MULTISCALE MODELING OF VISCOUS FLOW IN A POROUS MEDIUM. BASILISK

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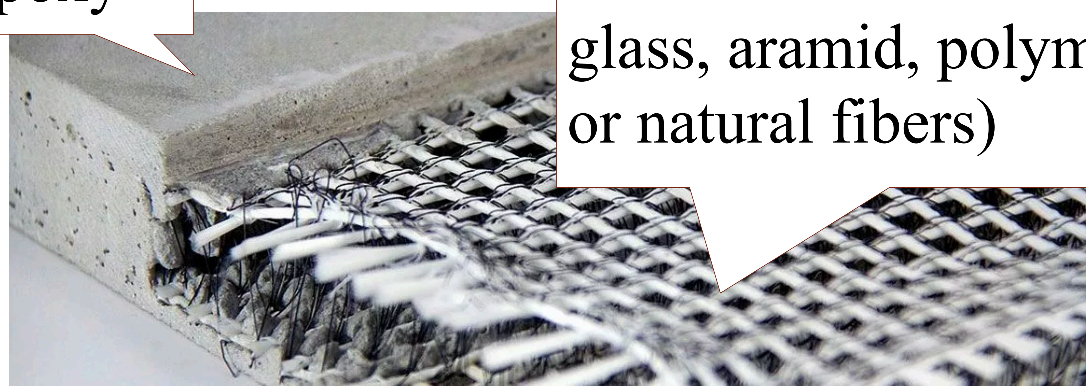
Outline

1. Background & Motivation
2. Formulation of the Problem
3. Basilisk. Numerical Methods.
4. Results
5. Computational & Modeling Challenges
6. Conclusion

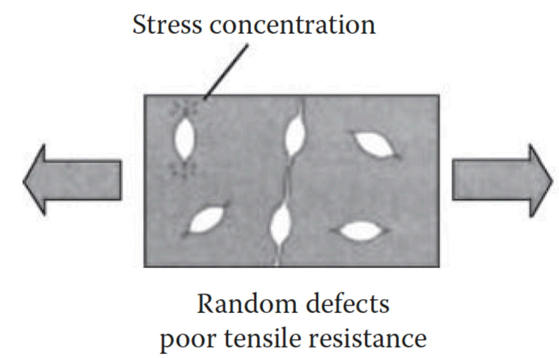
Background & Motivation

epoxy

Reinforced matrix (Carbon, glass, aramid, polymer or natural fibers)



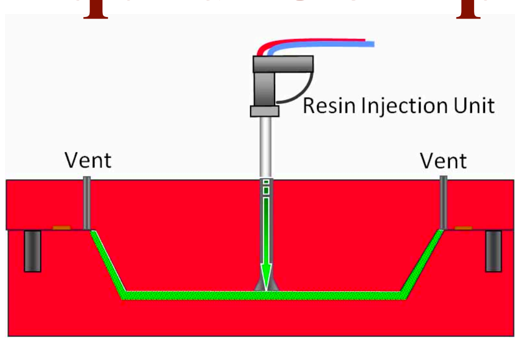
Manufacturing problems



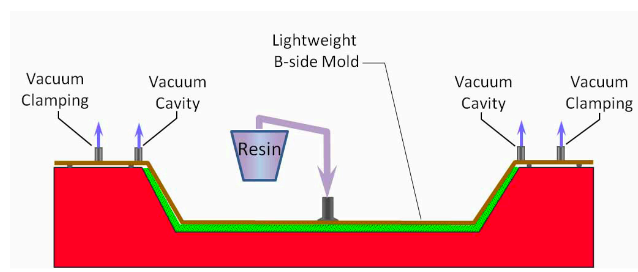
- Cracks

>5% of bubbles => inappropriate for practical use

Liquid Composite Molding (LCM)



Resin Transfer Molding

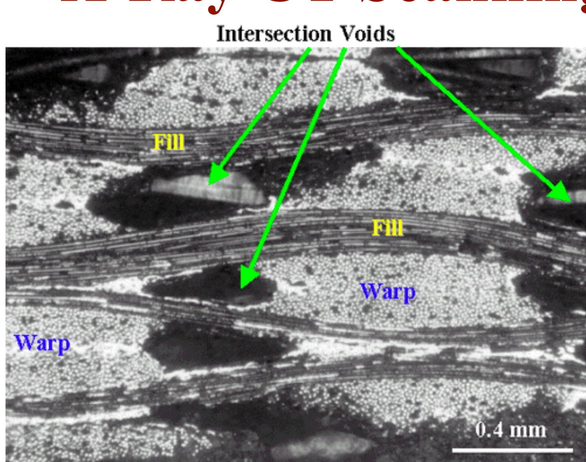


Vacuum Infusion

Simulation problems

1. Vast range of scales:
2. Multiphase (liquid resin, air bubbles)
3. Capillary/surface interaction effects
4. Polymerization process => Variable rheology
5. Complex topology of a fiber matrix

X-Ray CT Scanning



Sizes

$10-1000\mu m$	–bubble
$5-25\mu m$	–fibers
$1mm$	–tows
$1cm-m$	–part

Purpose & Steps

Purpose

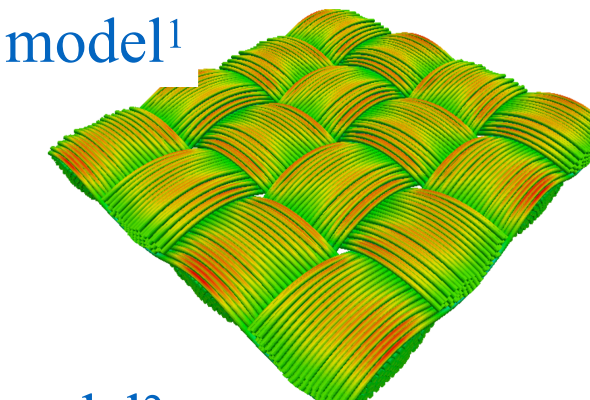
Develop a computational technology for **predictive modeling** and **simulation** of multi-scale resin flow through fiber reinforced material

Modeling levels

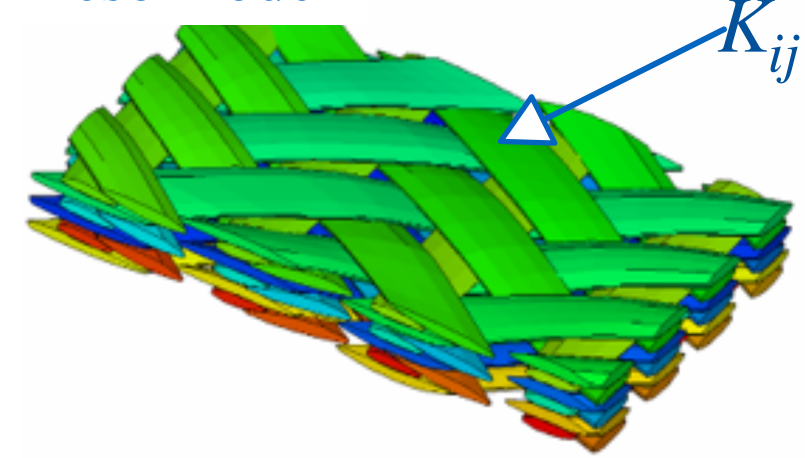
- **Micro**
- Meso
- Macro

A carbon fiber tow[3]

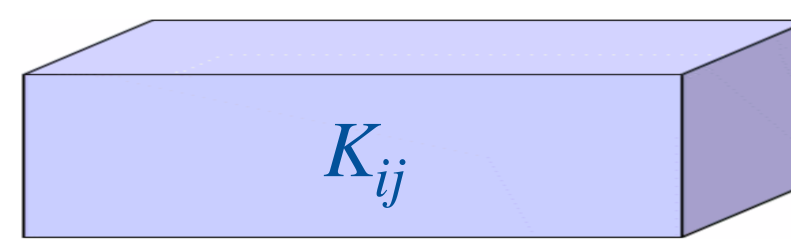
- Micro model[1]



- Meso model[2]



- Macro model



Modeling approaches

Scale	Domain size	Model	Medium
Micro	10μm – 10mm	Stokes surface tension	Solid
Meso	1-10mm	Stokes	Open gap
		Darcy	Porous
Macro	>0.1m	Darcy	Porous

[1]D. Durville, arxiv, 2012 [2]David Mollenhauer et al., 2009 [3]http://velozephyr.com/carbon-fiber

