A Volume-Of-Fluid Method for the Simulation of Liquid-Gas Free Surface Flows

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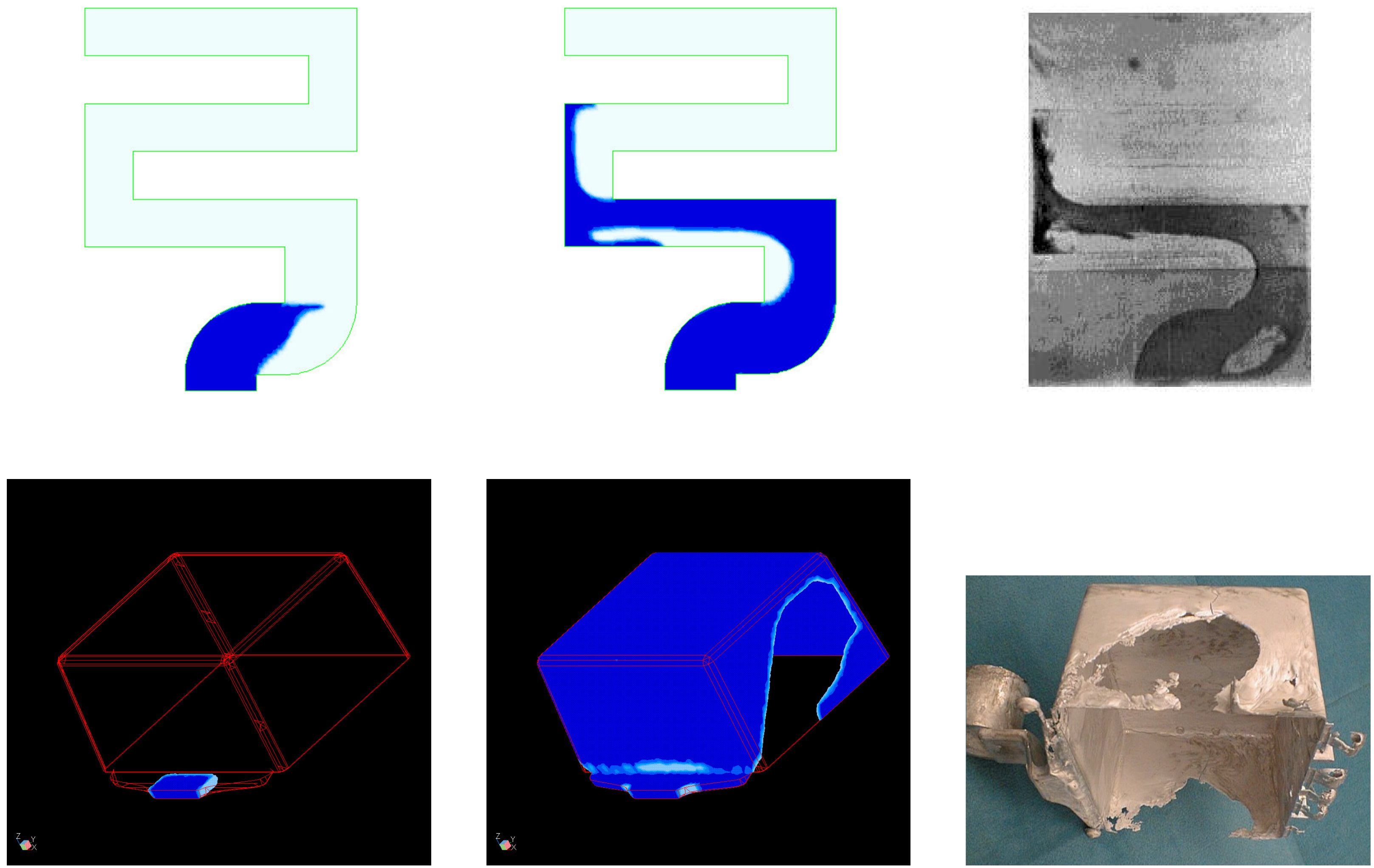
Motivations

- Mold filling - Injection filling.



Motivations

- Mold filling - Injection filling.

- **Features:**
  - Compressible gas - incompressible liquid;
  - Complex 3D geometries in mold filling applications;
  - Topological changes of the liquid domain;
  - High Reynolds numbers;
  - Conservation of the Mass of Liquid;

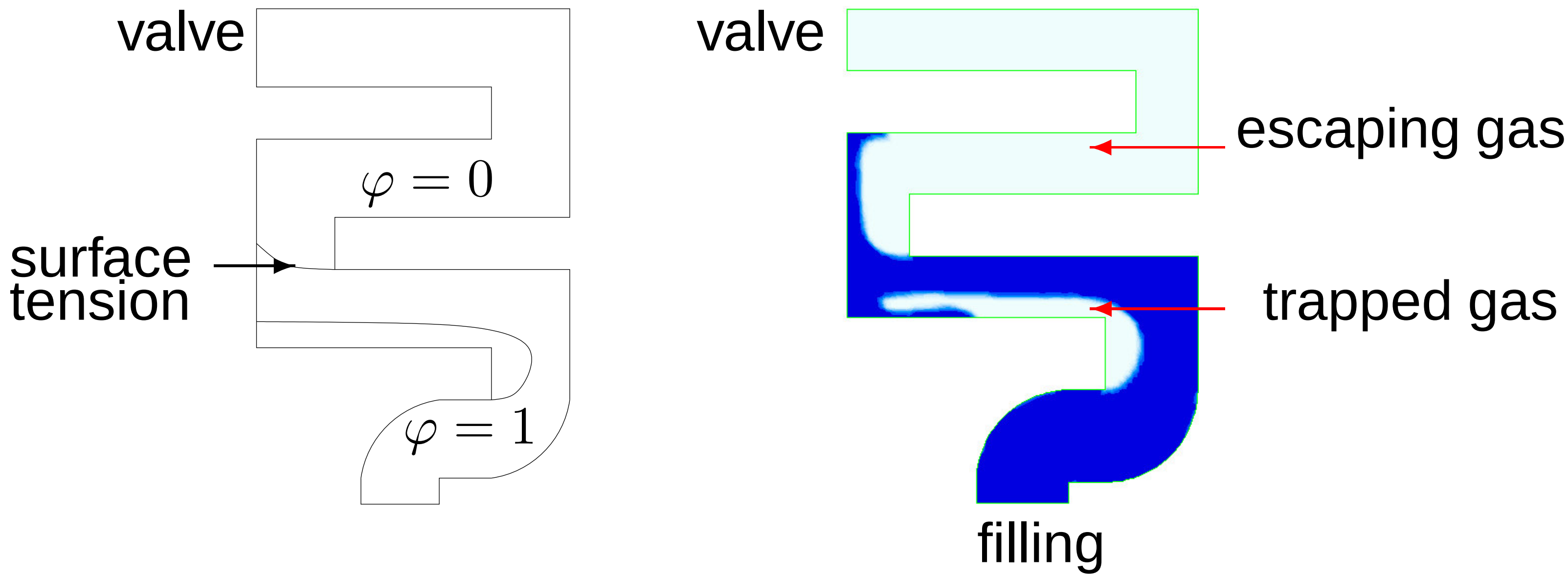
$\Rightarrow$ Eulerian approach
$\Rightarrow$ Volume-of-Fluid method

