DE LA RECHERCHE À L'INDUSTRIE

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Applications of the Front-Tracking algorithm of TrioCFD to turbulent bubbly flows in plane channels

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OUTLINE

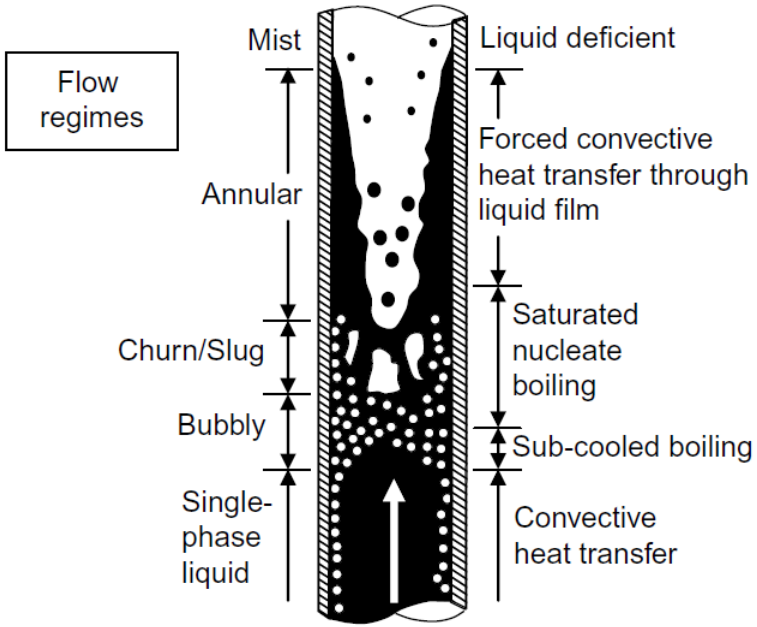
1. Introduction & context
2. Part 1. The numerical method: Front-Tracking algorithm
   - ➢ Governing equations: The One-fluid formulation
   - ➢ General algorithm
     - ✓ Remeshing
     - ✓ Mass & momentum conservation
     - ✓ Sharp discontinuities & interfacial source term
     - ✓ Ghost Fluid Method for phase change
3. Part 2. Quest for up-scaled models
   - ➢ Objectives
   - ➢ Working cases: Bubbly upward turbulent flows
   - ➢ Averaged analysis
     - ✓ Shear stress budget
     - ✓ Void fraction & velocity profiles
   - ➢ Two-fluid Model
     - ✓ Formulation
     - ✓ Closure relations
4. Conclusion & prospects