Void Formation in LCM. Models

Formation of 3 scales of voids

Void scale	Location
Micro	Inside tows
Meso	Between tows
Macro	Dry spots

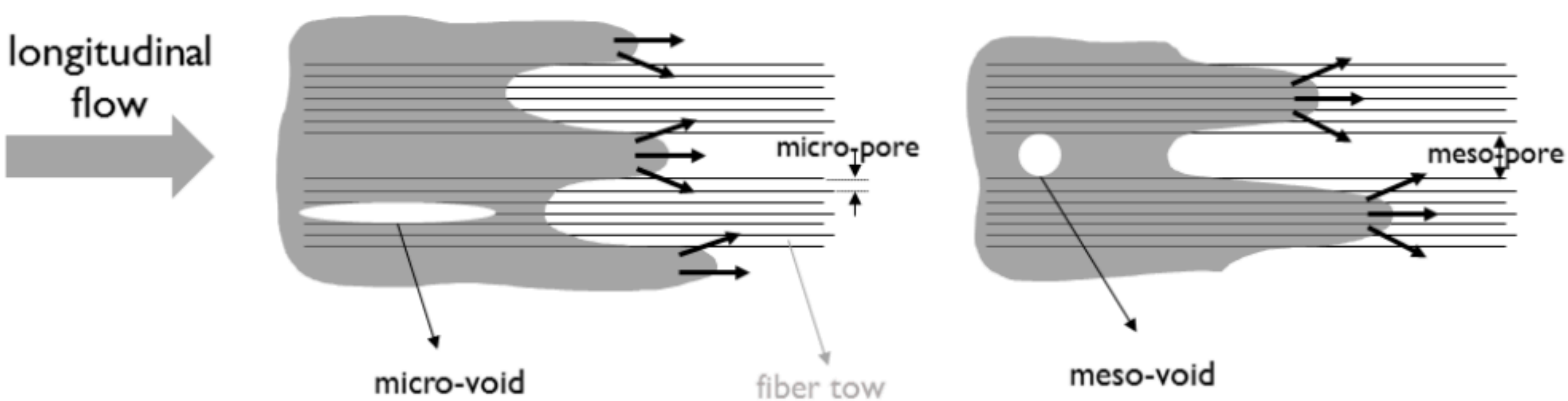
Capillary number

$$Ca = \frac{\mu V}{\gamma \cos\theta}$$

Reason

- competition of the hydrodynamic force and capillary force

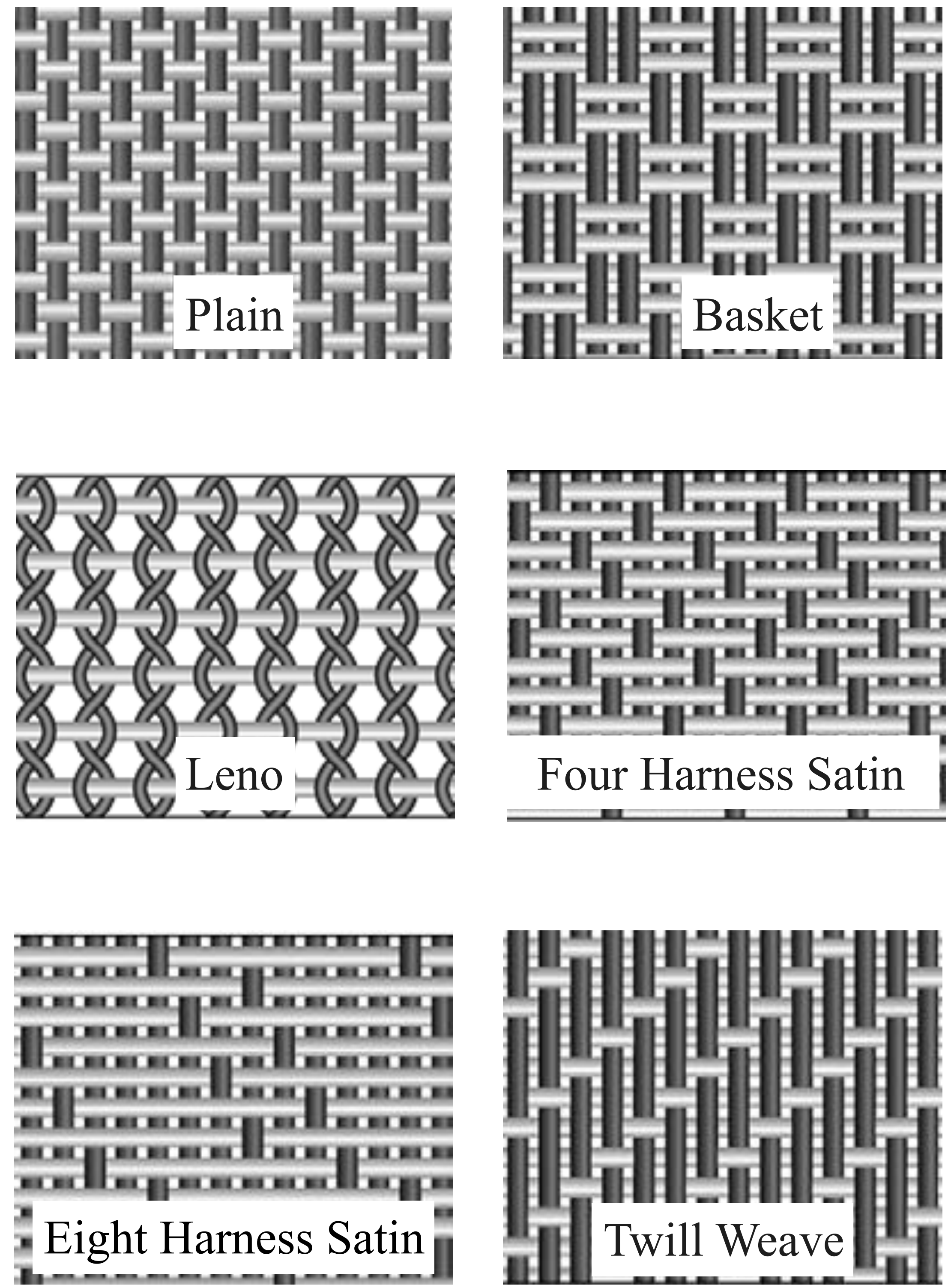
$Ca \gg 1$ $\qquad$ $Ca \ll 1$



M. Mehdikhani, L. Gorbatikh, S. Lomovet, SICOMP28 Conference, 2017

Parameters for Woven Fabric Selection

- **weave pattern**
- yarn weight
- thread count
- fabric finish
- stability
- pliability



Situation Now

- Mechanical properties neglecting porosity
- Big errors

Suggestion

1. Choose weaving geometry
2. Calculate resin flow through it
3. Compute mechanical properties for the resulting material with porous

Questions

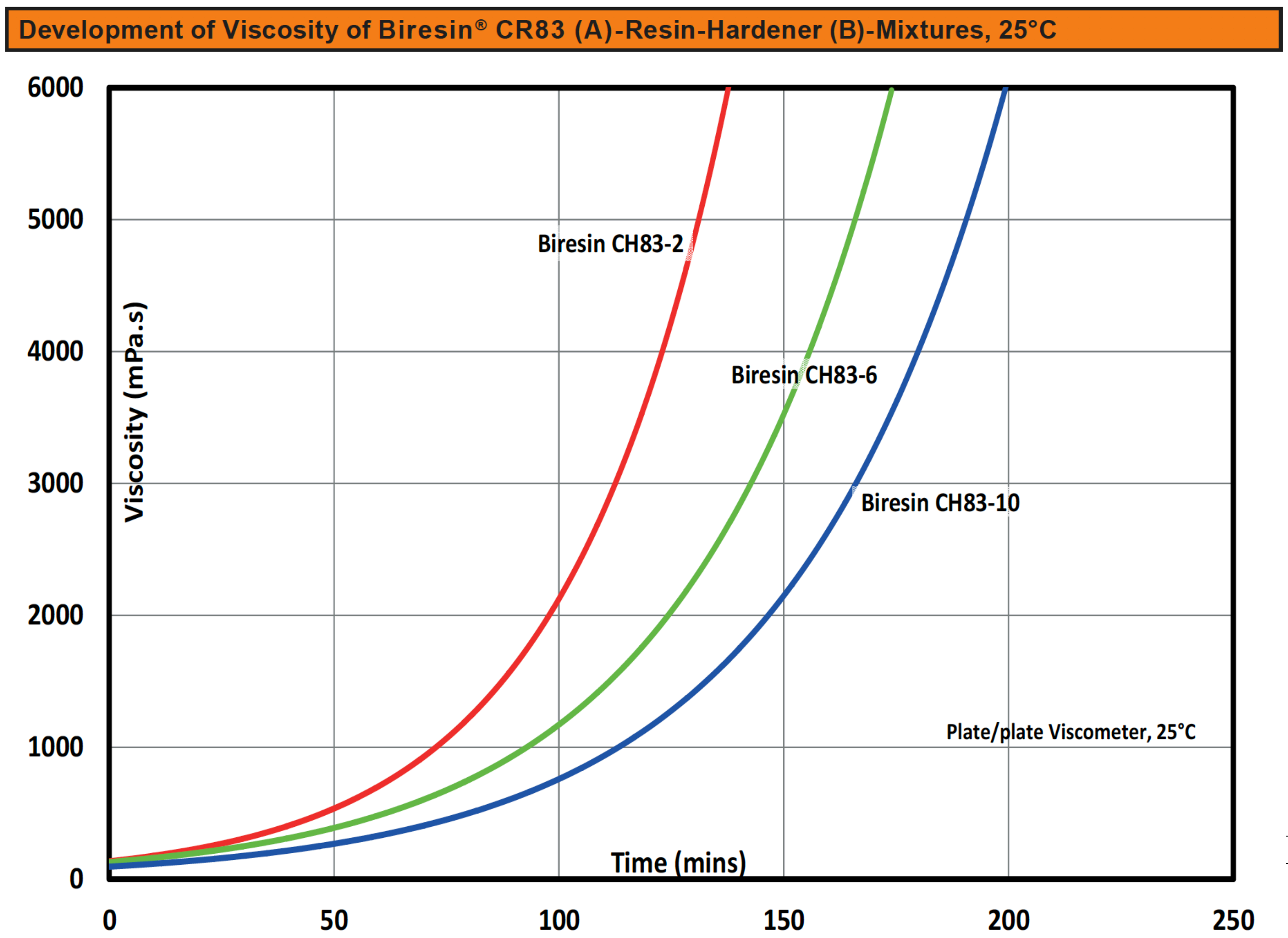
- How do weave patterns affect porosity?
- What is distribution of bubbles?