Contents

- Description of the model of liquid-gas free surface flow.
  - Incompressible liquid - Compressible gas flow.
  - Dynamical effects are neglected in the gas.
  - Volume-of-Fluid (VOF) formulation (No remeshing).
  - Surface tension on the interface between liquid and gas.
- Numerical method for the simulation of liquid-gas free surface flow.
  - Time splitting algorithm.
  - Two grids discretization.
- Numerical results.
  - Mold filling.
  - Bubbles simulations.

References: *AC, Maronnier, Picasso, Rappaz, LNCSE* ***35****, 2003;*
AC, Picasso, Rappaz, J. Comput. Phys., 2004, to appear;
AC, Computers and Fluids, 2004, submitted.

The Model : Volume-of-Fluid (VOF)



Unknowns:

- Volume fraction of liquid φ in the cavity.
- Velocity $\mathbf{u}$ and pressure p in the liquid (incompressible flow).
- Pressure P in each bubble (velocity is disregarded).
- Number and position of the connected components of gas.
- Curvature κ of the liquid-gas interface.

Governing Equations

- Advection equation for φ: the liquid particles move with the liquid along the characteristics ($\dot{\mathbf{X}} = \mathbf{u}$):

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = 0 \ .$$

- Incompressible Navier-Stokes equations in the liquid domain:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} - 2\nabla \cdot (\mu \mathbf{D}(\mathbf{u})) + \nabla p = \mathbf{f} \ ,$$
$$\nabla \cdot \mathbf{u} = 0 \ .$$

- Ideal gas law in the gas domain (bubbles):

$$P \cdot V = \text{ constant in each bubble of gas}$$

(velocity in the gas is disregarded).

Liquid - Gas Interaction

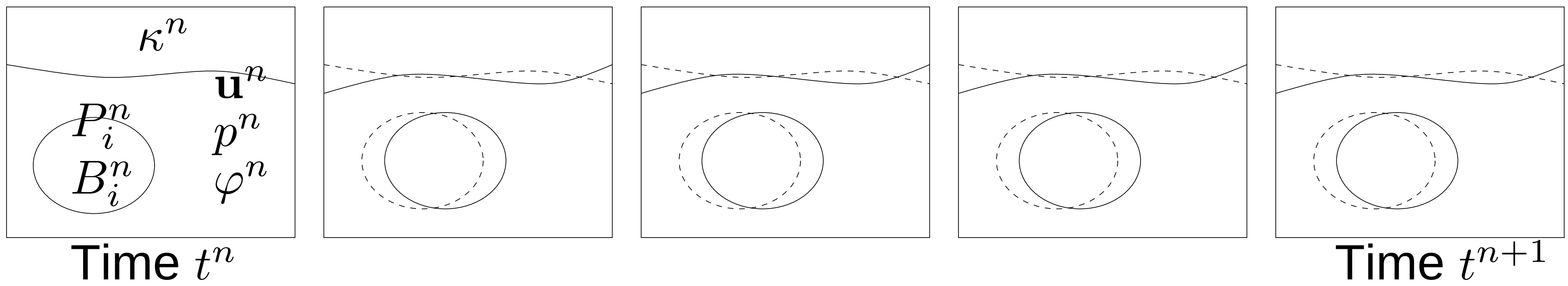
- On the liquid-gas free surface:
  - force induced by the compressibility of the gas;
  - force induced by the surface tension;

$$-p\mathbf{n} + 2\mu D(\mathbf{u})\mathbf{n} = -P\mathbf{n} + \sigma\kappa\mathbf{n} \ .$$

($\sigma =$ constant surface tension coefficient)

- Dirichlet and/or slip boundary conditions on the walls of the cavity.
- Initial conditions for the VOF function, the velocity in the liquid and the pressure in the gas.
- Simple turbulence modeling (turbulent viscosity).

Time Discretization : A Splitting Algorithm



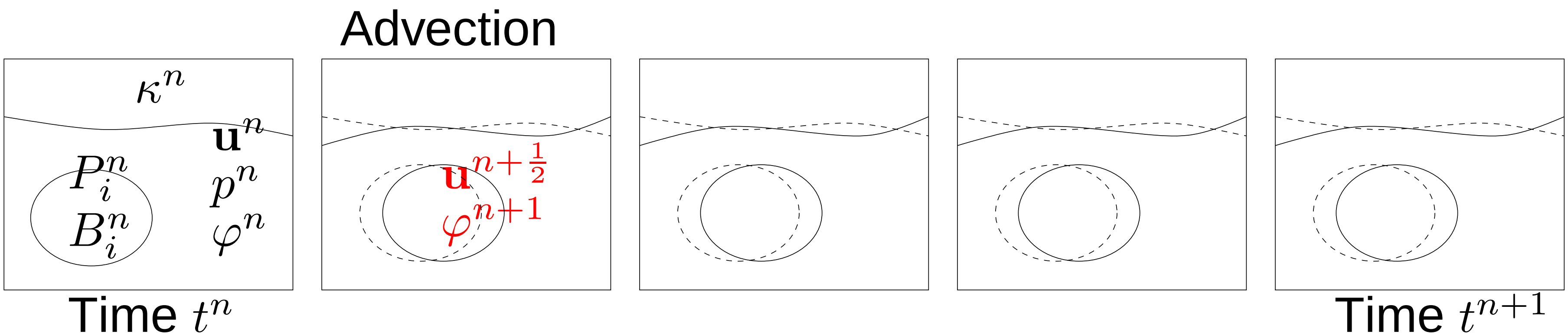
(1) Advection step.

