\frac{f_\Gamma - f_1}{d_1}\right)$$

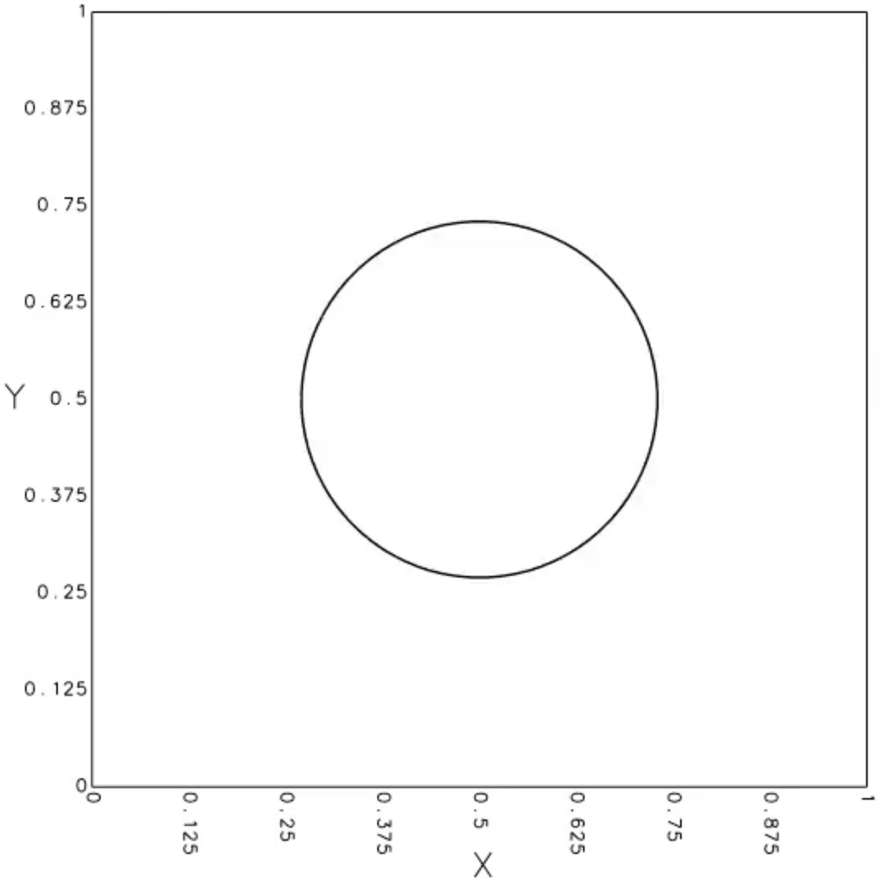
03

Numerical Results

- Constant Properties Validation
- Non-Constant Properties Simulations

Validation: Fixed Flux Evaporation of a Liquid Droplet

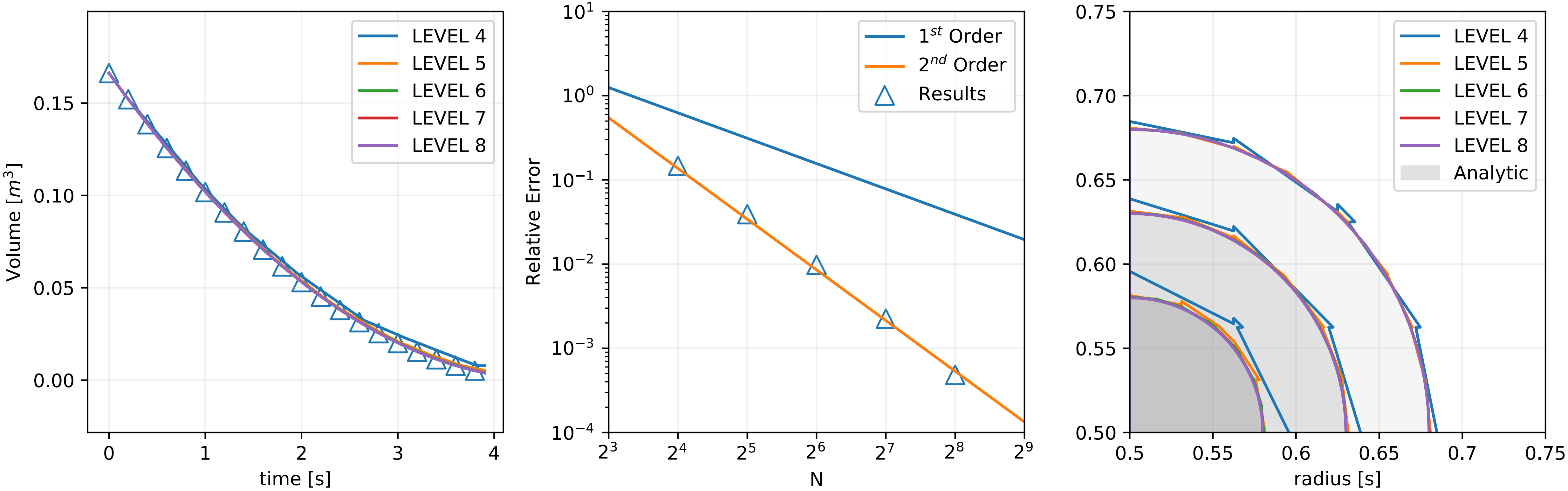
Evaporation of a liquid droplet with a constant vaporization flowrate, the mass balance on the liquid droplet is the analytic solution to the problem: $\frac{dR}{dt} = \frac{\dot{m}}{\rho_l}$



Malan et al. *Journal of Computational Physics* (2021)

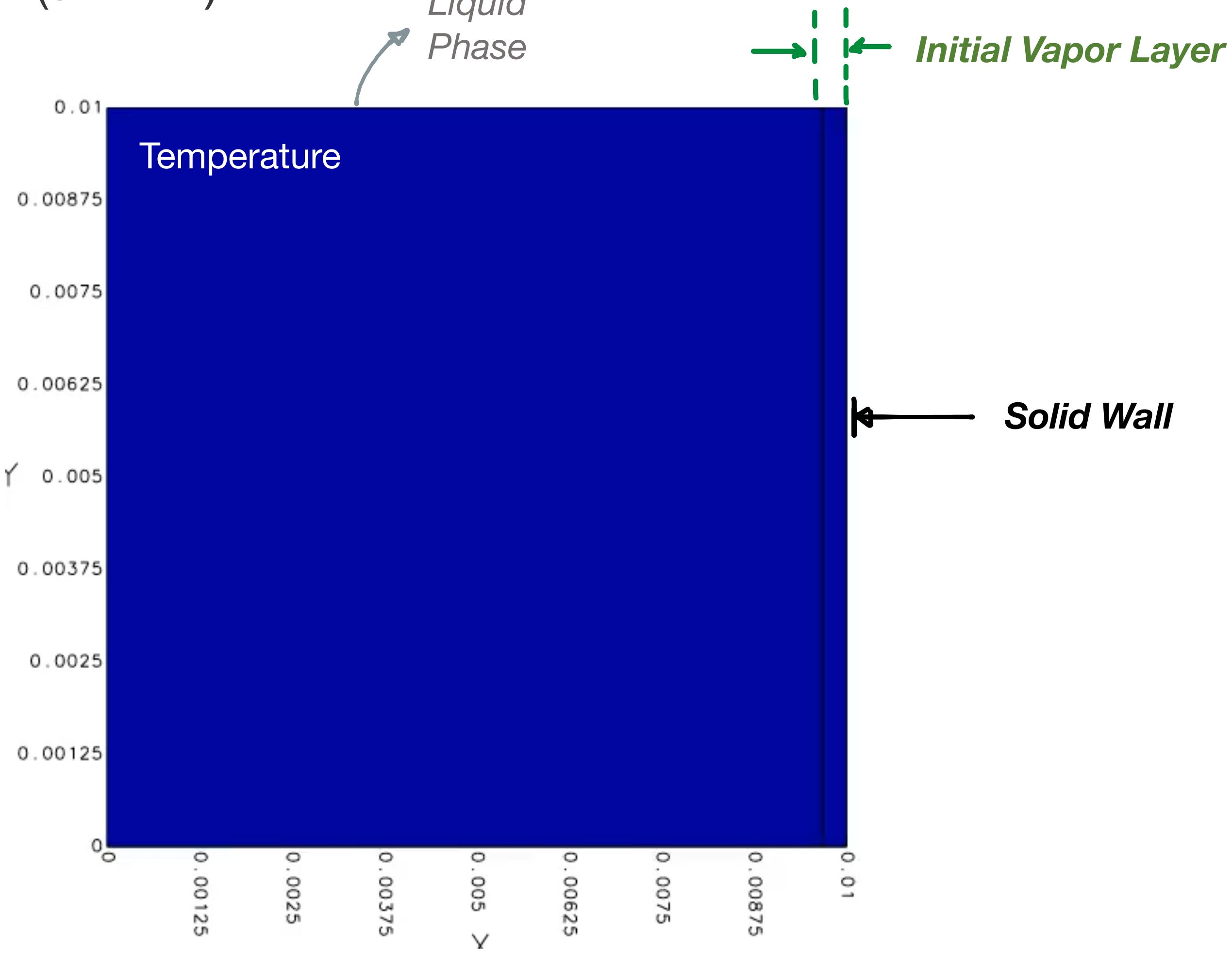
Validation: Fixed Flux Evaporation of a Liquid Droplet

Evaporation of a liquid droplet with a constant vaporization flowrate, the mass balance on the liquid droplet is the analytic solution to the problem: $\frac{dR}{dt} = \frac{\dot{m}}{\rho_l}$