Liquid Composite Molding

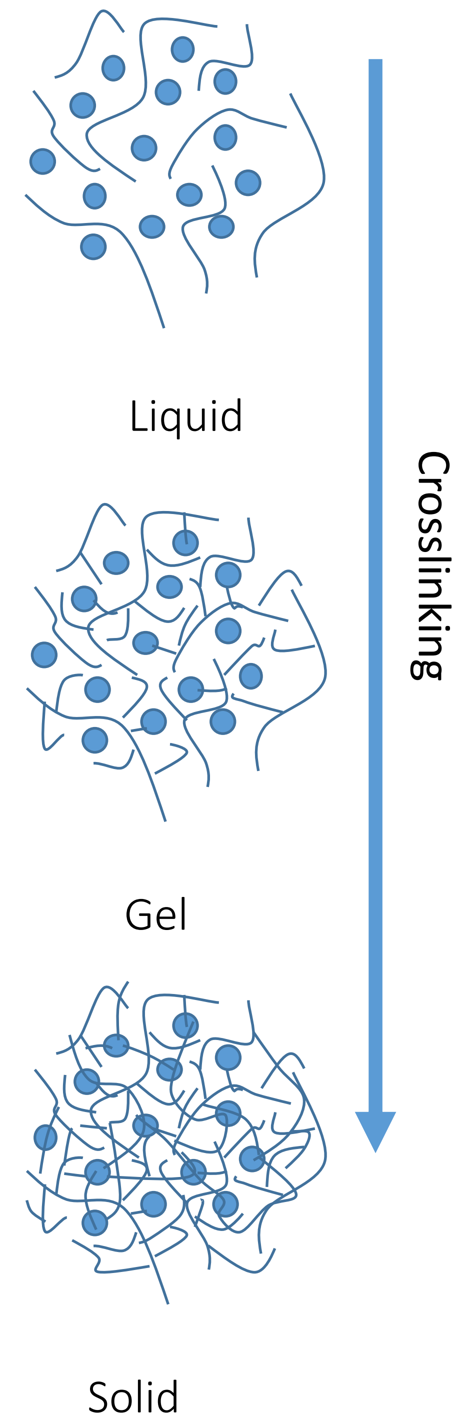
- Epoxy flows slowly: velocity is 0.1–1 mm/s
- High viscosity: starts from 100 mPa·s

Assumptions

- Stokes flow
- Non-cavitation regime
- Incompressible flow



Solidification



Biresin® CR83 Data sheet

General Problem Formulation. Micromodel

$\nabla \cdot \mathbf{u} = 0$	***Incompressible flow***
$\partial_t \rho \mathbf{u} = -\nabla p + \nabla \cdot (2\mu \overline{\overline{D}}) + \overbrace{\sigma \kappa \nabla \varphi_r}^{\text{surface tension}}$	***Momentum***
$\partial_t \varphi_r + \mathbf{u} \cdot \nabla \varphi_r = 0$	***Phase tracer***
$\rho C_p \left(\partial_t T + \mathbf{u} \nabla T \right) = \nabla \cdot \kappa \nabla T + \overbrace{H_{tr} \rho_r \varphi_r \frac{D\alpha}{Dt}}^{\text{polymerization}}$	***Heat transfer and chemical reactions***
$\frac{D\alpha}{Dt} = \partial_t \alpha + \mathbf{u} \nabla \alpha = A(1-\alpha)^n \exp(-E/RT)$	***Polymerization. Degree of cure***
$\varphi_b + \varphi_r + \varphi_f = 1$	***Identity***
$f = \varphi_f f_f + \varphi_r f_r + \left(1 - \varphi_f - \varphi_r\right) f_b$	***Homogenized mixture***
$f = \left(\rho, C_p, \kappa\right)$	***for material values***

κ curvature
σ surface tension coeff.
φ_r volume fraction of resin
φ_b volume fraction of bubbles
φ_f volume fraction of fibres

α degree of cure
A rate constant
E activation energy
n material constant
$D\alpha/Dt$ reaction rate

H_{tr} total heat during reaction
$H(t)$ heat generated up to t

Current Problem Formulation. Micromodel

$$
\begin{cases}
\nabla \cdot \mathbf{u} = 0 & \textit{Incompressible flow} \\
\partial_t \rho \mathbf{u} = -\nabla p + \nabla \cdot (2\mu \overline{\overline{\mathrm{D}}}) + \overbrace{\sigma \kappa \nabla \varphi_r}^{\text{surface tension}} & \textit{Momentum} \\
\partial_t \varphi_r + \mathbf{u} \cdot \nabla \varphi_r = 0 & \textit{Phase tracer} \\
\varphi_b + \varphi_r + \varphi_f = 1 & \textit{Identity} \\
f = \varphi_f f_f + \varphi_r f_r + \left(1 - \varphi_f - \varphi_r\right) f_b & \textit{Homogenized mixture for material values} \\
f = \left(\rho, C_p, \kappa\right) &
\end{cases}
$$