(2) Computation of gas pressure.

(3) Computation of the curvature and surface tension effects.

(4) Diffusion step.

Time Discretization : A Splitting Algorithm



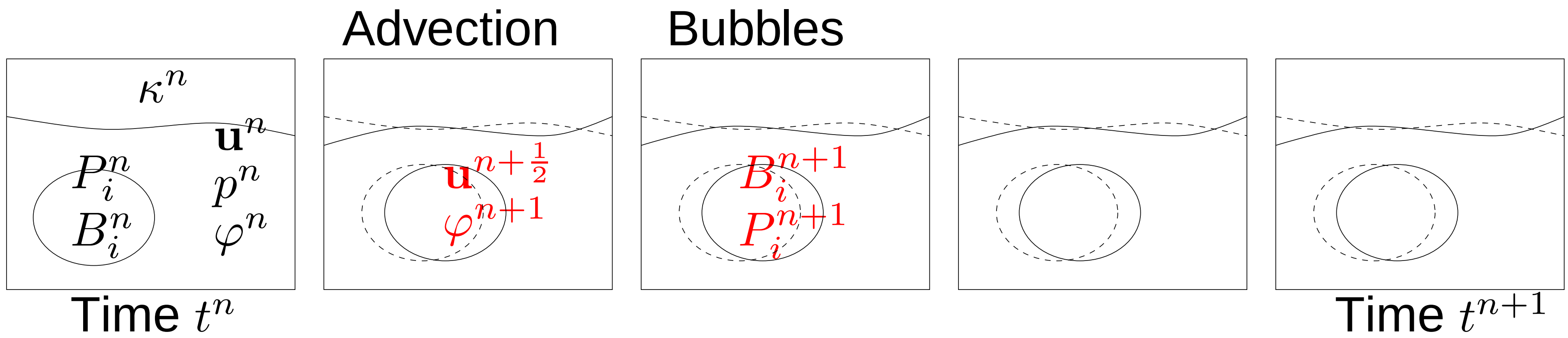
(1) Advection step.
  $\Rightarrow$ Prediction $\mathbf{u}^{n+1/2}$ of the velocity.
  $\Rightarrow$ Volume fraction of liquid φ^{n+1} and new liquid domain Ω^{n+1}.

(2) Computation of gas pressure.

(3) Computation of the curvature and surface tension effects.

(4) Diffusion step.

Time Discretization : A Splitting Algorithm



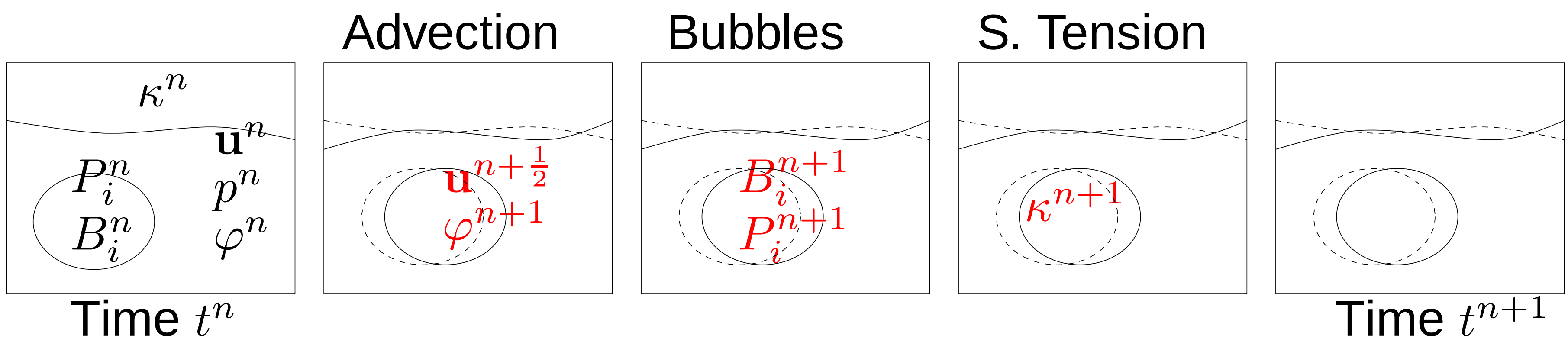
(1) Advection step.

(2) Computation of gas pressure.
$\Rightarrow$ Pressure P_i^{n+1} constant in each bubble of gas B_i^{n+1}.

(3) Computation of the curvature and surface tension effects.

(4) Diffusion step.

Time Discretization : A Splitting Algorithm



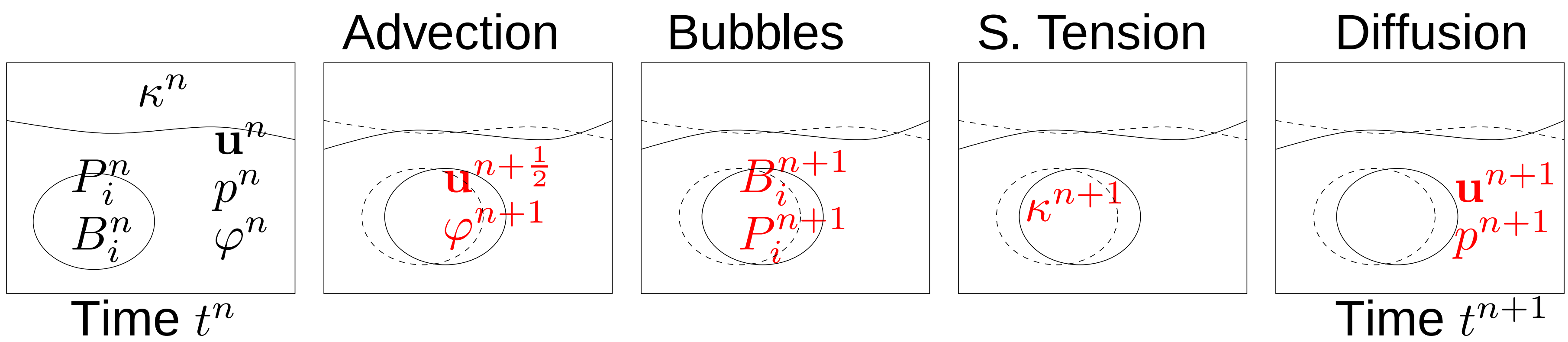
(1) Advection step.