Validation: Stefan Problem

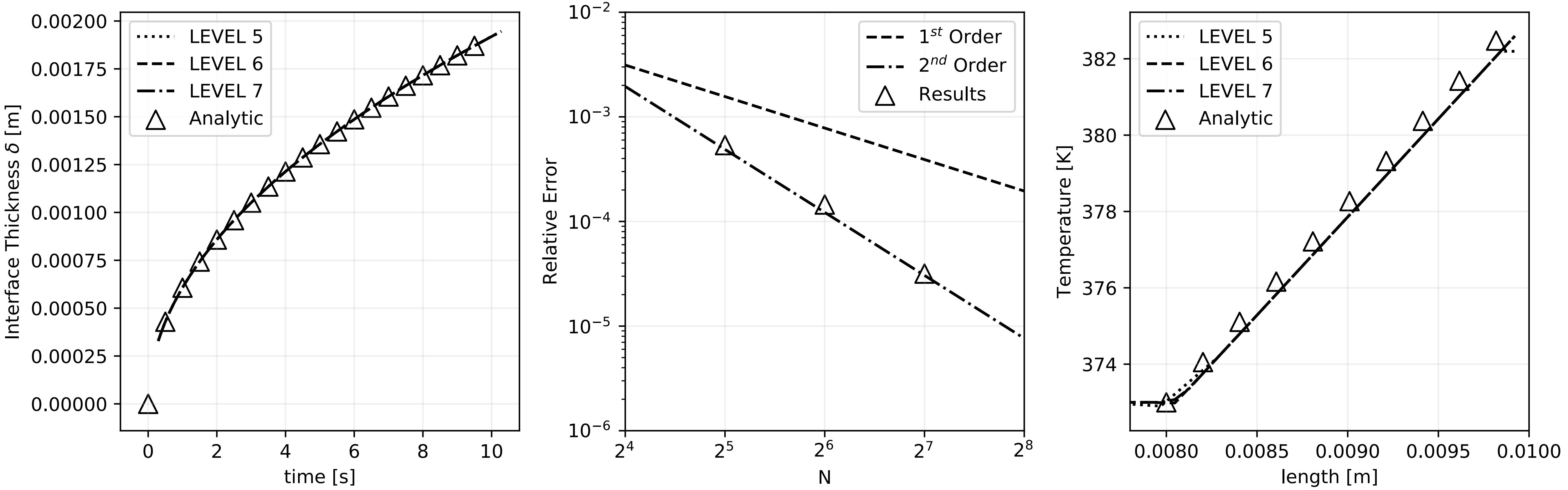
Evaporation of a liquid plane, induced by a temperature gradient between a hot wall and a vapor layer in contact with the liquid (Ja=0.5).



Malan et al. *Journal of Computational Physics* (2021)

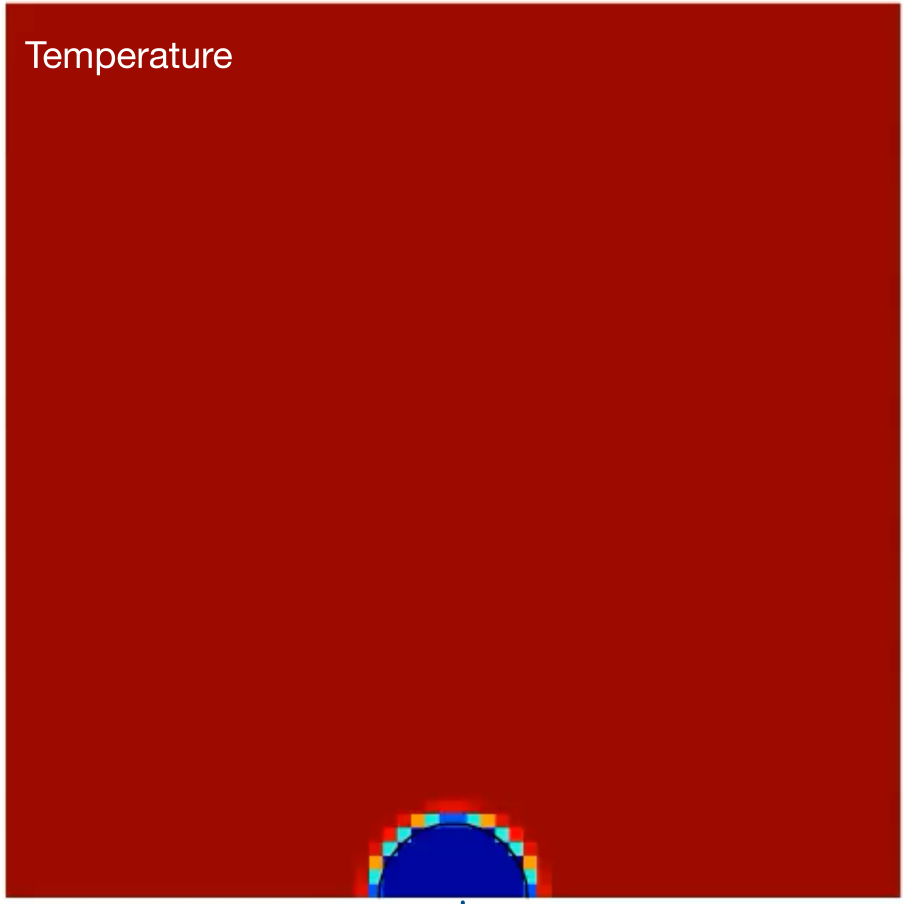
Validation: Stefan Problem

Evaporation of a liquid plane, induced by a temperature gradient between a hot wall and a vapor layer in contact with the liquid (Ja=0.5).



Validation: Scriven Problem

Growth of a bubble in a superheated liquid (Ja = 3).



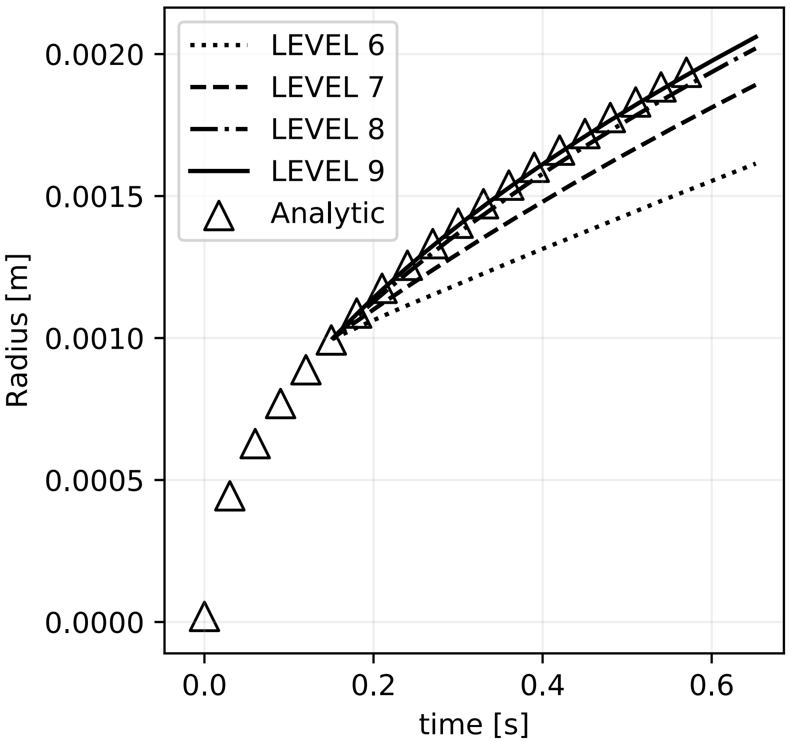
Superheated Liquid

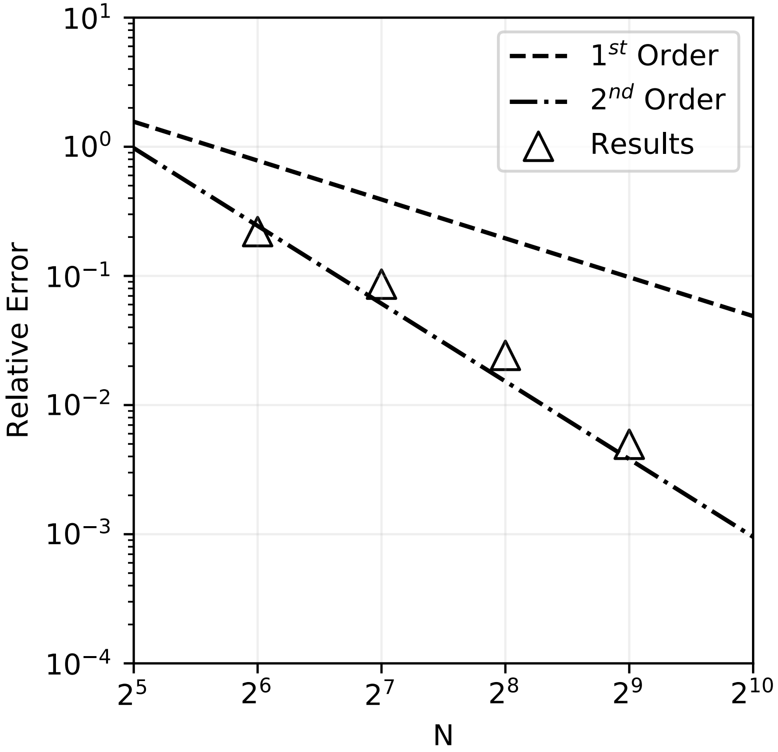
Bubble at saturation temperature

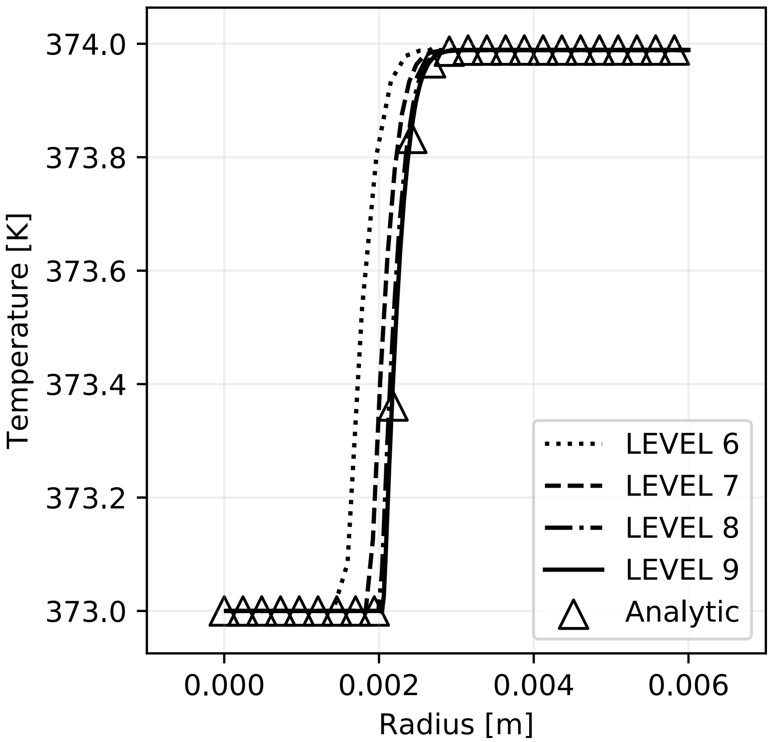
Tanguy et al. *Journal of Computational Physics* (2014)

Validation: Scriven Problem

Growth of a bubble in a superheated liquid (Ja = 3).