Boundary and Initial Conditions

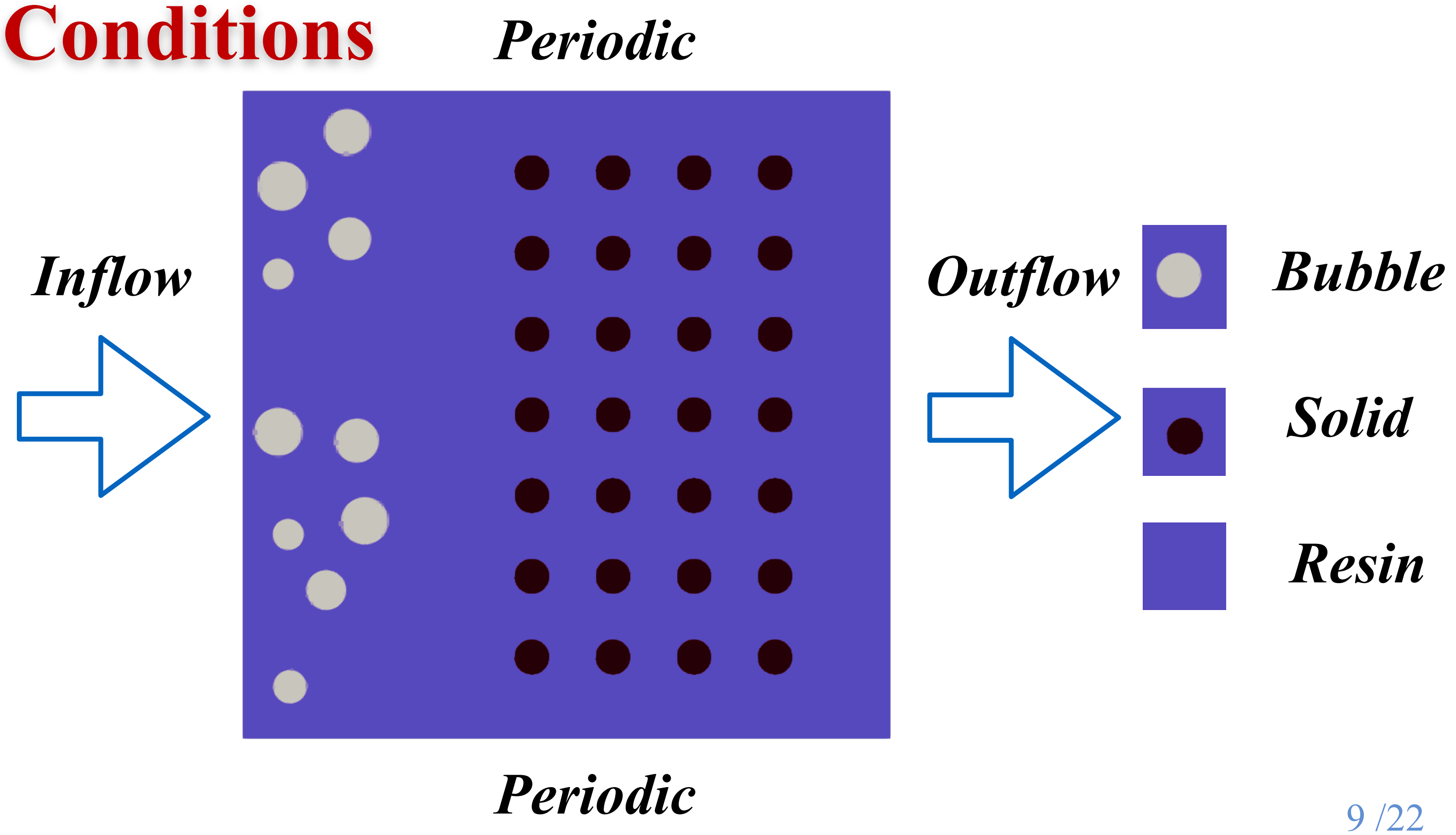
left :
$v_n = 1$
$p = 0$
$f = 1$

right :
$\partial_x v = 0$
$\partial_x p = 0$
$\partial_x f = 1$

top & bottom :
periodic

solid :
$v_n = 0$

$$
f = \begin{cases} 0 & non-wetting \\ 1 & wetting \end{cases}
$$



The Nearest Goal

$$Ca = \frac{\mu V}{\gamma \cos\theta} \qquad\qquad Re = \frac{VL\rho}{\mu}$$

I need to find dependency of porosity $\varphi(Re, Ca)$

Research Open Source Code Basilisk

My requirements

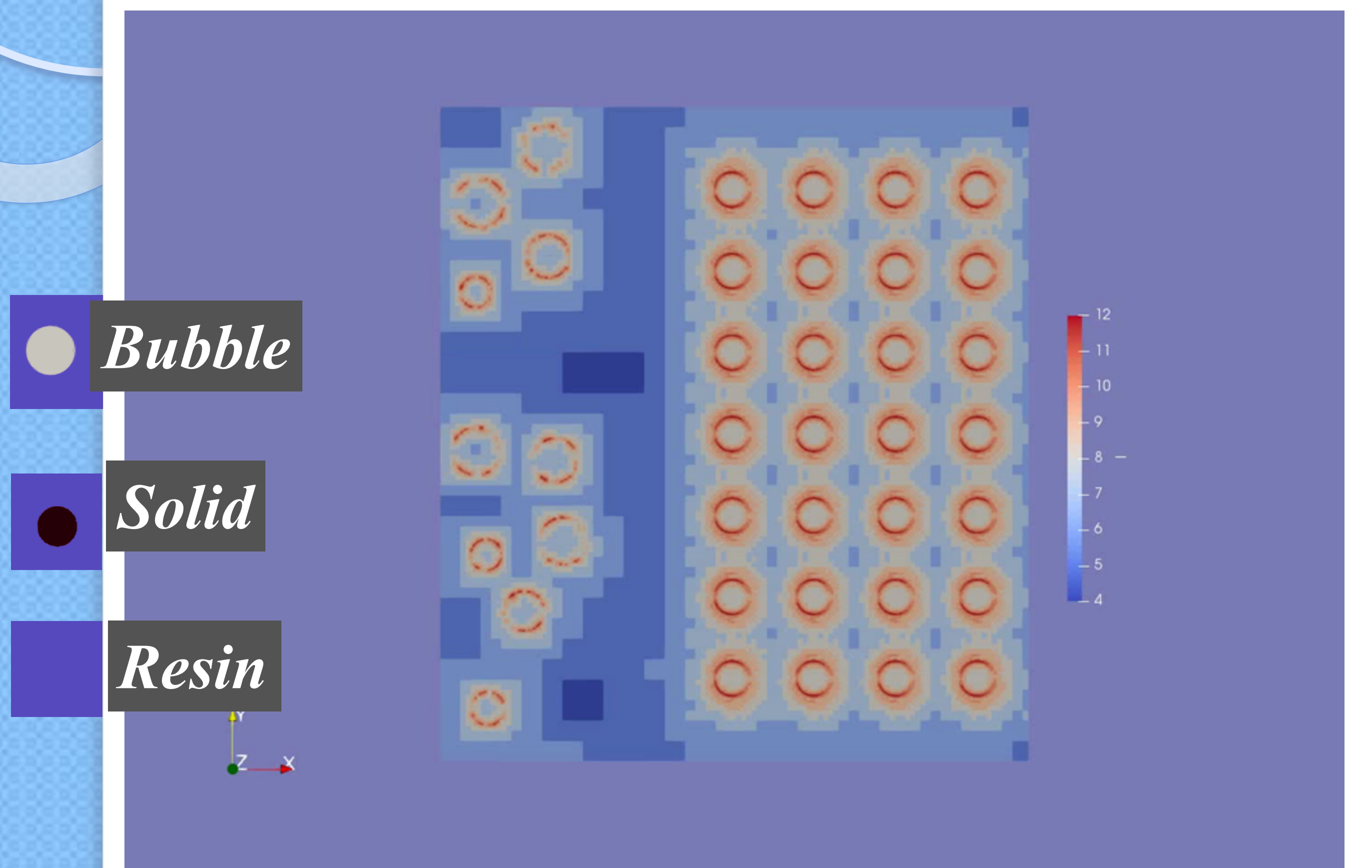
- Adaptive grid
- Flexible in adding equations
- Two-phase
- Surface tension
- Set complex geometry
- Free of charge

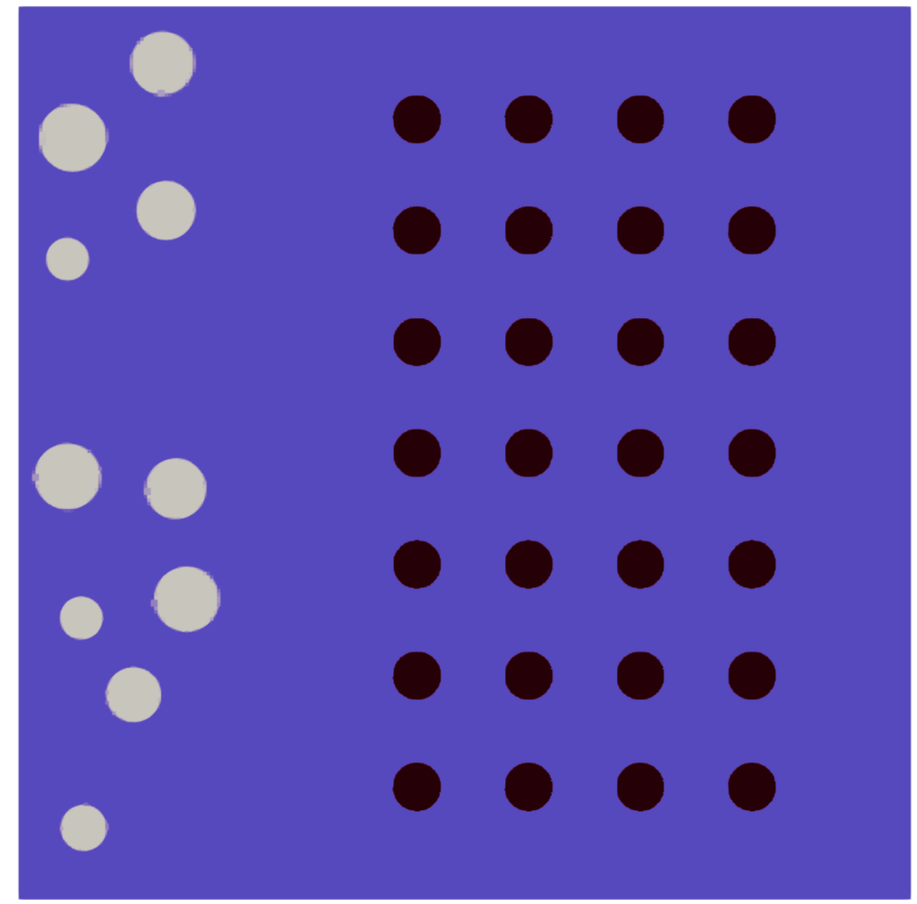
Results

- Saturated flow through cylinders
- Non-saturated flow through cylinders
- Non-saturated flow through staggered cylinders

- BASILISK: navier-stokes + surface-tension + VOF + Popinet's trick

Saturated Flow Through cylinders.Wetting Solids





Initial condition

Grid

interface of bubbles and obstacles

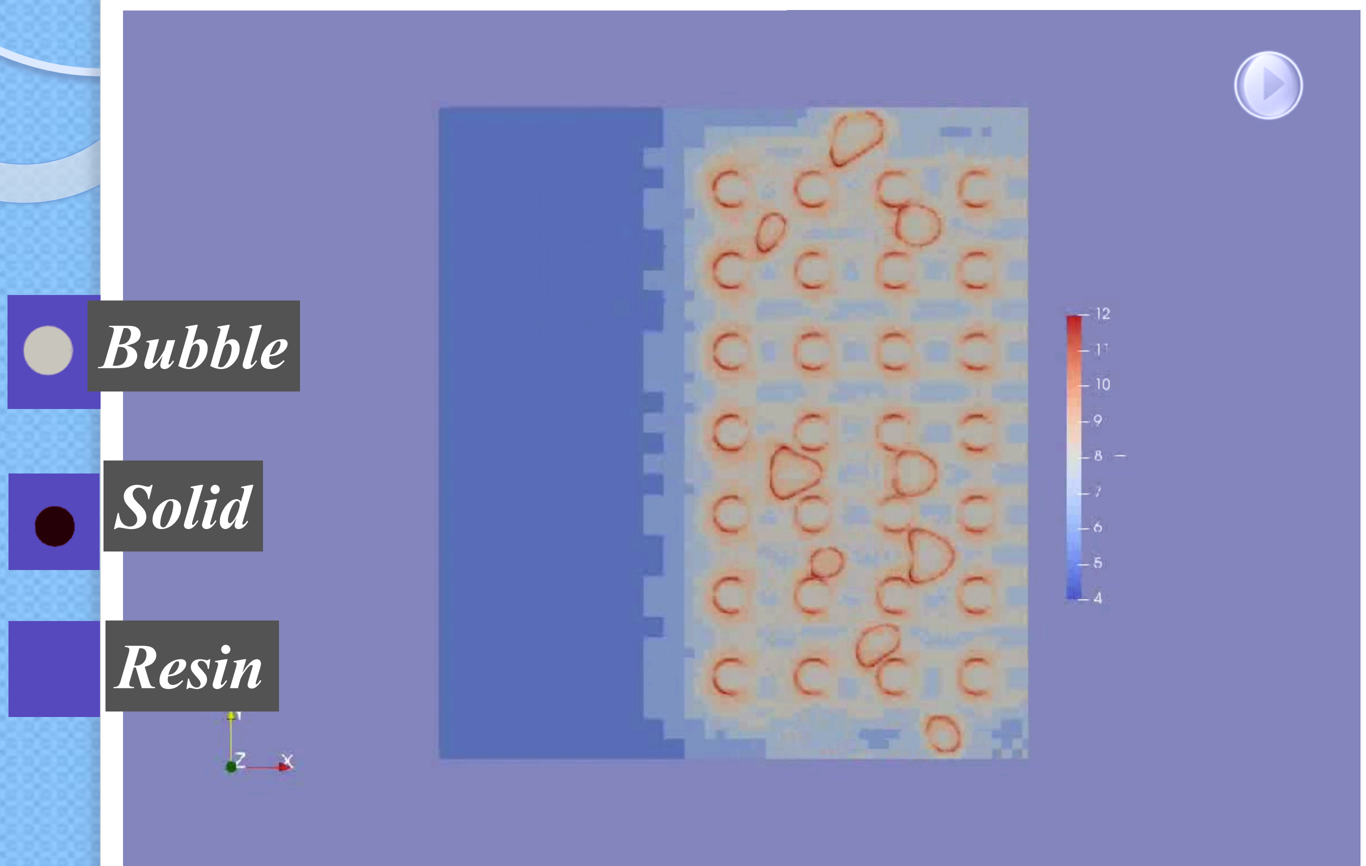
$$\frac{\rho_r}{\rho_b} = 1000 \quad \frac{\mu_r}{\mu_b} = 100 \quad Re = \frac{u_0 L \rho_r}{\mu_r} = 100 \quad Ca = \frac{\mu_r u_0}{\sigma_0} = 0.1 \quad \epsilon = 10^{-2} \quad CFL = 0.8 \quad Level_{max} = 12$$