(2) Computation of gas pressure.

(3) Computation of the curvature and surface tension effects.
$\Rightarrow$ Curvature κ^{n+1} and unit normal vector $\mathbf{n}^{n+1}$ on the liquid-gas interface.

(4) Diffusion step.

Time Discretization : A Splitting Algorithm



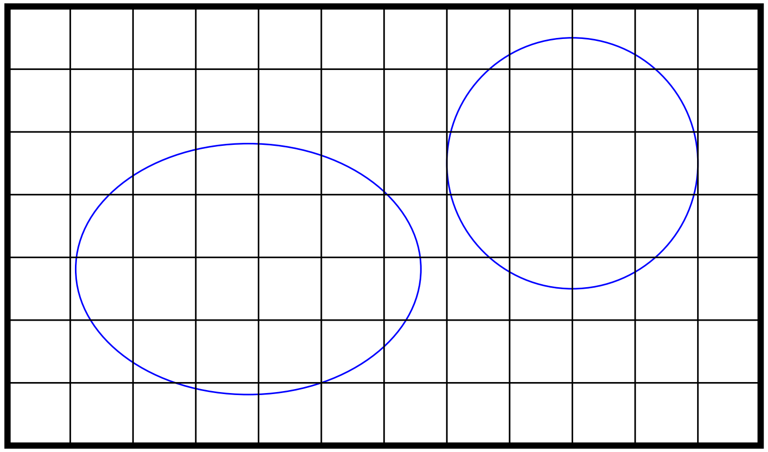
(1) Advection step.

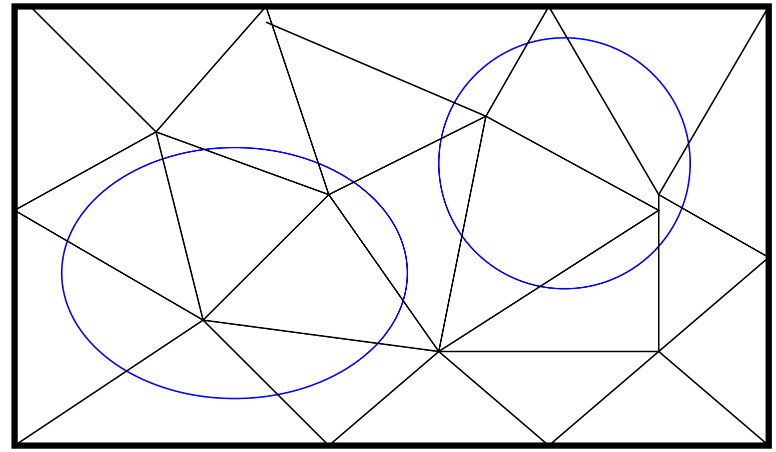
(2) Computation of gas pressure.

(3) Computation of the curvature and surface tension effects.

(4) Diffusion step.
$\Rightarrow$ Velocity $\mathbf{u}^{n+1}$ (correction) and pressure p^{n+1} in the liquid domain.

A Two Grids Method





- Structured grid of small cells (finer);
  - Resolution of the advection step with a characteristics method;
- Unstructured finite element mesh (coarser);
  - Computation of the gas pressure;
  - Computation of the curvature on the interface;
  - Resolution of the diffusion step (Stokes problem) with continuous (stabilized) piecewise linear finite elements;
- Projection/Interpolation methods.

Advection Step

- Solve the two advection problems between t^n and t^{n+1}:

$$\frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = 0 \ ,$$
$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = 0$$

  with initial conditions

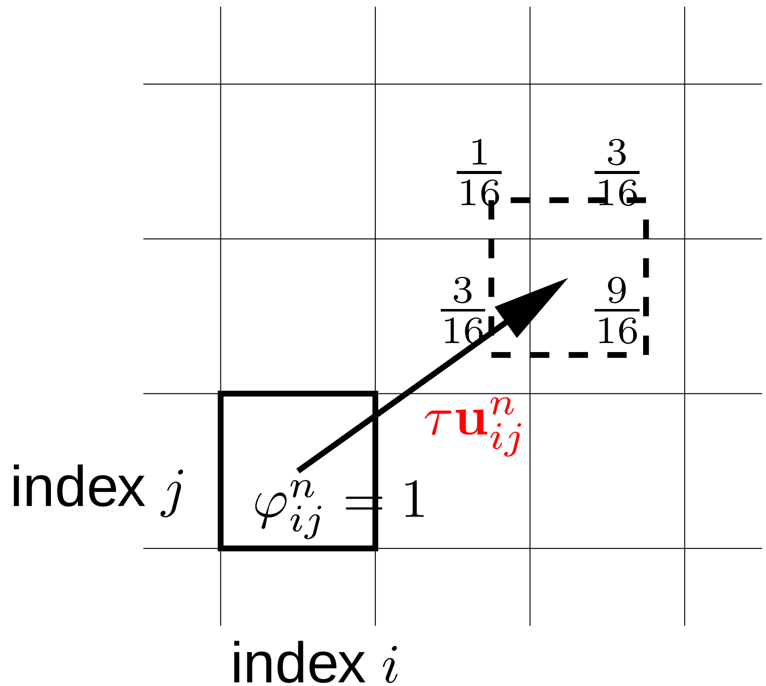
$$\mathbf{u}(t^n) = \mathbf{u}^n \ , \quad \varphi(t^n) = \varphi^n \ .$$

- Forward characteristics method: $\forall \mathbf{x} \in \Omega^n$:

$$\mathbf{u}^{n+\frac{1}{2}}(\mathbf{x} + \tau^{n+1}\mathbf{u}^n(\mathbf{x})) = \mathbf{u}^n(\mathbf{x}) \ ,$$
$$\varphi^{n+1}(\mathbf{x} + \tau^{n+1}\mathbf{u}^n(\mathbf{x})) = \varphi^n(\mathbf{x}) \ .$$

Advection Step (2)

- Forward characteristics method with projection on the regular grid of small cells.



- Numerical diffusion (SLIC algorithm, *Chorin, 1980*); Computation of an interface line in each cell such that $0 < \varphi < 1$;
- Numerical compression (post-processing);
- Not restricted by any CFL condition.