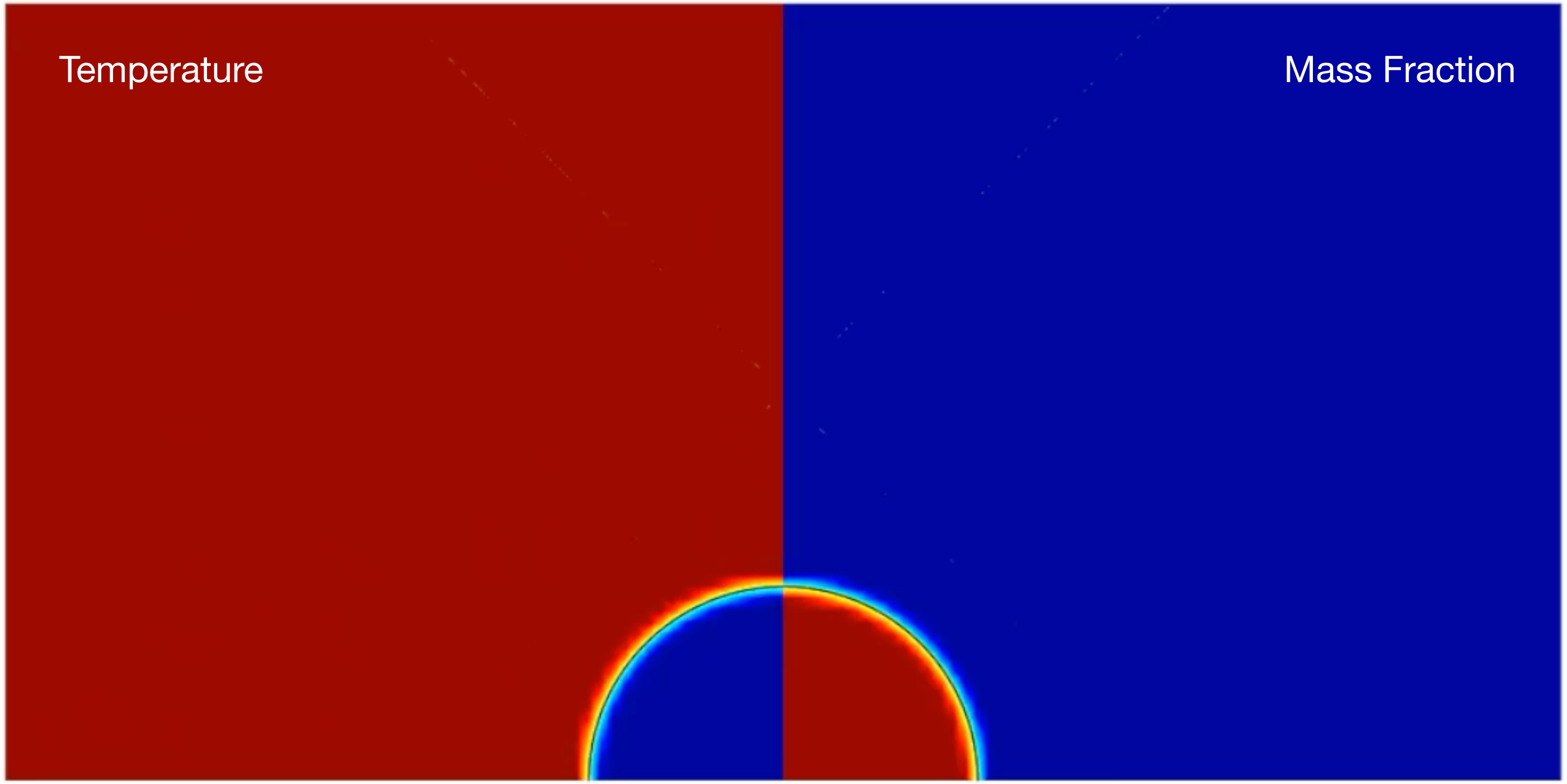






Validation: Non-Isothermal Evaporation of a N-Heptane Droplet

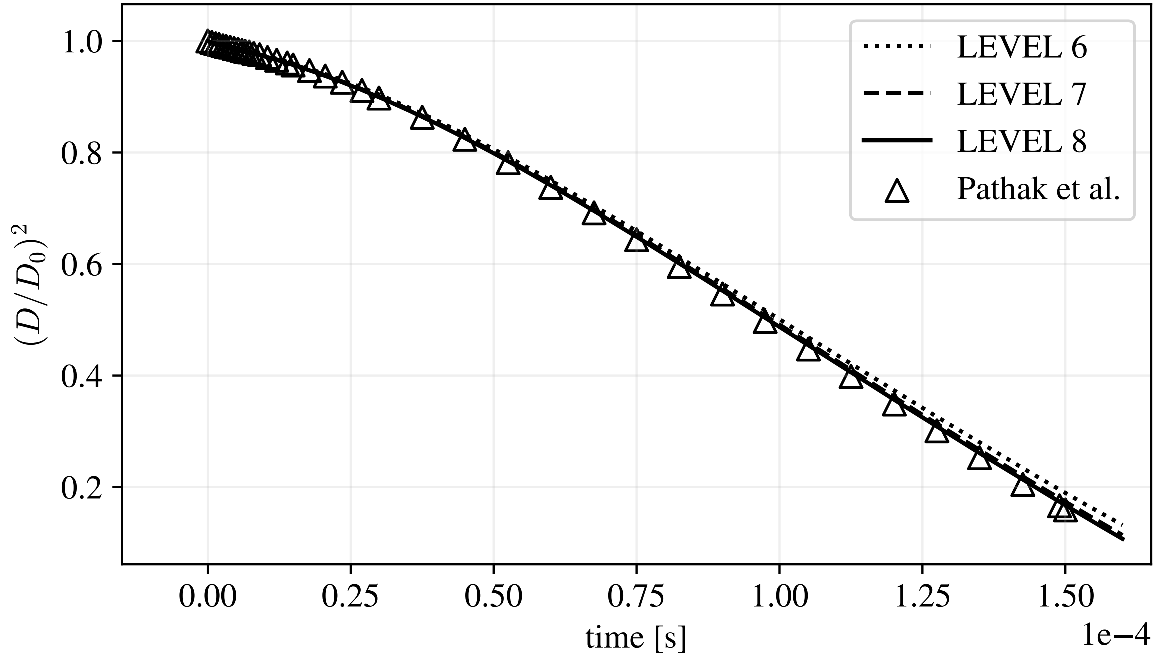
Evaporation of a n-heptane droplet in a non-isothermal environment. The material properties are assumed to be constant in space and time during the entire simulation.

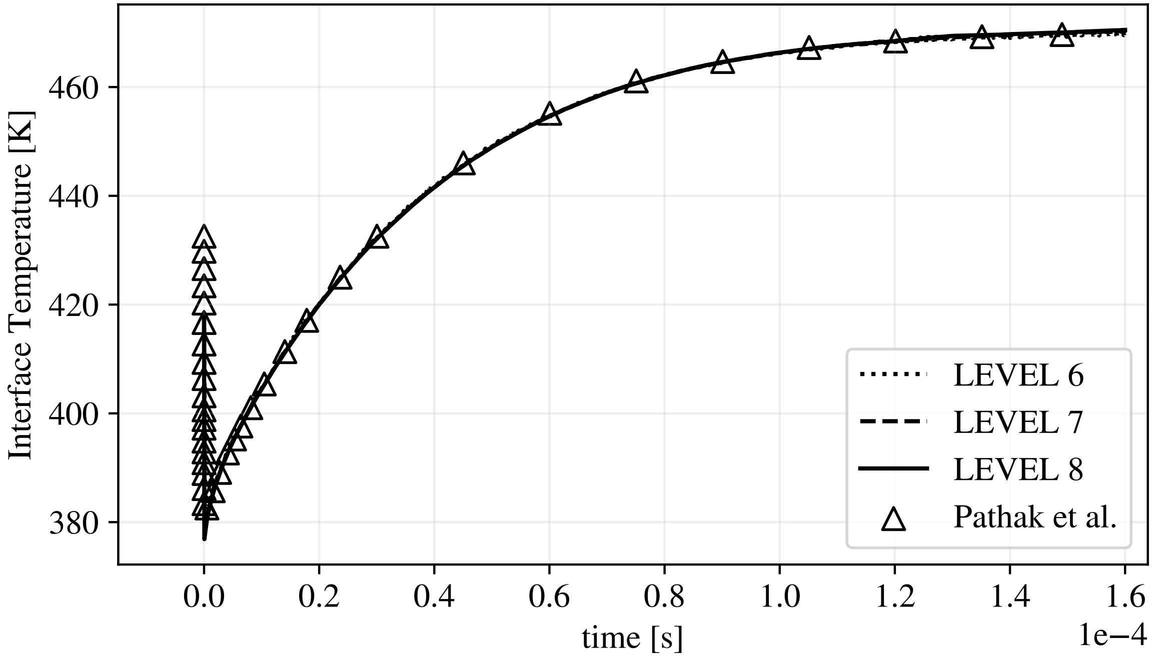


Pathak et al. *International Journal of Heat and Mass Transfer* (2018)