Wetting solids

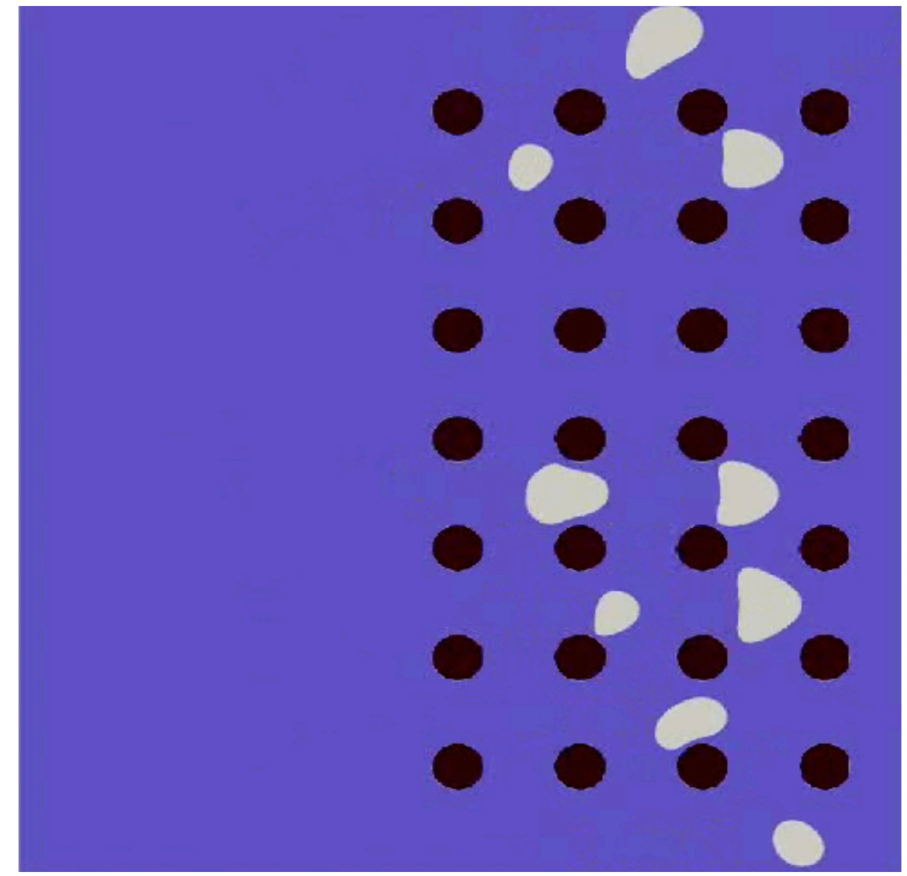
$4L$ is channel width; ϵ is threshold parameter

u_0 is inflow velocity; CFL is stability parameter

Saturated Flow Through cylinders.Wetting Solids



Grid



interface of bubbles and obstacles

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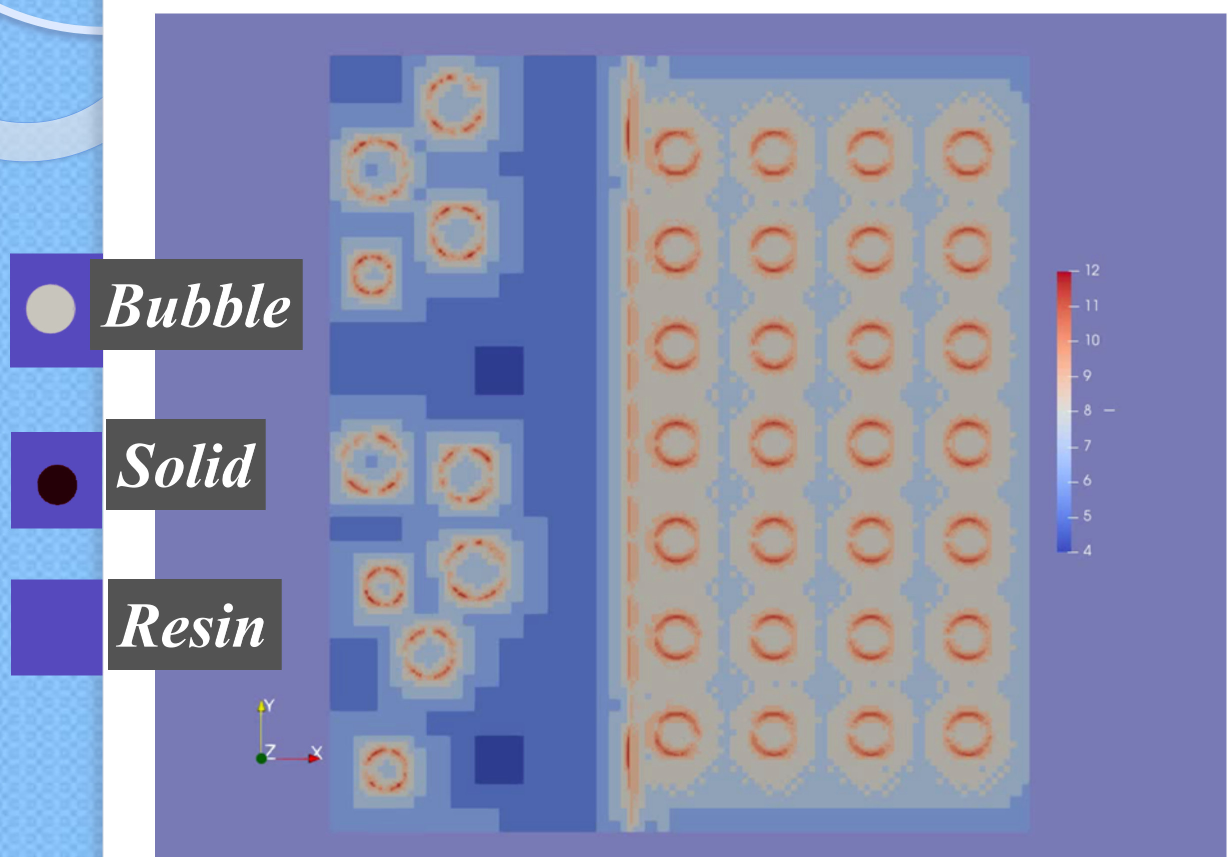
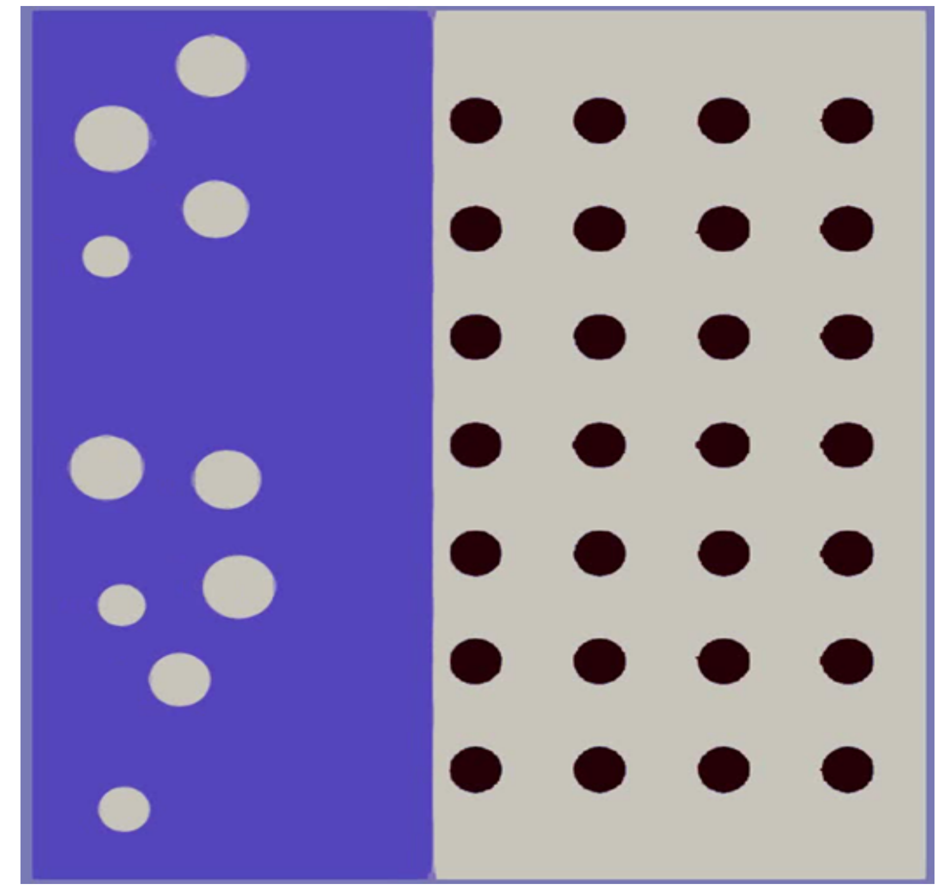
Wetting solids

$4L$	is channel width	ϵ	is threshold parameter
u_0	is inflow velocity	CFL	is stability parameter

Non-Saturated Flow Through Cylinders. No-Wetting Solids





Initial condition

Grid

interface of bubbles and obstacles

$$\frac{\rho_r}{\rho_b} = 1000 \frac{\mu_r}{\mu_b} = 100 Re = \frac{u_0 L \rho_r}{\mu_r} = 100 Ca = \frac{\mu_r u_0}{\sigma_0} = 0.1 \epsilon = 10^{-2} CFL = 0.8 Level_{max} = 12$$