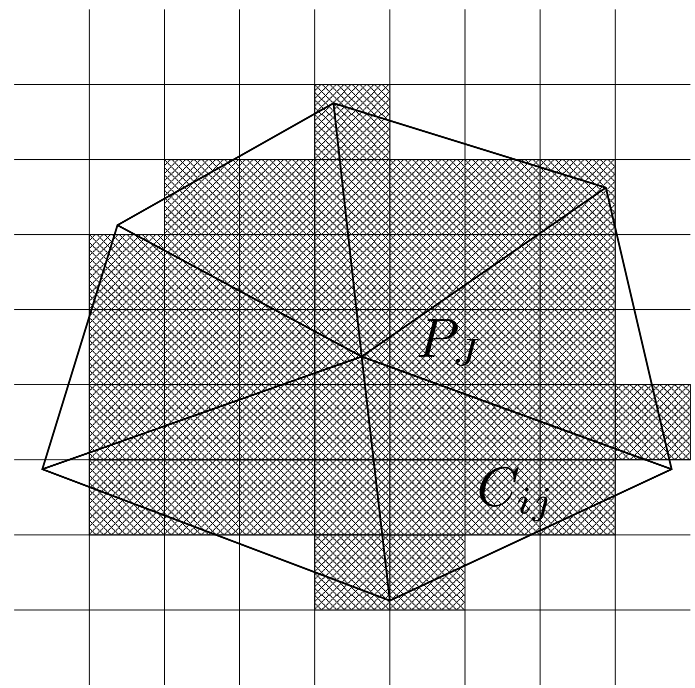
From the Cells to the Finite Elements

- Projection of the piecewise constant approximation on the cells on the piecewise linear finite element space:

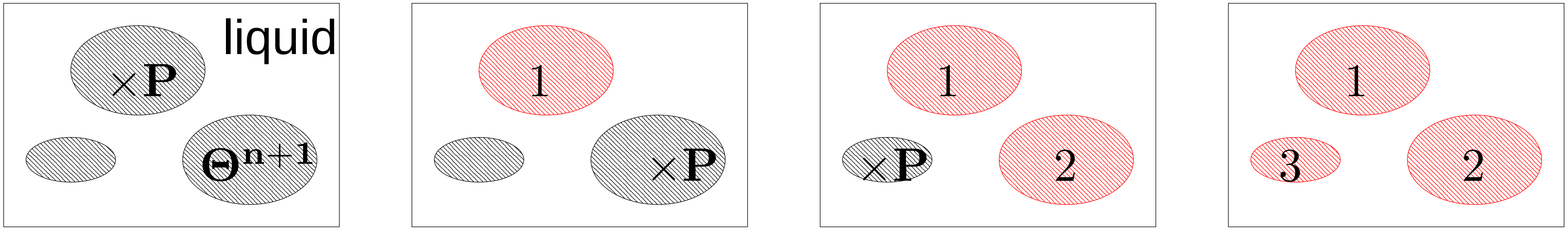
$$\int_\Lambda u_{FE}^{n+1/2} \psi_J dx = \int_\Lambda u_{CELLS}^{n+1/2} \psi_J dx, \quad \forall J \ .$$

- Projection is approximated by an interpolation procedure.

$$u_P^{n+1/2} = \frac{\displaystyle\sum_{\substack{K \\ P \in K}} \sum_{\substack{ijk \\ C_{ijk} \in K}} \psi_P(C_{ijk}) u_{ijk}^{n+1/2}}{\displaystyle\sum_{\substack{K \\ P \in K}} \sum_{\substack{ijk \\ C_{ijk} \in K}} \psi_P(C_{ijk})}$$



Bubbles Step : Numbering



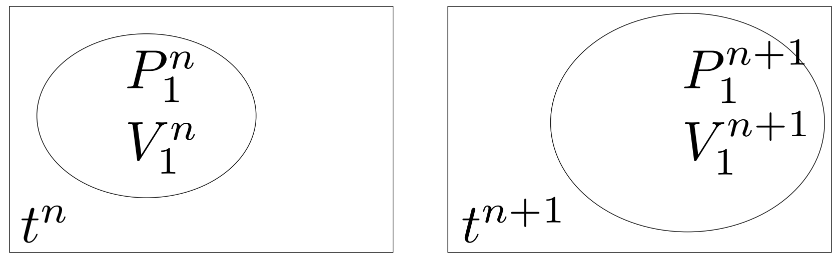
- Choose a point P in the gas domain Θ^{n+1} and solve:

$$\begin{cases} -\Delta u = \delta_P, & \text{in } \Theta^{n+1}; \\ u = 0, & \text{on } \partial\Theta^{n+1}. \end{cases}$$

- If $u(x) \neq 0$ then $x \in$ connected component number 1.
- Increment bubble number, update domain Θ^{n+1} and repeat until all the bubbles are numbered...
- Solve Poisson problems with continuous, piecewise linear finite elements.

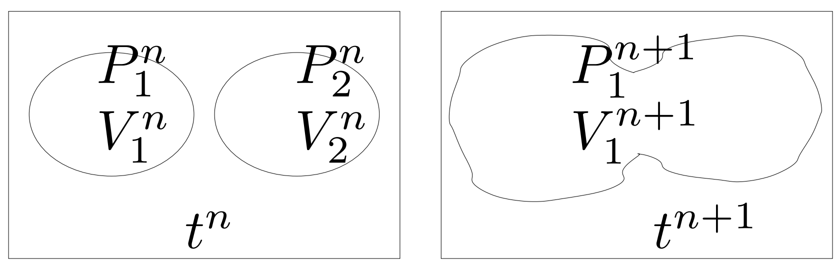
Bubbles Step : Gas Pressure

- Evolution of a single bubble.



$$P_1^{n+1} V_1^{n+1} = P_1^n V_1^n \quad .$$

- Merging of two bubbles.



$$P_1^{n+1} V_1^{n+1} = P_1^n V_1^n + P_2^n V_2^n \quad .$$

- Splitting of one bubble into two bubbles.
- General case is a mixing of these three basic situations.