Validation: Non-Isothermal Evaporation of a N-Heptane Droplet

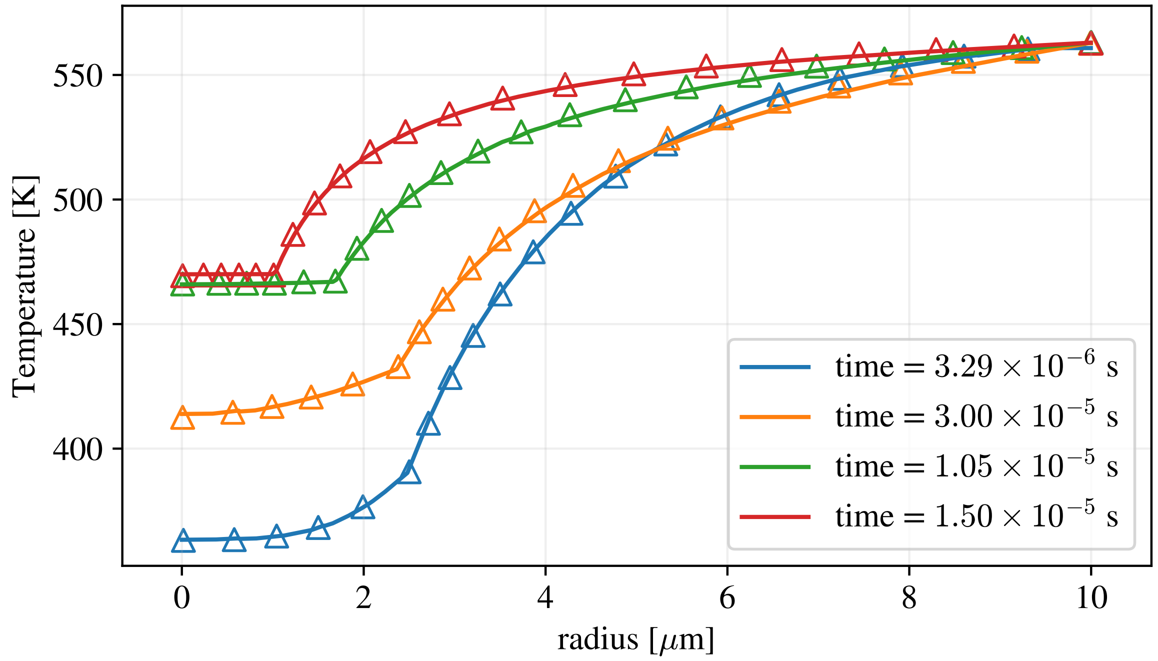
Evaporation of a n-heptane droplet in a non-isothermal environment. The material properties are assumed to be constant in space and time during the entire simulation.

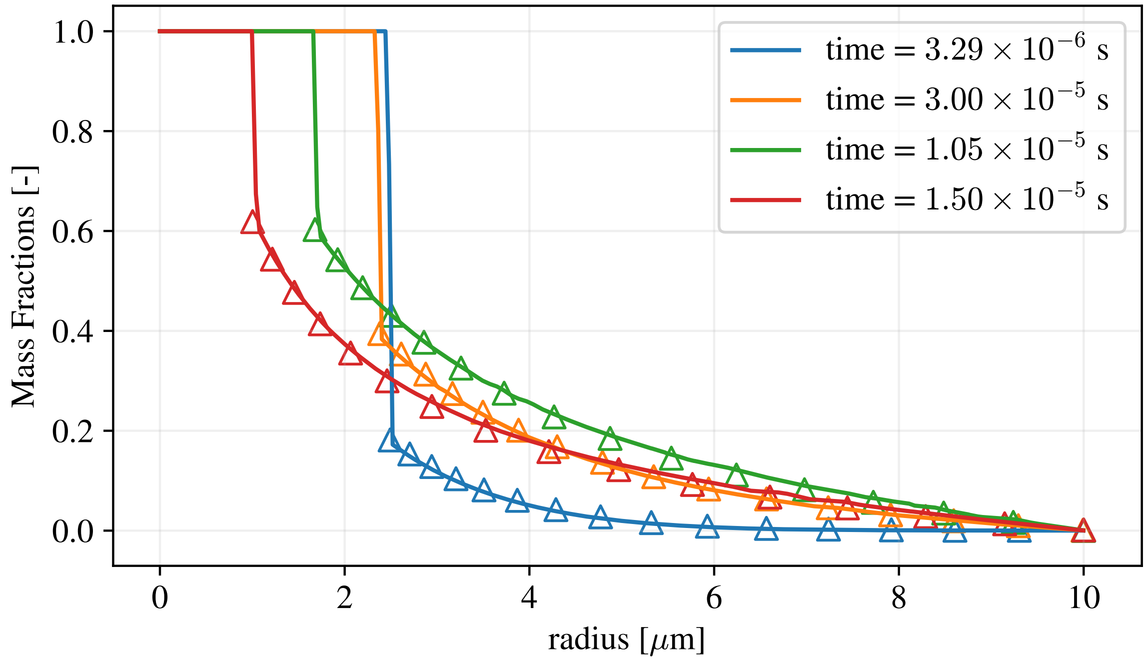




Validation: Non-Isothermal Evaporation of a N-Heptane Droplet

Evaporation of a n-heptane droplet in a non-isothermal environment. The material properties are assumed to be constant in space and time during the entire simulation.





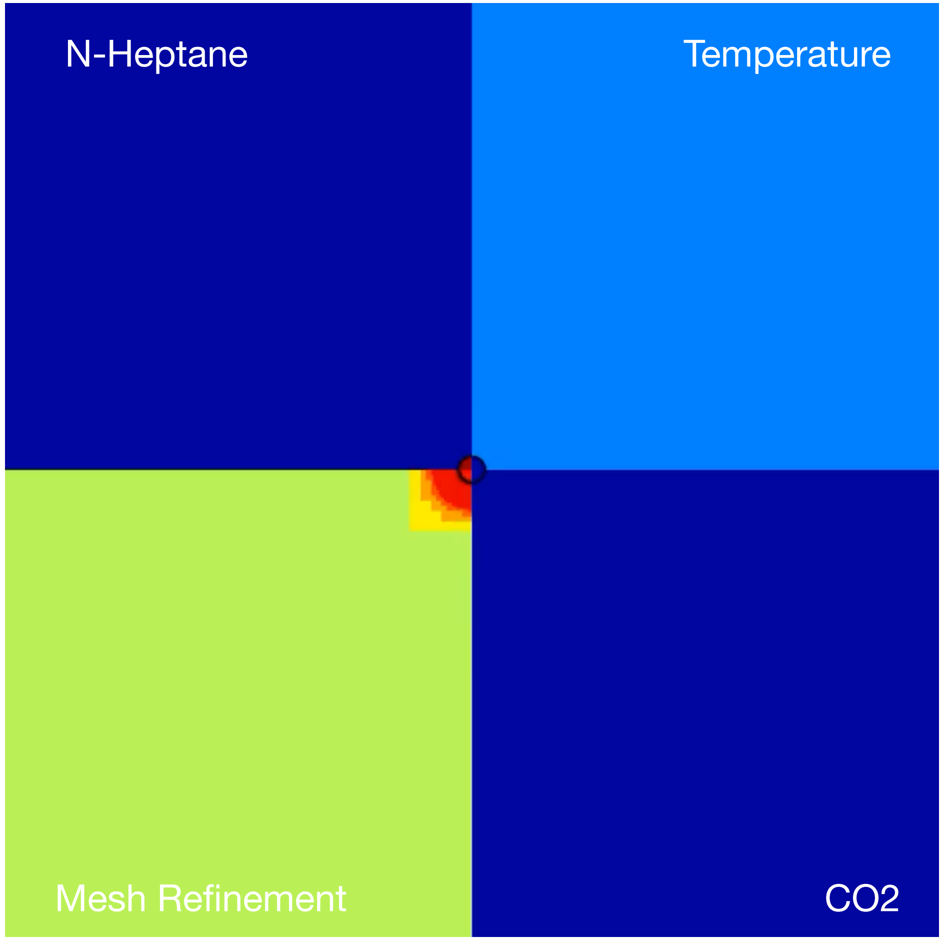
Results: Combustion of a N-Heptane Droplet

Combustion of a n-heptane droplet in microgravity: experiment on the International Space Station.

Dietrich et al. *Microgravity Science and Technology* (2014)

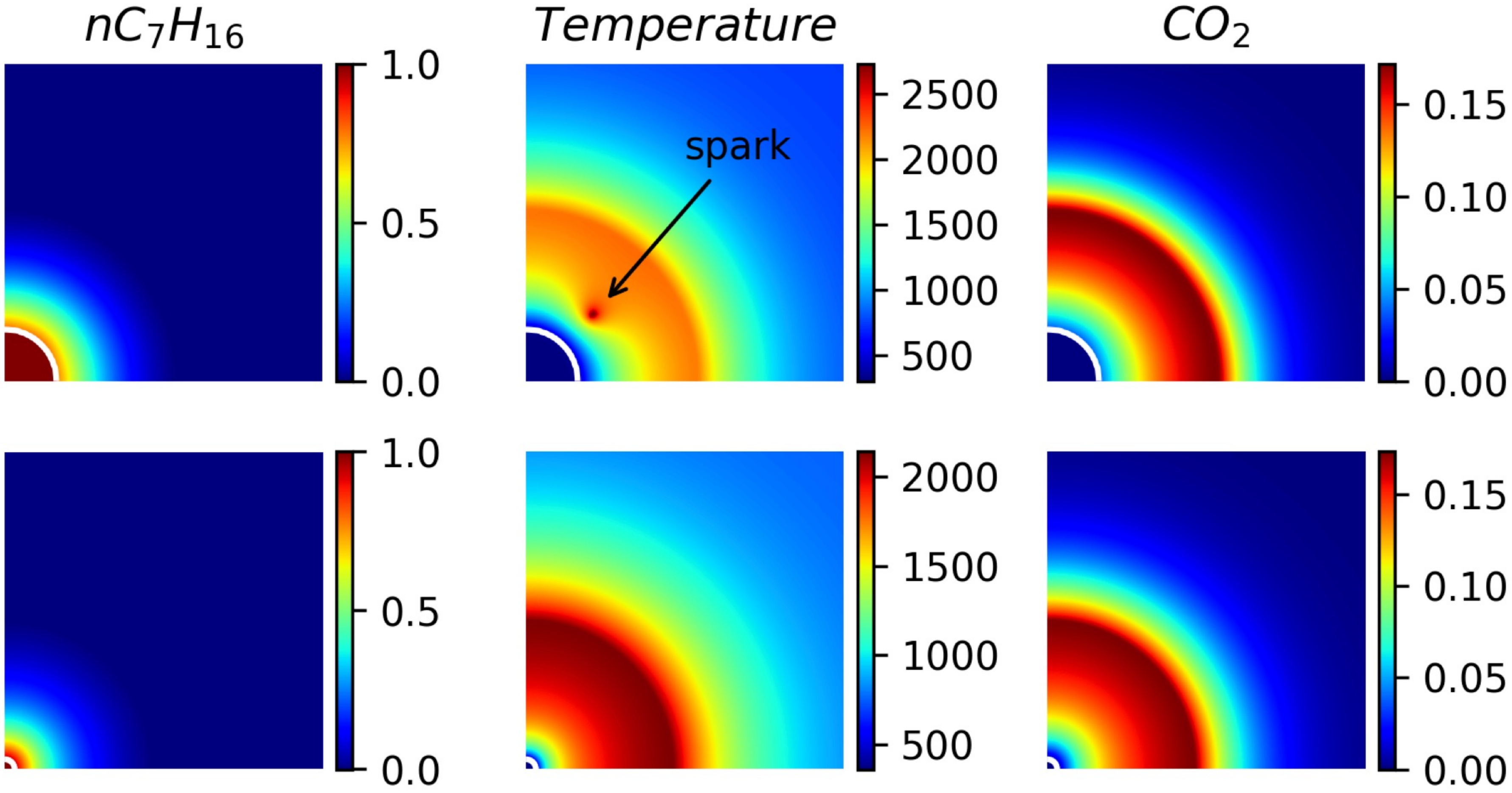
Results: Combustion of a N-Heptane Droplet

Combustion of a n-heptane droplet in a non-isothermal with constant properties and a global kinetic scheme.