No-Wetting solids

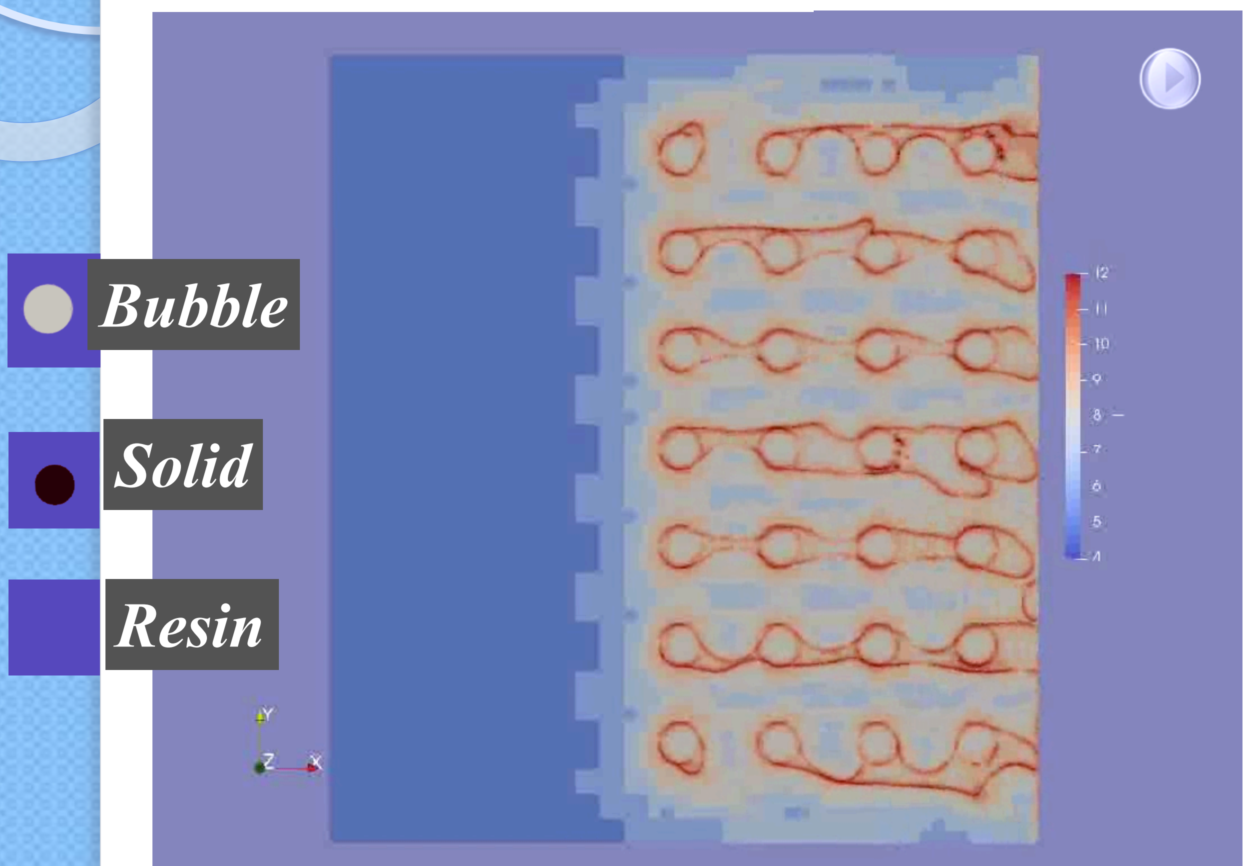
$4L$ is channel width

u_0 is inflow velocity

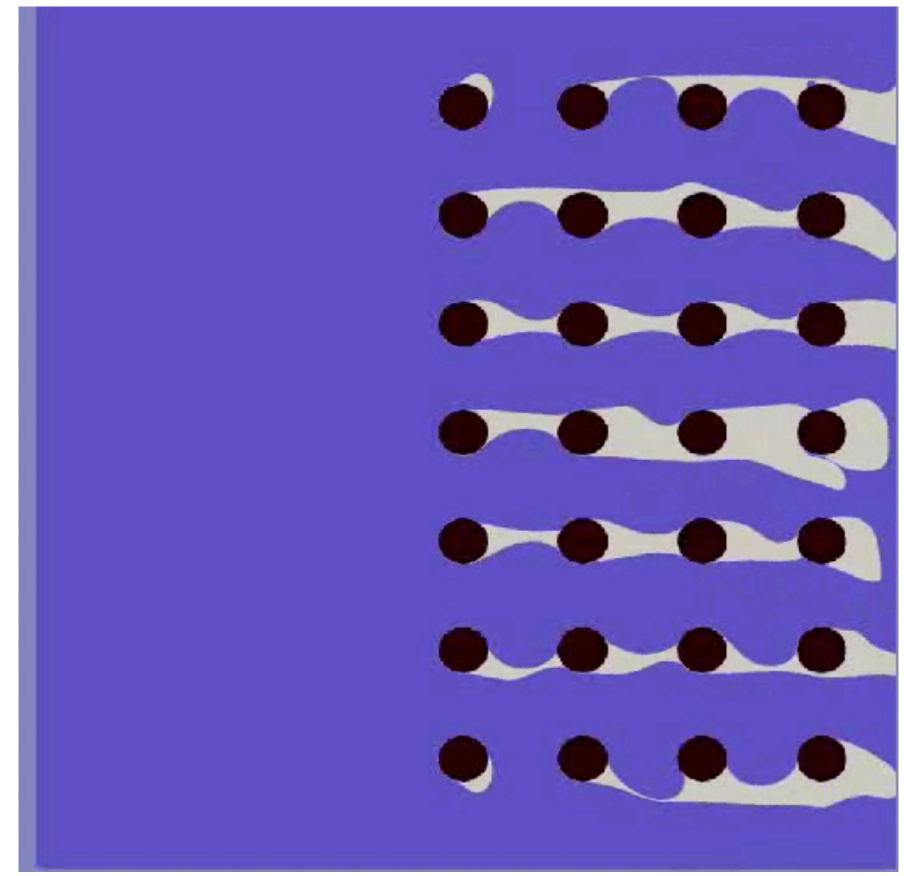
ϵ is threshold parameter

CFL is stability parameter

Non-Saturated Flow Through Cylinders. No-Wetting Solids



Grid



interface of bubbles and obstacles

$$\frac{\rho_r}{\rho_b} = 1000 \quad \frac{\mu_r}{\mu_b} = 100 \quad Re = \frac{u_0 L \rho_r}{\mu_r} = 100 \quad Ca = \frac{\mu_r u_0}{\sigma_0} = 0.1 \quad \epsilon = 10^{-2} \quad CFL = 0.8 \quad Level_{max} = 12$$

No-Wetting solids

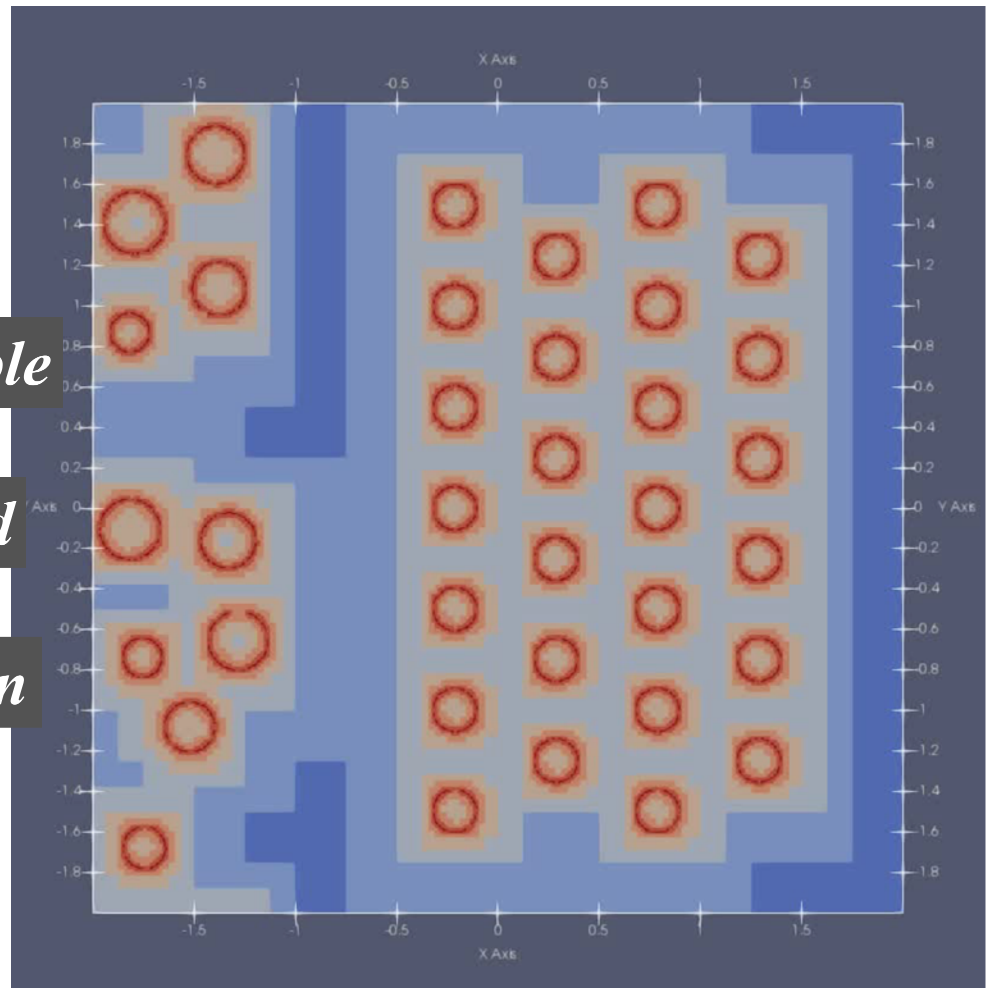
$4L$	is channel width	ϵ	is threshold parameter
u_0	is inflow velocity	CFL	is stability parameter