Curvature Step

- Curvature:

$$\kappa^{n+1} = \nabla \cdot \ \mathbf{n}^{n+1} = -\nabla \cdot \ \frac{\nabla \varphi^{n+1}}{|\nabla \varphi^{n+1}|} \ .$$

- Smoothing of VOF function φ^{n+1} by convolution of φ^{n+1} with a smooth kernel function K_ε:

$$\tilde{\varphi}^{n+1}(x) = \int_\Lambda \varphi^{n+1}(y) K_\varepsilon(x-y) dy \ .$$

- Computation of curvature (L^2-projection on FE space with mass lumping):

$$\int_\Lambda \kappa^{n+1} \varphi_j dx \quad = \quad \int_\Lambda -\nabla \cdot \ \frac{\nabla \tilde{\varphi}^{n+1}}{|\nabla \tilde{\varphi}^{n+1}|} \varphi_j dx \ .$$

- Computations on the finite element unstructured mesh.

Diffusion Step

- Diffusion step (velocity correction): solve Stokes problem in Ω^{n+1} with an implicit scheme:

$$\rho \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2}}{\tau} - 2\,\nabla \cdot \big(\mu \mathbf{D}(\mathbf{u}^{n+1})\big) + \nabla p^{n+1} = \mathbf{f} \;,$$

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

with boundary conditions on the free surface:

$$-p^{n+1}\mathbf{n}^{n+1} + 2\mu \mathbf{D}(\mathbf{u}^{n+1})\mathbf{n}^{n+1} = -P^{n+1}\mathbf{n}^{n+1} + \sigma \kappa^{n+1}\mathbf{n}^{n+1} \;.$$

and given boundary conditions on the wall boundary.

Diffusion Step (2)

- Solve Stokes problem in Ω^{n+1} with continuous, piecewise linear ($\mathbb{P}_1 - \mathbb{P}_1$) stabilized finite elements (Galerkin Least Squares Method) (*Franca, Frey, 1992*):

$$\int_{\Omega^{n+1}} \frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2}}{\tau^{n+1}} \mathbf{w} dx + 2\mu \int_{\Omega^{n+1}} \mathbf{D}(\mathbf{u}^{n+1}) : \mathbf{D}(\mathbf{w}) dx$$
$$- \int_{\Omega^{n+1}} p^{n+1} \,\text{div}\, \mathbf{w} dx - \int_{\Omega^{n+1}} \mathbf{f}\mathbf{w} dx$$
$$+ \int_{\Gamma^{n+1}} (P^{n+1}\mathbf{n}^{n+1} - \sigma\kappa^{n+1}\mathbf{n}^{n+1}) \mathbf{w} dS - \int_{\Omega^{n+1}} \text{div}\, \mathbf{u}^{n+1} q dx$$
$$- \sum_{K \subset \Omega^{n+1}} \alpha_K \int_K \left(\frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2}}{\tau^{n+1}} + \nabla p^{n+1} - \mathbf{f} \right) \cdot \nabla q dx = 0$$

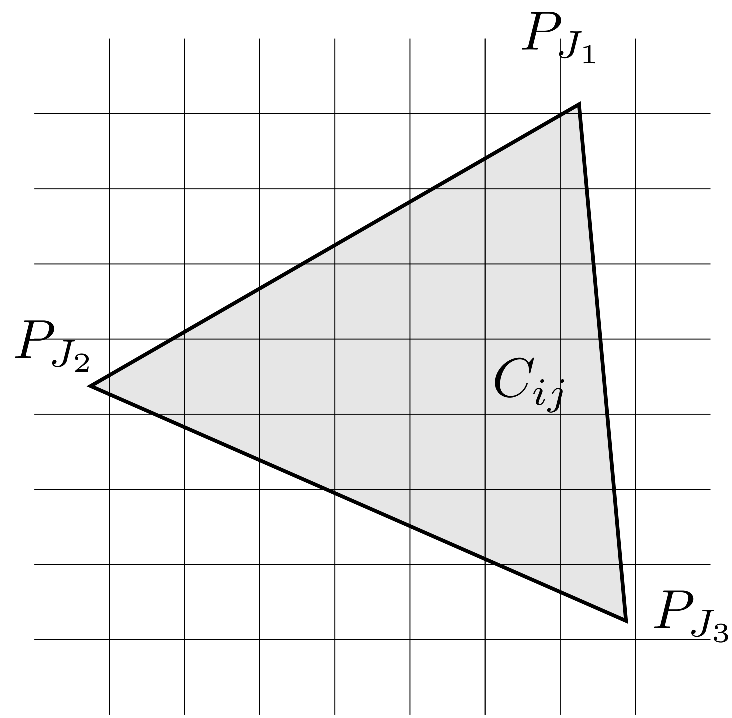
for all 'compatible' test functions $\mathbf{w}$ and q.