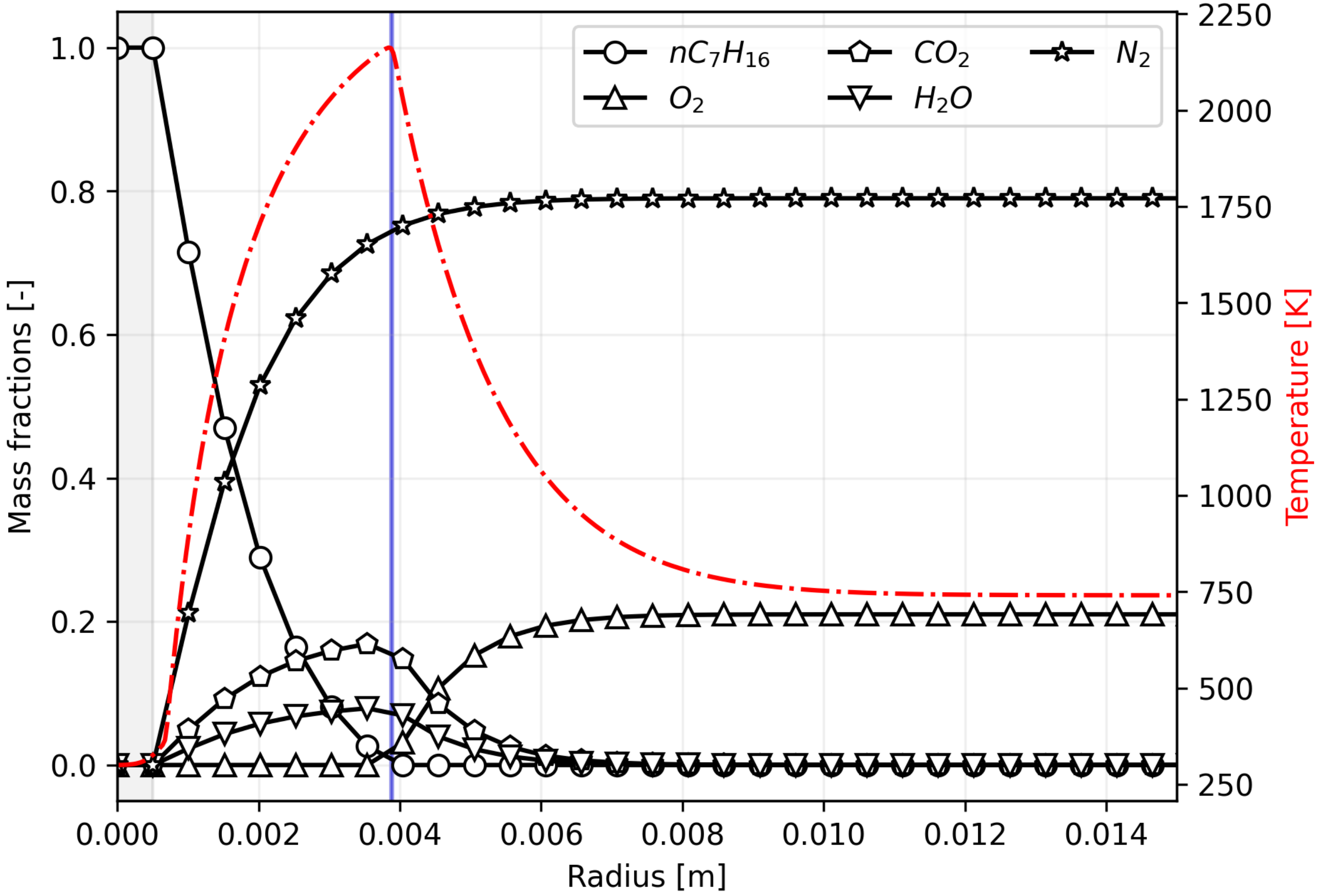
Results: Combustion of a N-Heptane Droplet

Combustion of a n-heptane droplet in a non-isothermal with constant properties and a global kinetic scheme: $nC_7H_{16} + 11O_2 \Rightarrow 7CO_2 + 8H_2O$



Results: Combustion of a N-Heptane Droplet

Combustion of a n-heptane droplet in a non-isothermal with constant properties and a global kinetic scheme: $nC_7H_{16} + 11O_2 \Rightarrow 7CO_2 + 8H_2O$



Numerical Model: Variable Properties Formulation

We introduce and equation of state:

$$\rho = EoS(T, P, \boldsymbol{x})$$

The continuity equation is corrected in order to consider density changes:

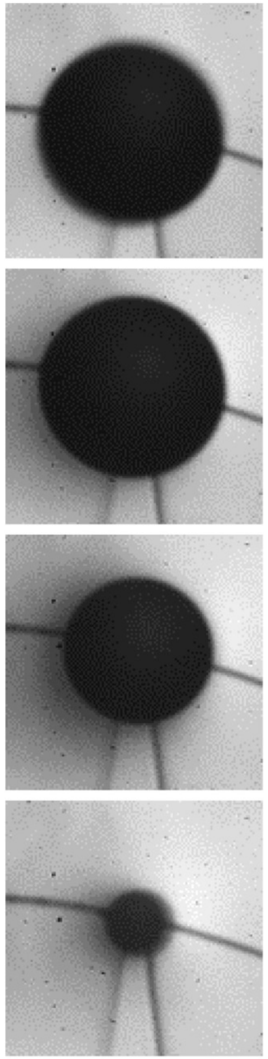
$$\nabla \cdot \boldsymbol{u} = -\frac{\beta}{\rho c_p} \nabla \cdot (\lambda \nabla T) + \dot{m} \left(\frac{1}{\rho_g} - \frac{1}{\rho_l} \right) \delta_\Gamma$$

The scalar fields equations are re-written in a conservative form:

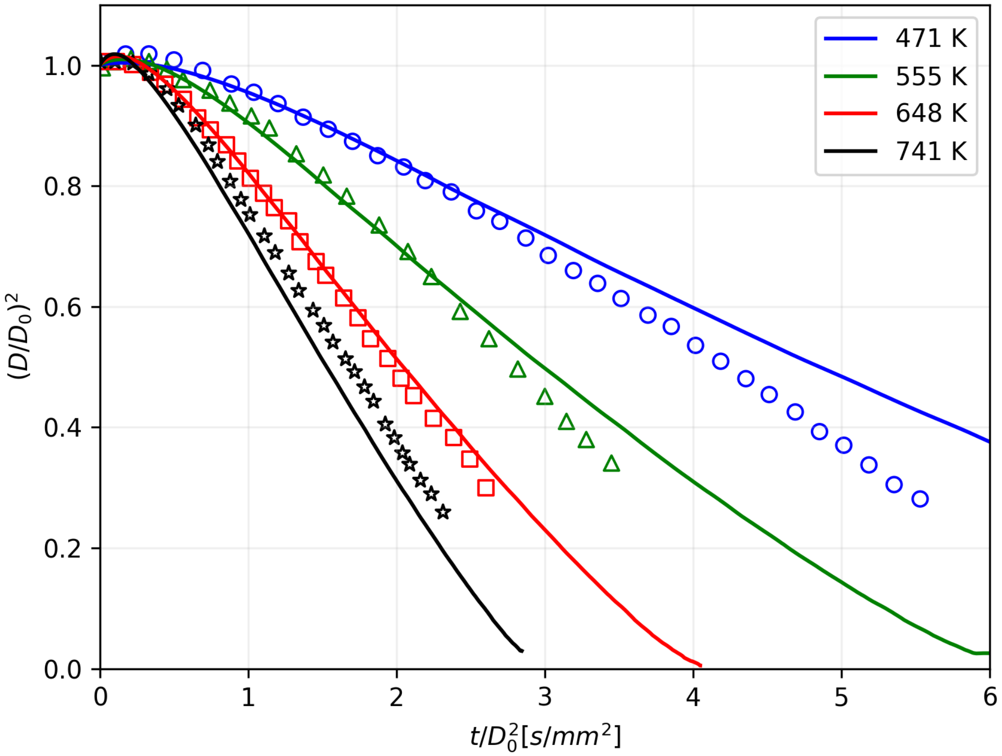
$$\frac{\partial \left(\rho c \omega_{i,l} \right)}{\partial t} + \nabla \cdot \left(\rho c \omega_{i,l} \boldsymbol{u} \right) = \nabla \cdot \left(\rho D c \nabla \omega_{i,l} \right) - \dot{m}_i$$

Wang Y., et al *Journal of Computational Physics* (2019)

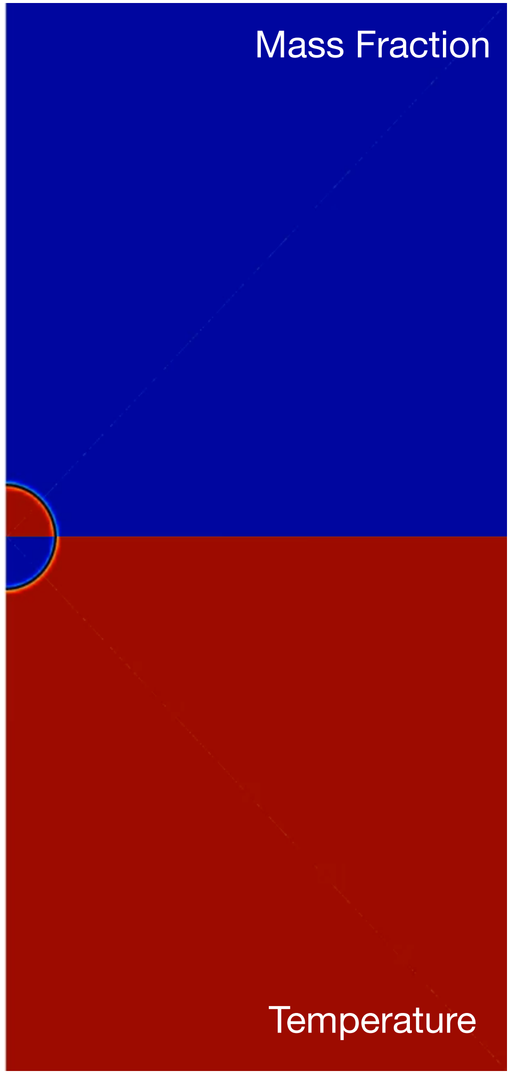
Results: N-Heptane Microgravity Droplet Evaporation