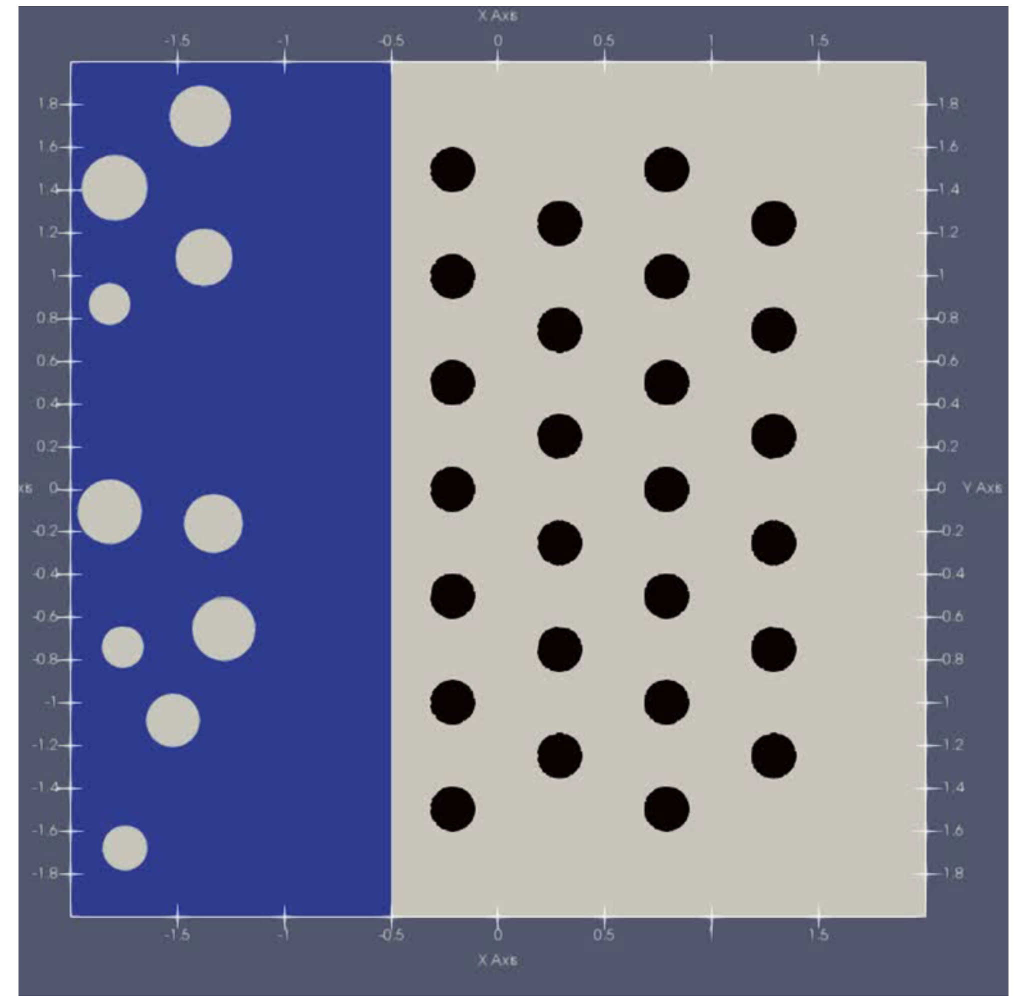
Saturated Flow With Through Staggered Cylinders. No-Wetting Solids

Bubble

Solid

Resin





Initial condition

Grid

interface of bubbles and obstacles

$$\frac{\rho_r}{\rho_b} = 1000 \quad \frac{\mu_r}{\mu_b} = 100 \quad Re = \frac{u_0 L \rho_r}{\mu_r} = 100 \quad Ca = \frac{\mu_r u_0}{\sigma_0} = 0.1 \quad \epsilon = 10^{-2} \quad CFL = 0.8 \quad Level_{max} = 12$$

No-Wetting solids

$4L$ is channel width

u_0 is inflow velocity

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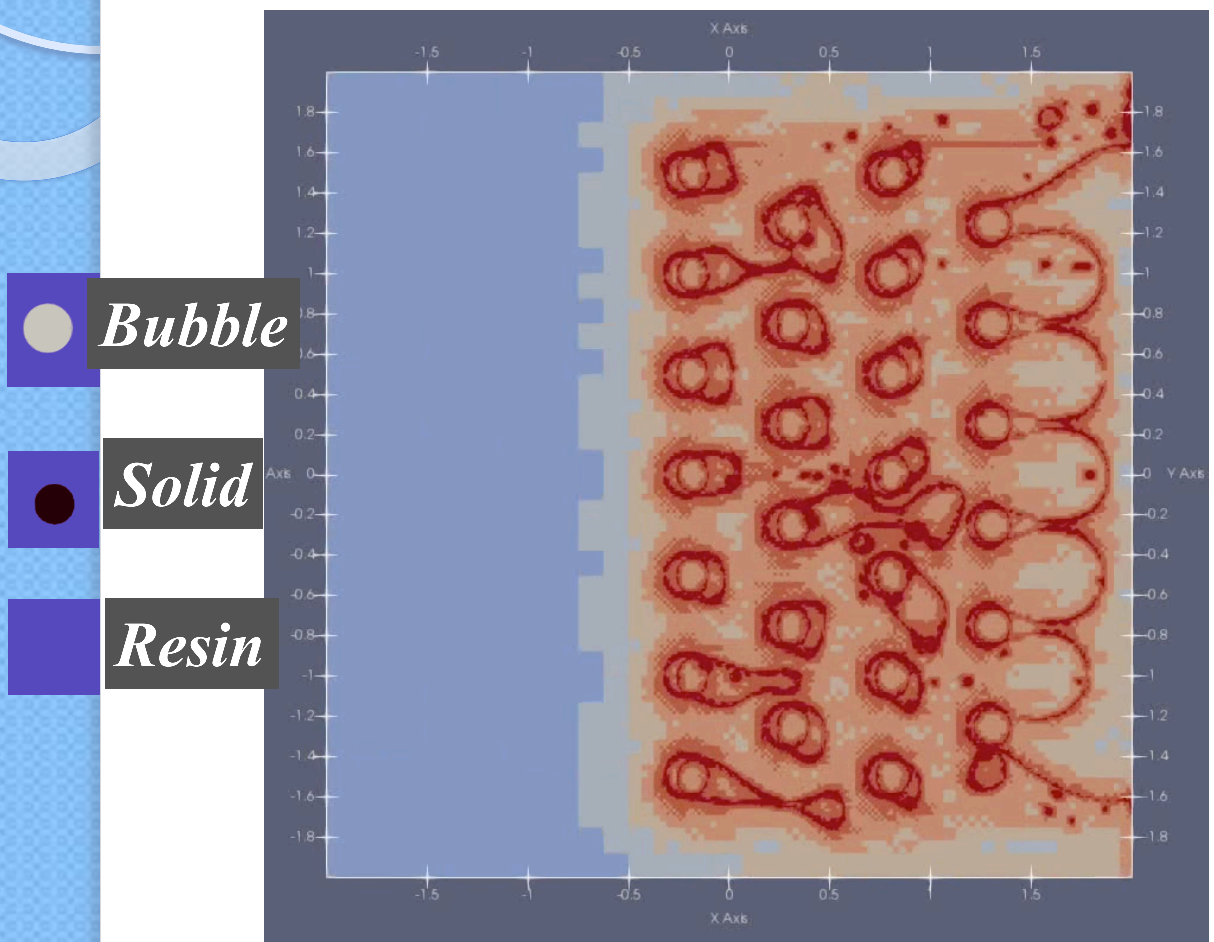
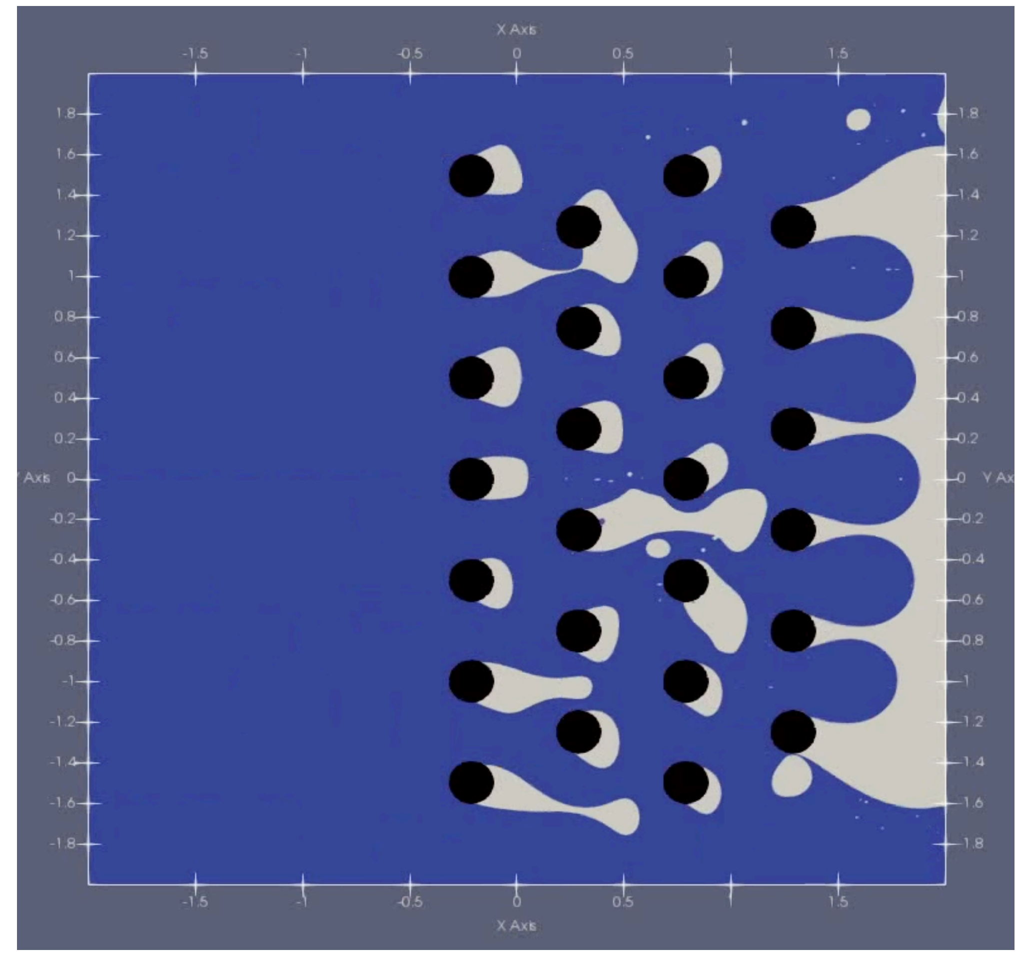
Saturated Flow With Through Staggered Cylinders. No-Wetting Solids