From the Finite Elements to the Cells

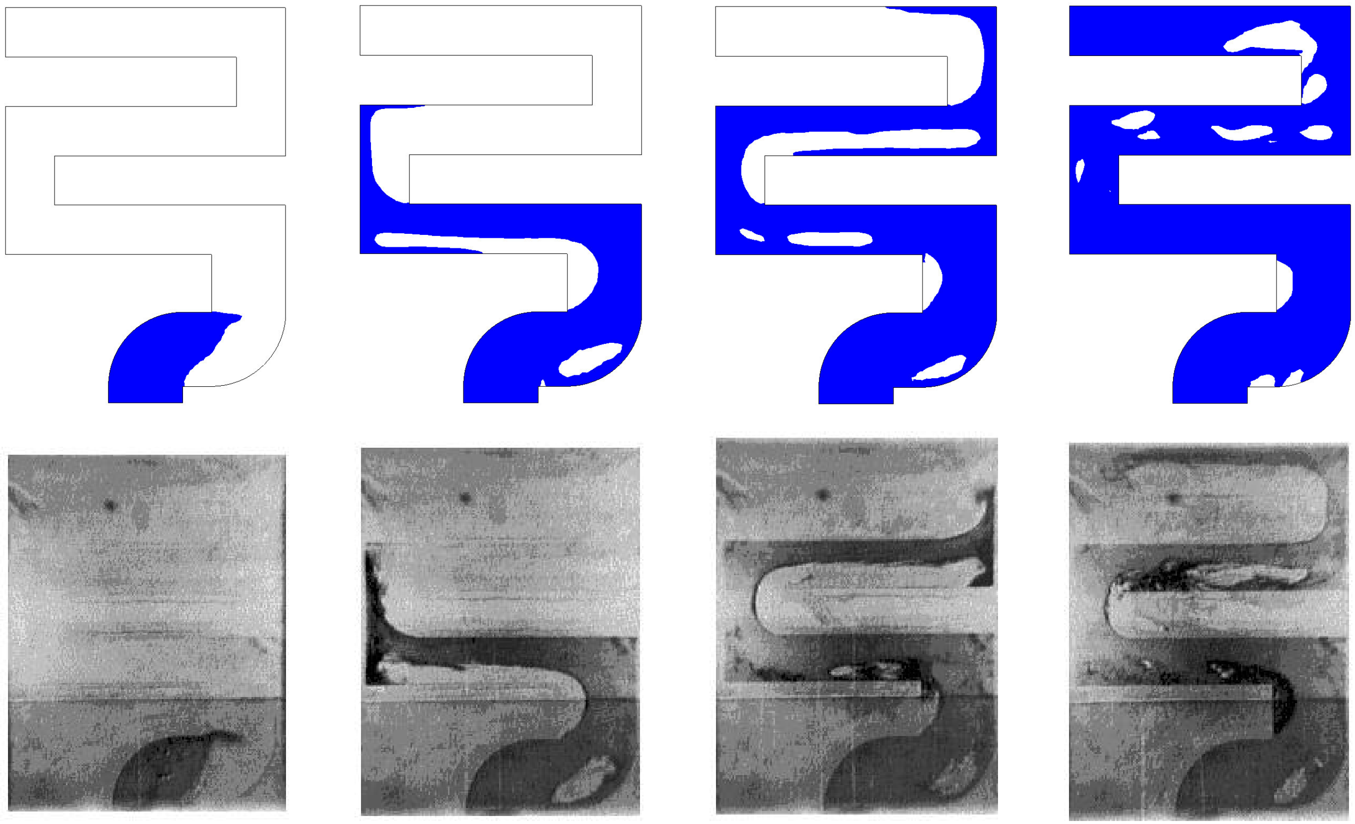
- Projection (Restriction to the center of mass of C_{ijk}) from the piecewise linear approximations to the piecewise constant approximations on the cells:

$$\int_\Lambda u^{n+1}_{CELLS}\psi_{ijk}dx = \int_\Lambda u^{n+1}_{FE}\psi_{ijk}dx, \quad \forall(i,j,k) \ .$$

$$u^{n+1}_{CELLS}(C_{ijk}) = u^{n+1}_{FE}(C_{ijk}) \ .$$



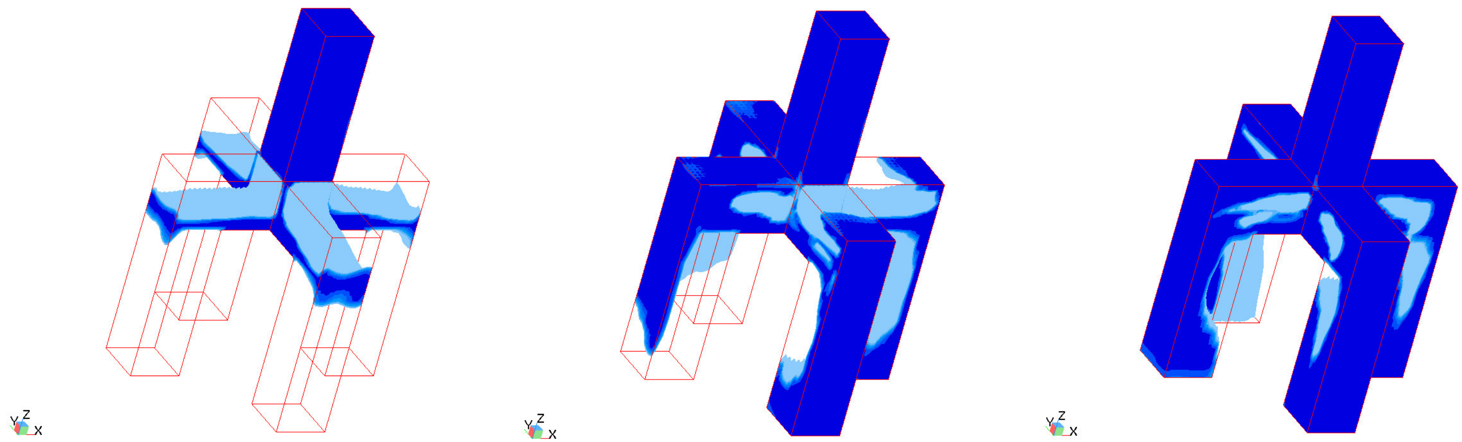
S-shaped channel



[anim]

- Persistence of the bubbles of gas (bubbles are scratched if no compressible gas, 10 % CPU time overhead for gas treatment).
- $21'000$ nodes and $100'000$ elements for FE mesh. $1'500'000$ cells. CPU ~ 350 minutes on a PC. $Re \simeq 10^6$.