D_0 0.7 mm - P 0.1 MPa
Effect of the Ambient Temperature

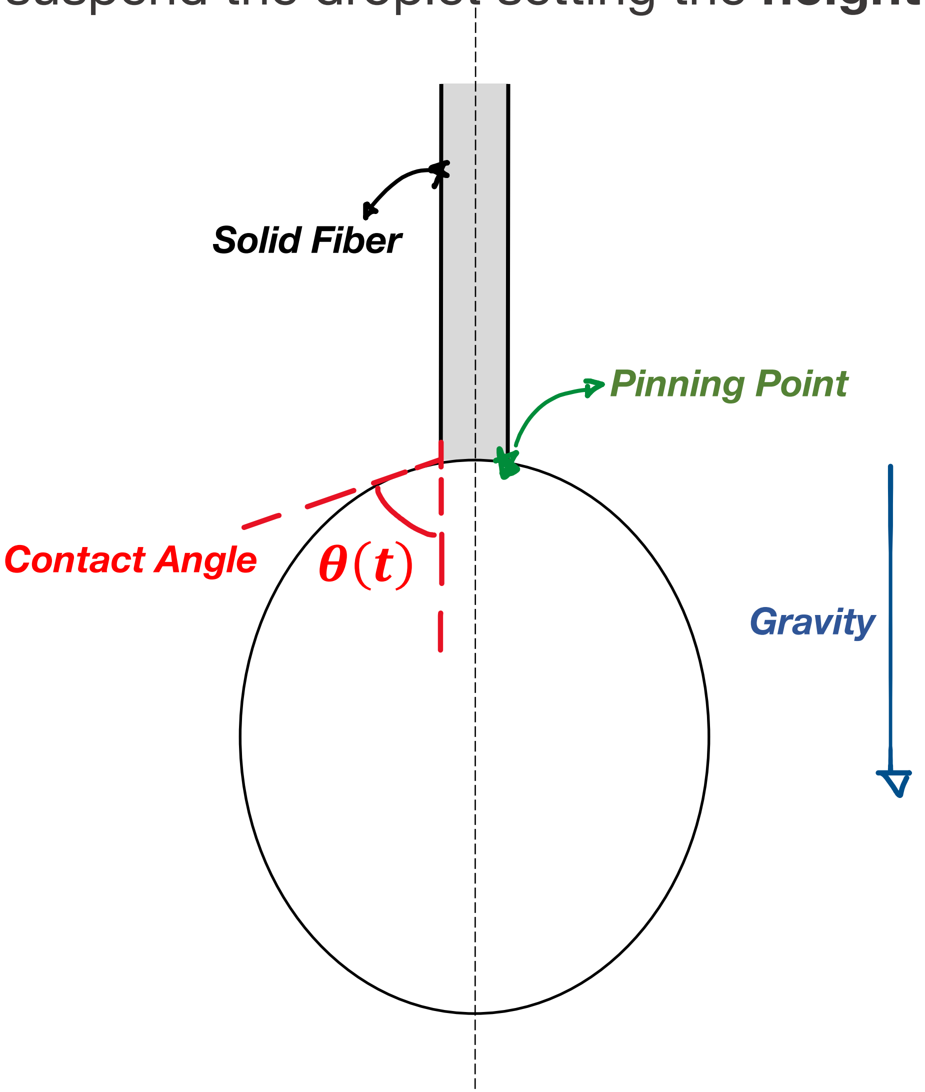


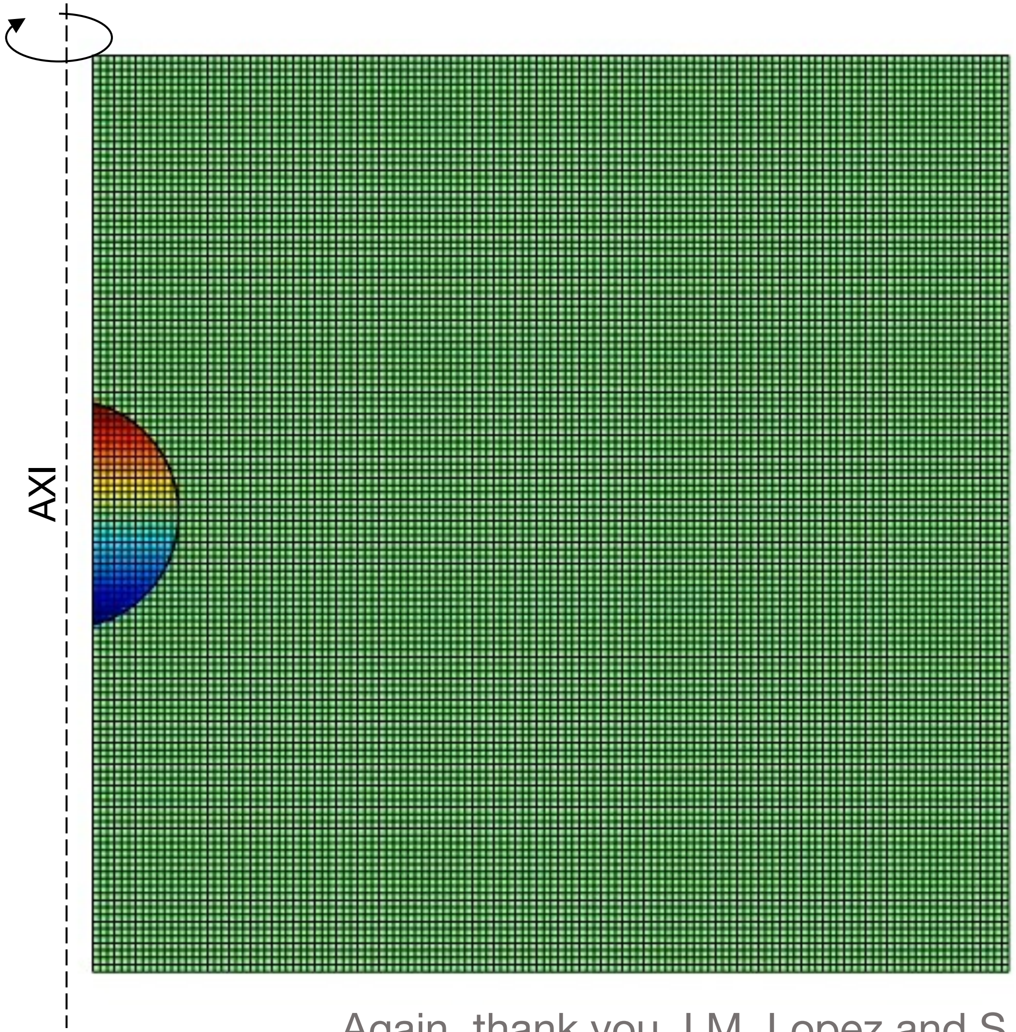
Nomura H., et al *Symposium (International) on Combustion* (1996)



Results: Suspended Droplets in Normal Gravity Conditions

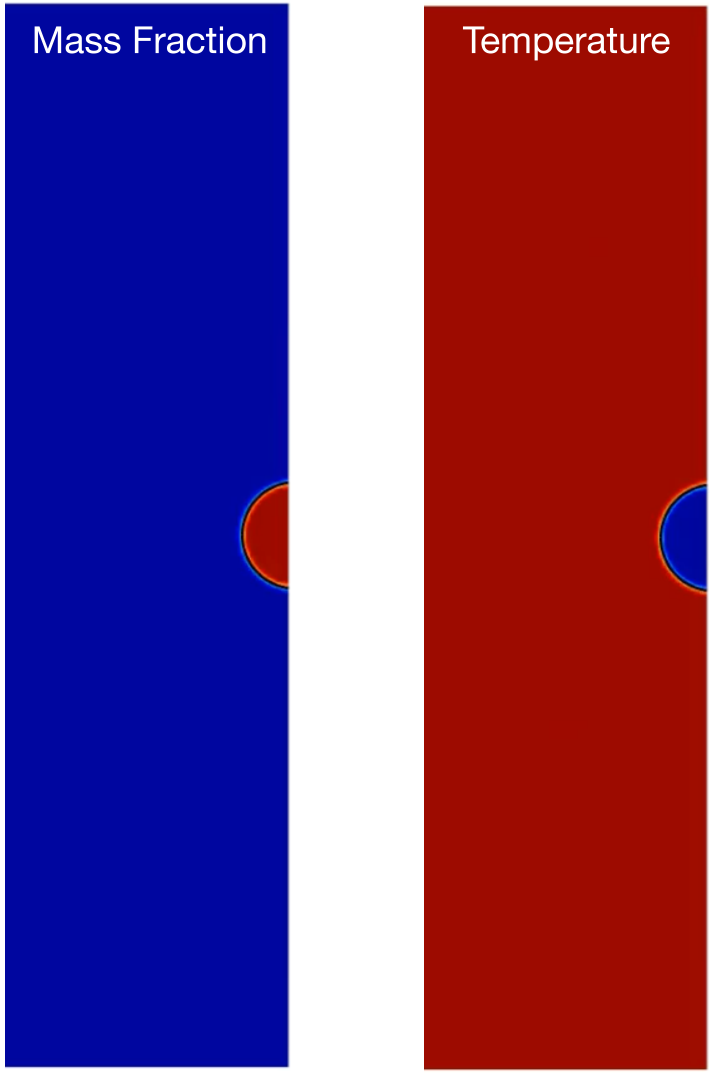
We suspend the droplet setting the **height-function boundary conditions**.