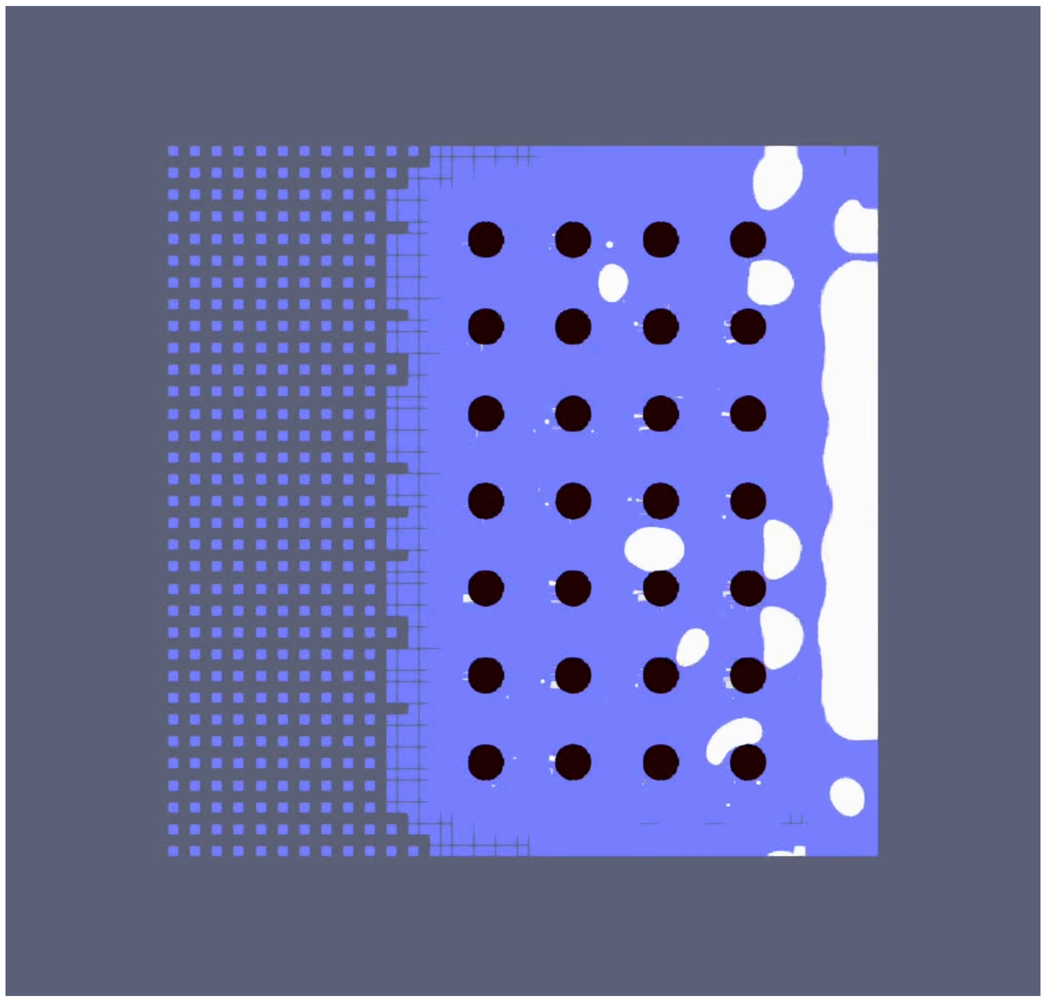
Grid — interface of bubbles and obstacles

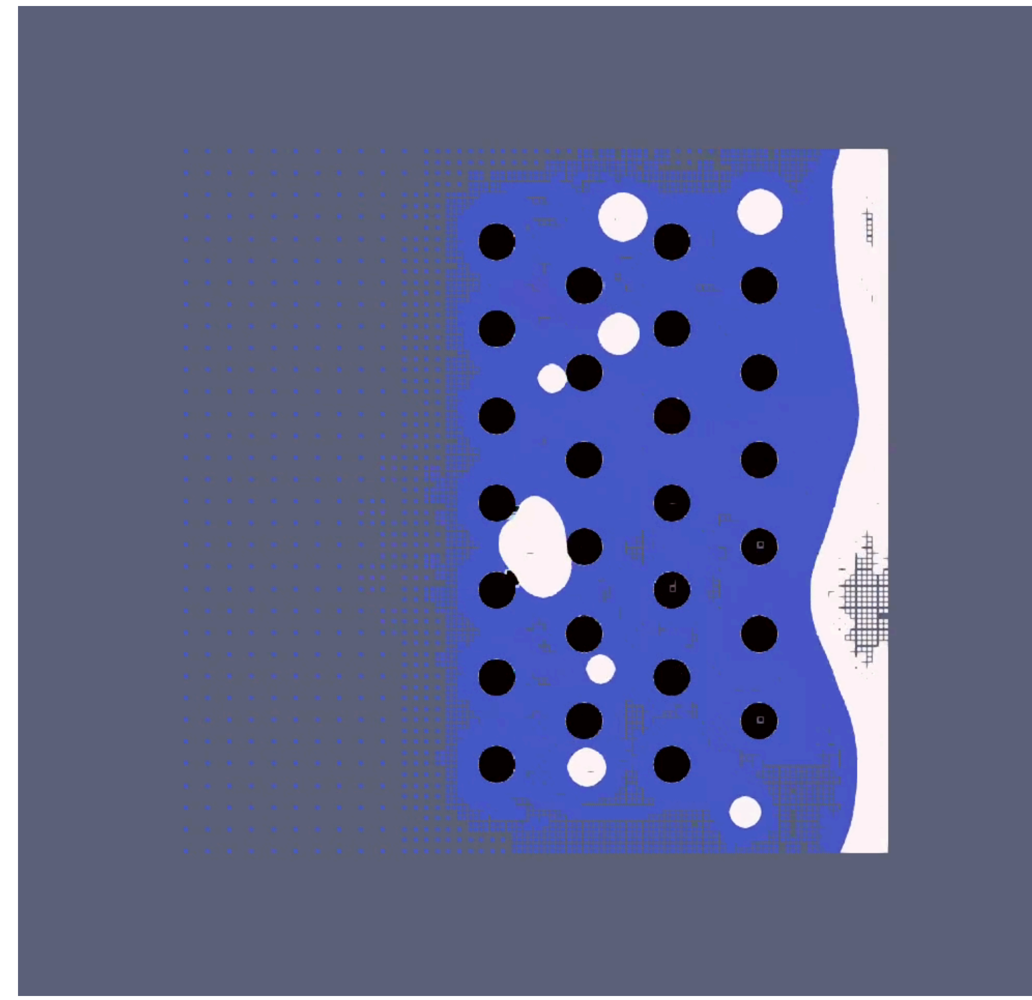
$$\frac{\rho_r}{\rho_b} = 1000 \quad \frac{\mu_r}{\mu_b} = 100 \quad Re = \frac{u_0 L \rho_r}{\mu_r} = 100 \quad Ca = \frac{\mu_r u_0}{\sigma_0} = 0.1 \quad \epsilon = 10^{-2} \quad CFL = 0.8 \quad Level_{max} = 12$$

No-Wetting solids

$4L$ is channel width
u_0 is inflow velocity
ϵ is threshold parameter
CFL is stability parameter

Saturated Flow With Through Straight & Staggered Cylinders. Perfect Wetting





$$\frac{\rho_r}{\rho_b} = 1000 \quad \frac{\mu_r}{\mu_b} = 100 \quad Re = \frac{u_0 L \rho_r}{\mu_r} = 100 \quad Ca = \frac{\mu_r u_0}{\sigma_0} = 0.1 \quad \epsilon = 10^{-2} \quad CFL = 0.8 \quad Level_{max} = 10$$

Wetting solids

$4L$ is channel width

u_0 is inflow velocity

ϵ is threshold parameter

CFL is stability parameter

Computational Aspects and Challenges

- Complex geometry treatment
    - mask
    - embedded boundaries
    - Popinet's trick $u = u_*(1 - \varphi_f)$

Methods	***Advantages***	***Problem***
Mask	*User friendly* *Easy to set*	*Single*
Embedded boundaries	*MPI*	*Time consuming &* *no for 2 phase flow* *No contact*
Popinet's trick	***MPI*** ***Very cheap***	***Solid is a little bit porous***

Conclusion and Future Work

- A two-phase model (gas-liquid) of resin through a porous medium, surface tension
- The results show the dynamics of viscous **saturated** and **unsaturated** flows and bubble formation

- Coupling of incompressible and compressible flows
- In practice, the dependence of the effect of wettability and viscosity on temperature is highly nonlinear, which will greatly affect the transfer and the appearance of bubbles
- A study of the role of wettability and temperature in these processes is the topic of our future research

Thank you for you attention!

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