Mold Filling

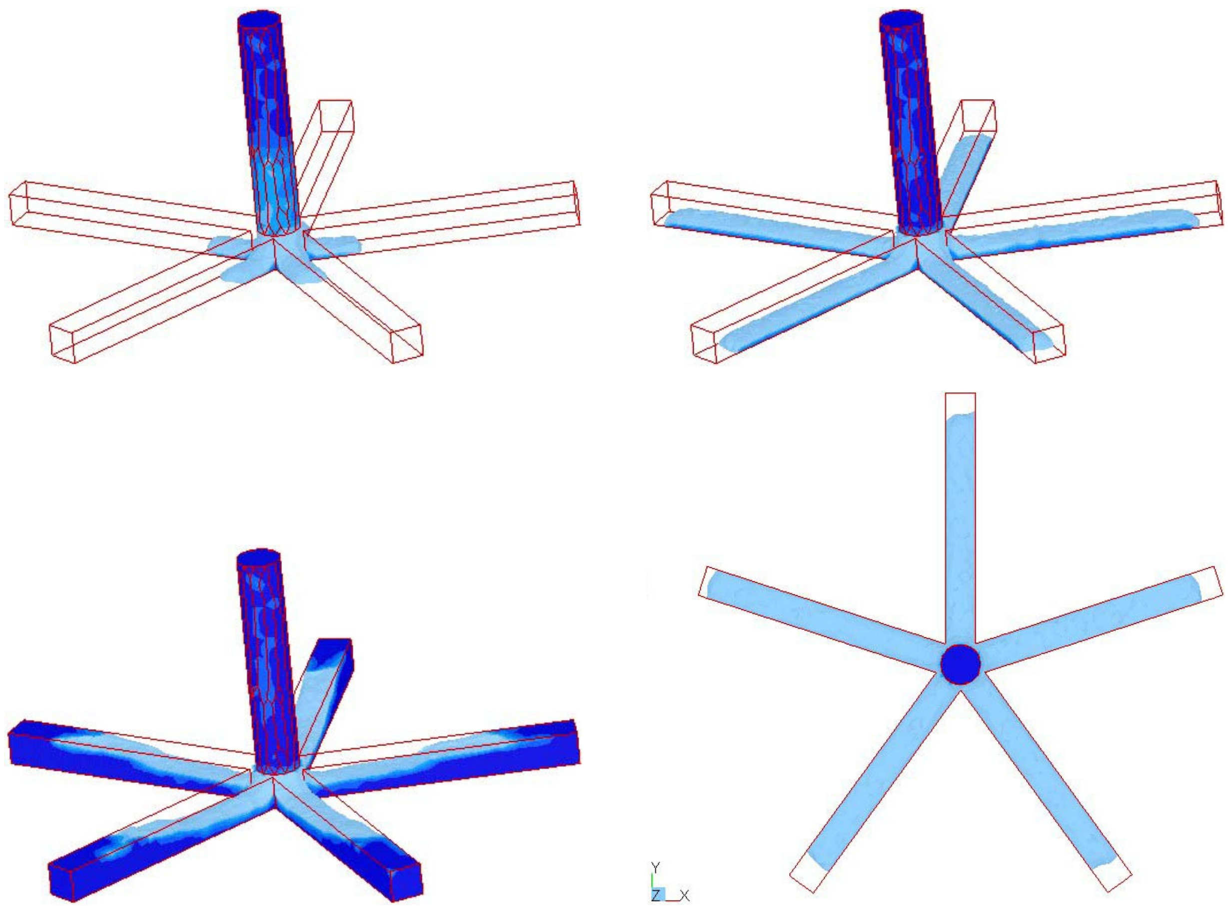


- $31'961$ nodes and $168'000$ elements for the FE mesh. $50'000'000$ cells. CPU ~ 24 hours on a PC.
- Arms with a valve (escaping gas) are filled faster.
- Determination of the location of valves.

[anim]

Star-shaped Mold Filling

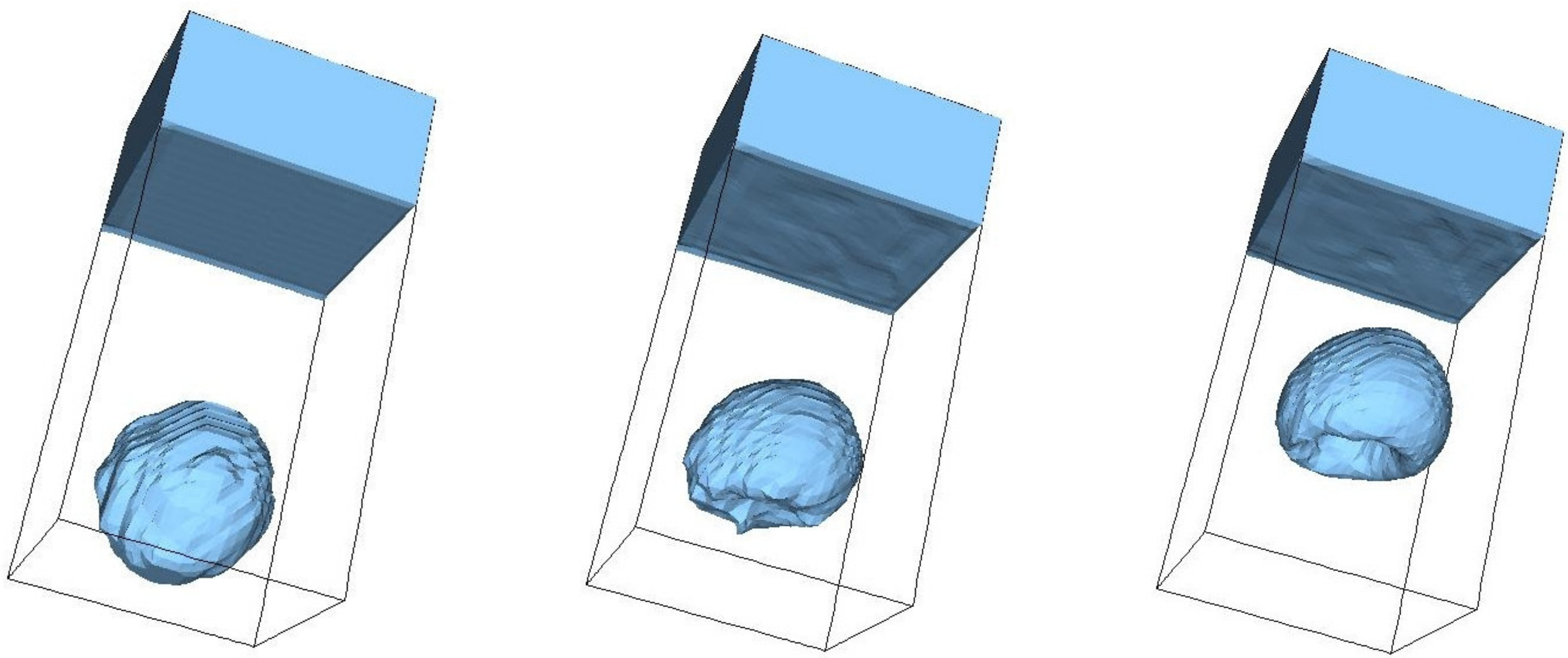
- Star-shaped mold with five arms.
- Hierarchical structure of the cells in order to save memory.



[anim]

Rising Bubble Flow

- Rising Bubble Flow with surface tension effects ($\sigma = 0.0738$ Nm^{-1});
- Convergence with surface tension effects when the mesh size tends to zero.



[anim]

Conclusions and Perspectives

- Simulations of incompressible liquid - compressible gas free surface flow with surface tension.
- Navier-Stokes equations solved only in the liquid.
- Gas treatment with a low computational cost.
- Well adapted to mold filling.
- Full use of the two grids by using projections.

- Coupling with heat equation for the simulation of mold casting.
- Multigrids methods for Stokes solver.
- Simulation of viscoelastic (non-Newtonian) flows [anim].