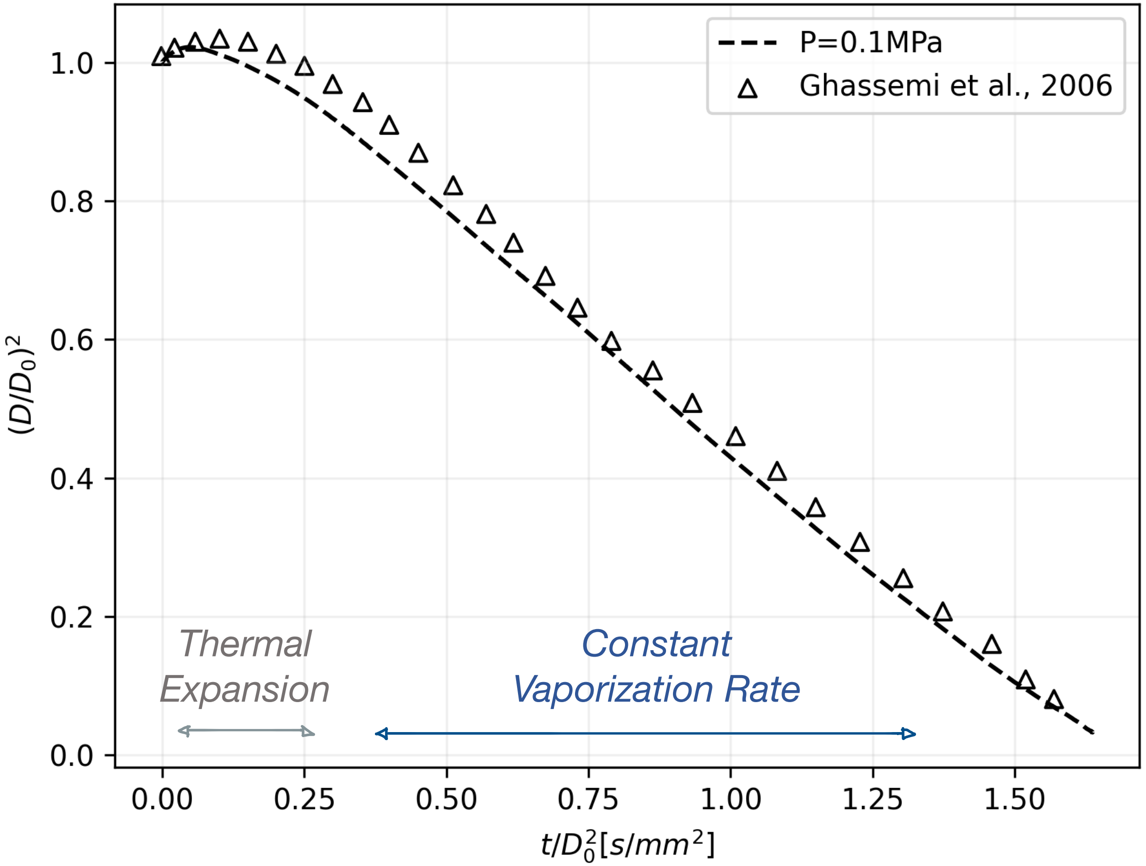


Again, thank you J.M. Lopez and S. Popinet

Results: Suspended N-Heptane Droplet Evaporation

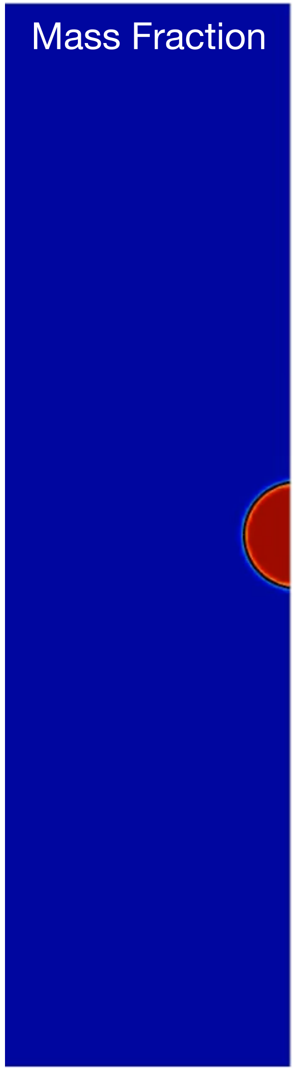


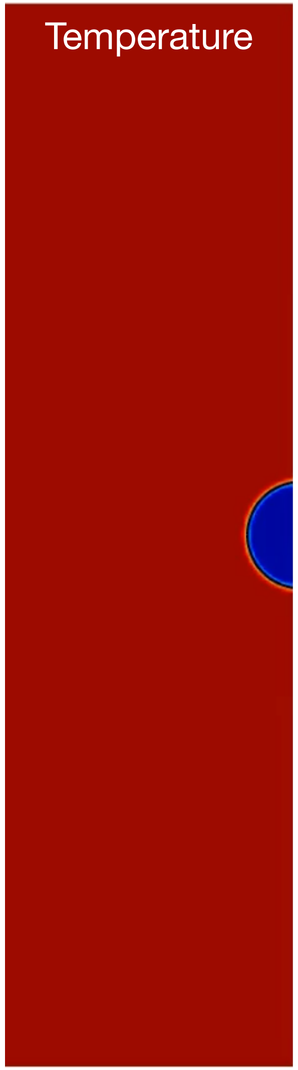
D_0 1mm - P 0.1MPa – T 973K



***Ghassemi H., et al,** Combustion science and technology* (2006)

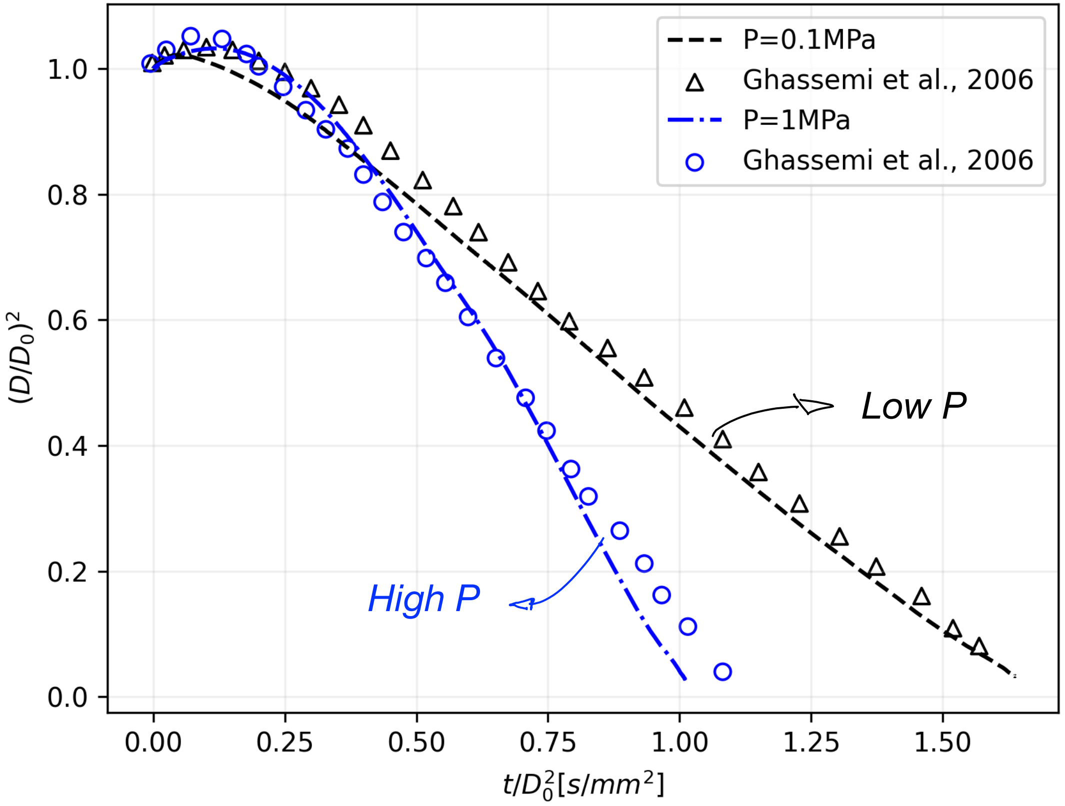
Results: Suspended N-Heptane Droplet Evaporation





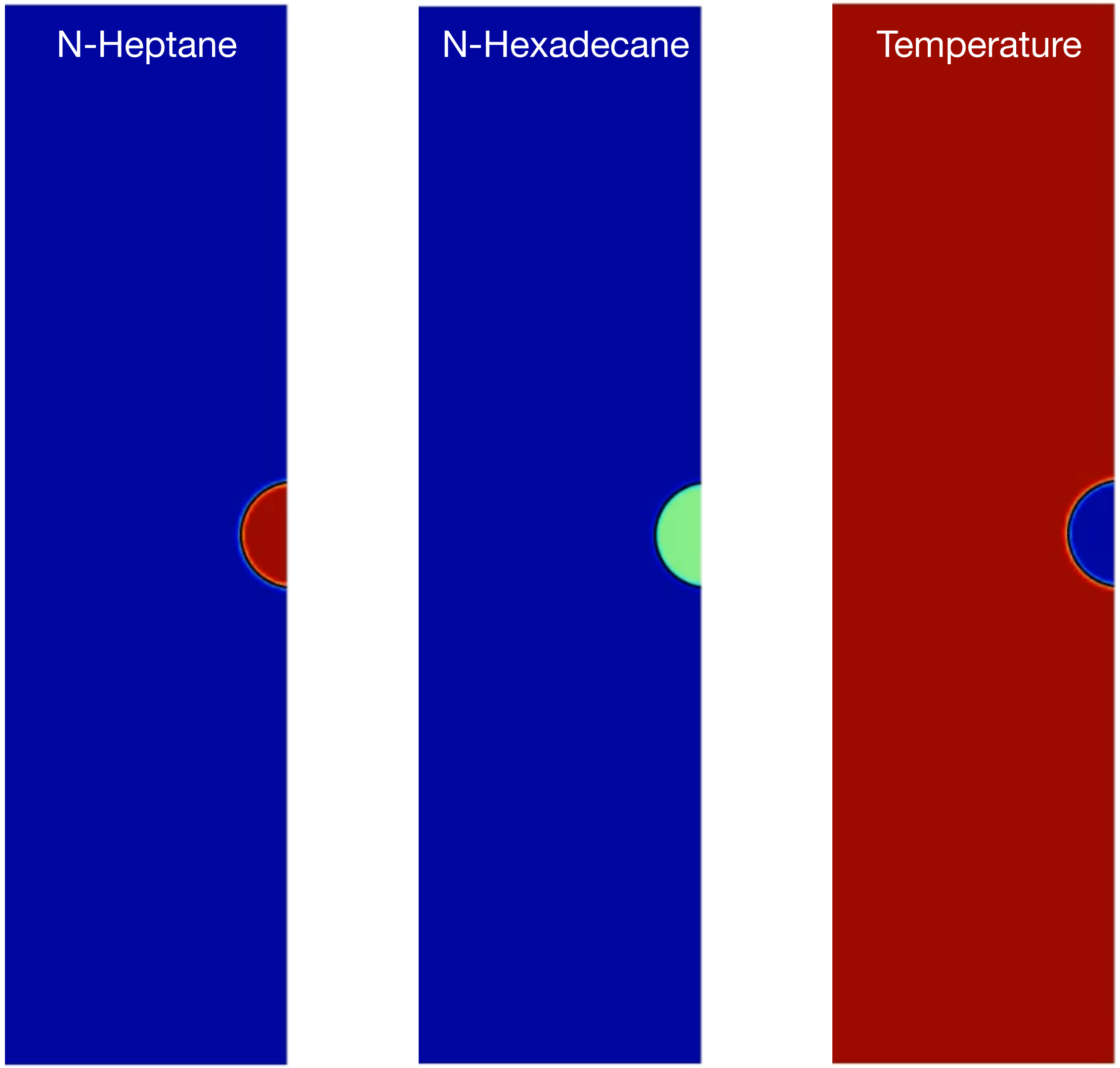
D_0 1mm - P 1MPa – T 973K

✓ Stronger Wake



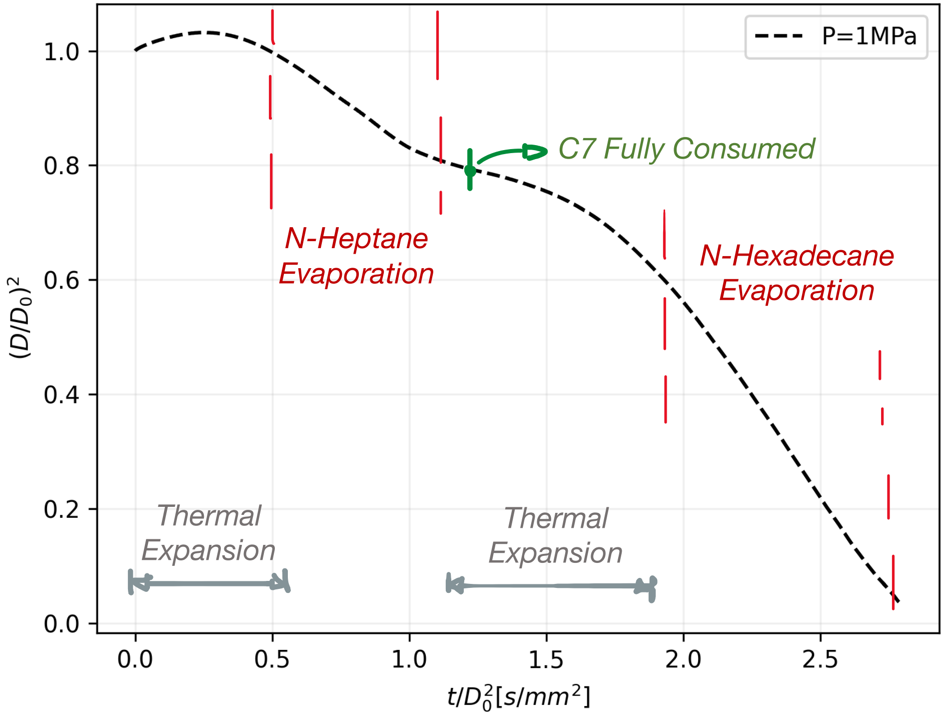
***Ghassemi H., et al,** Combustion science and technology* (2006)

Results: Suspended N-Heptane/N-Hexadecane Droplet Evaporation



D_0 1mm - P 1MPa – T 773K

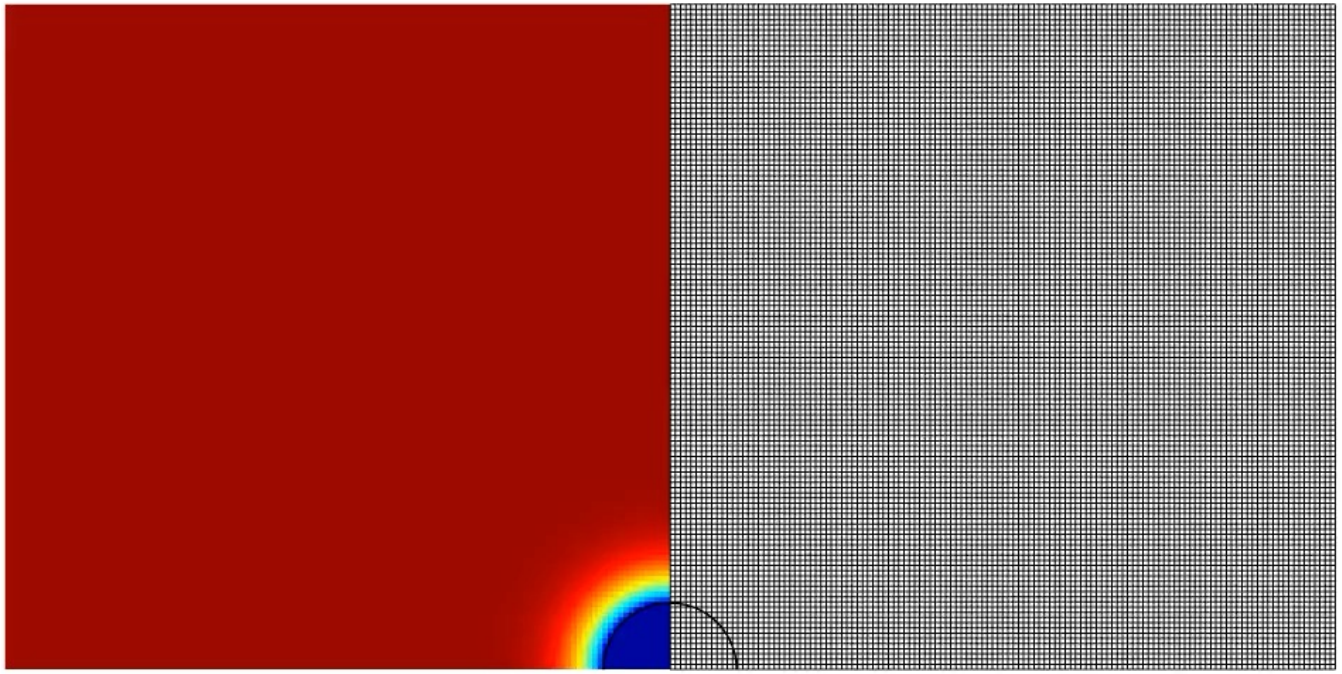
- ✓ Preferential Vaporization
- ✓ Accumulation of the heavy species
- ✓ Double saddle behavior
- ✓ Liquid Phase internal recirculation



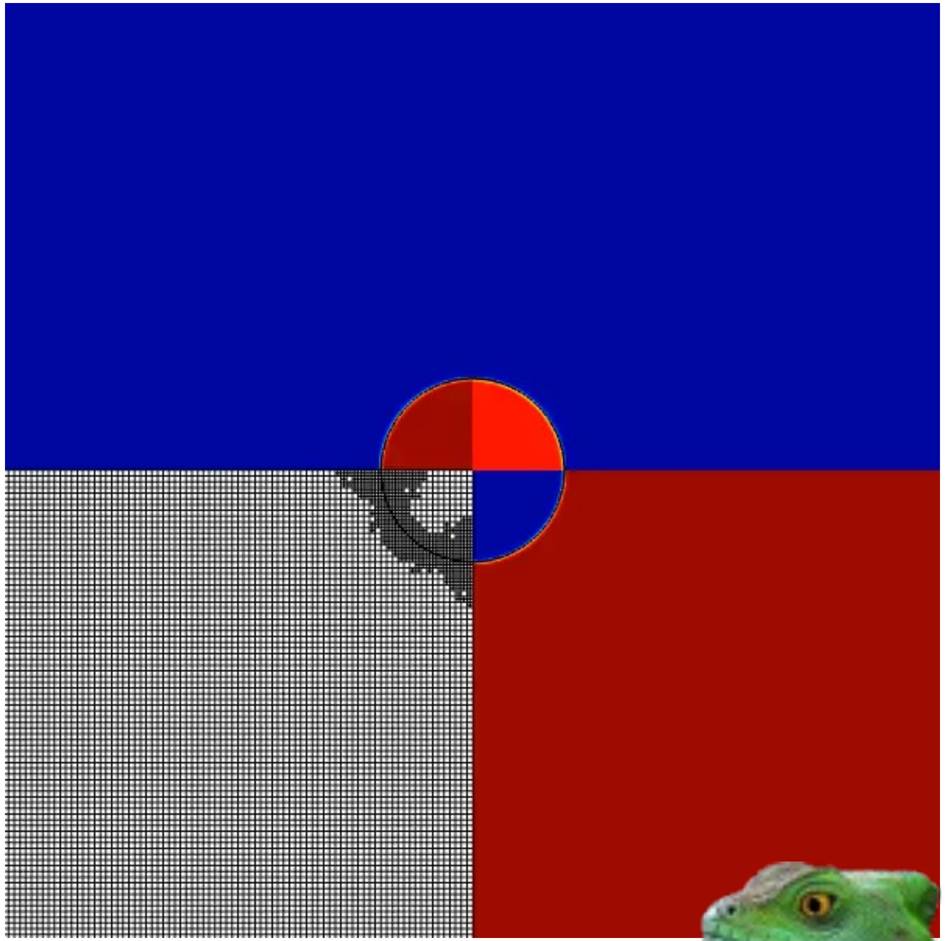
Check Out the Codes on the Basilisk websites

http://basilisk.fr/sandbox/ecipriano/

bubblecontact.c



staticbi.c



Edoardo Cipriano – BGUM 2023

Thank you for your attention

(edoardo.cipriano@polimi.it)