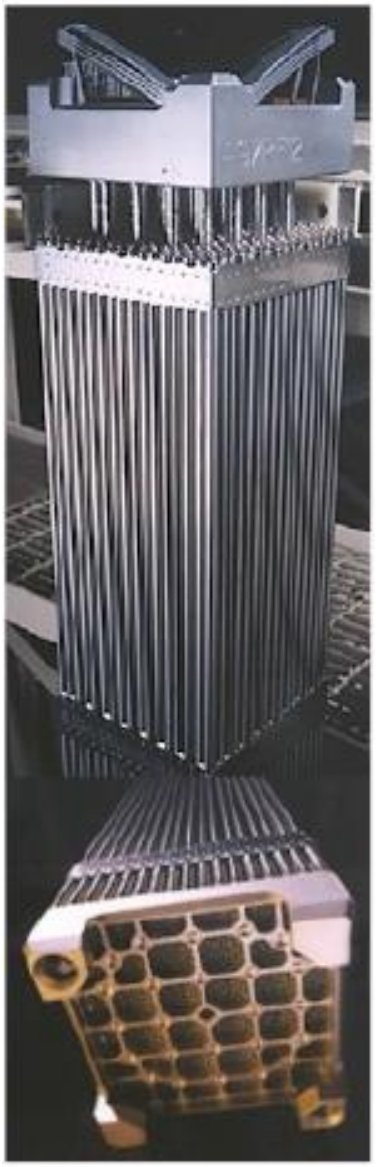
INTRODUCTION & CONTEXT

Context

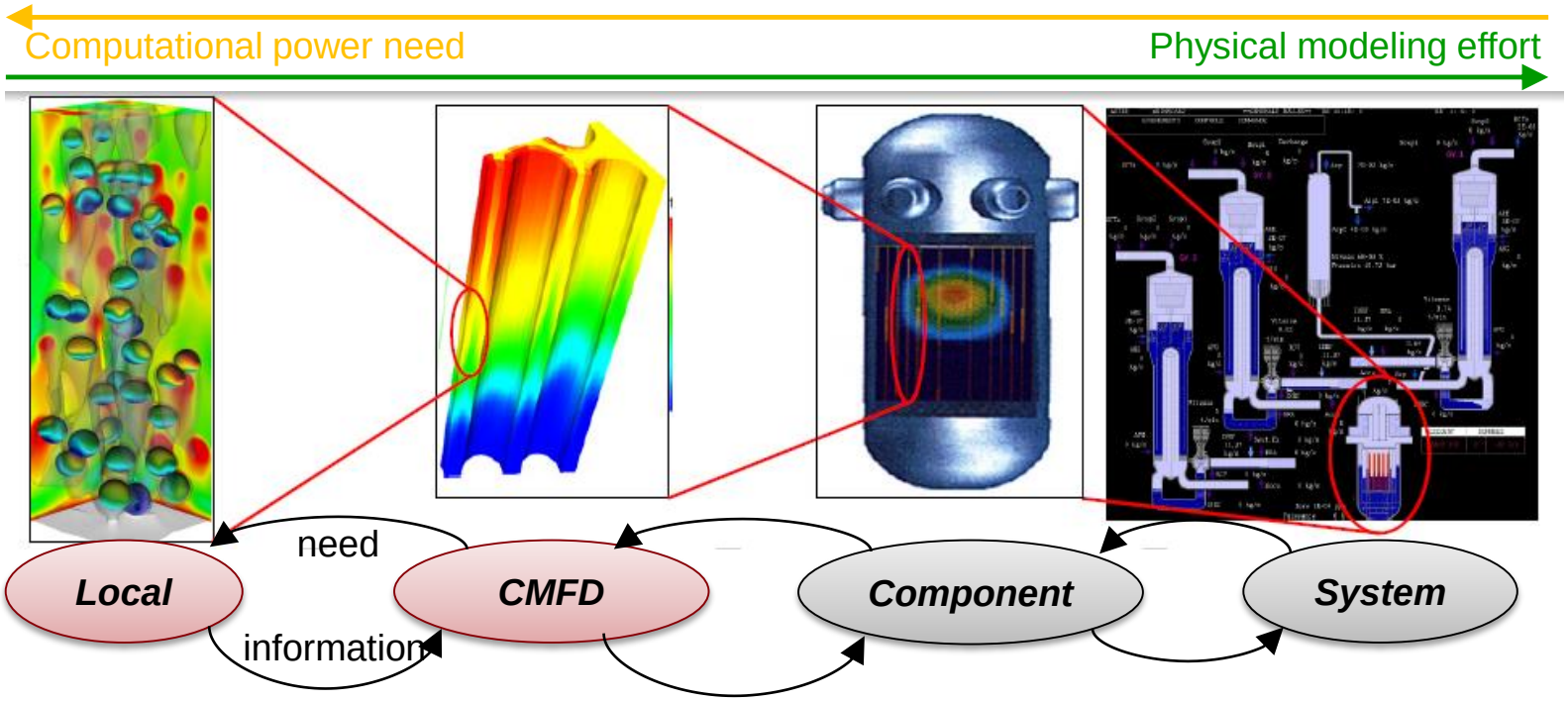
Boiling flows in Nuclear Reactor Safety analysis

- Many applications of two-phase flows to nuclear engineering;
- Transient accidental scenarios: fearing CHF;
- Prediction requires:
  - Accurate modeling of all the intermediate regimes;
  - Understanding of local phenomena.





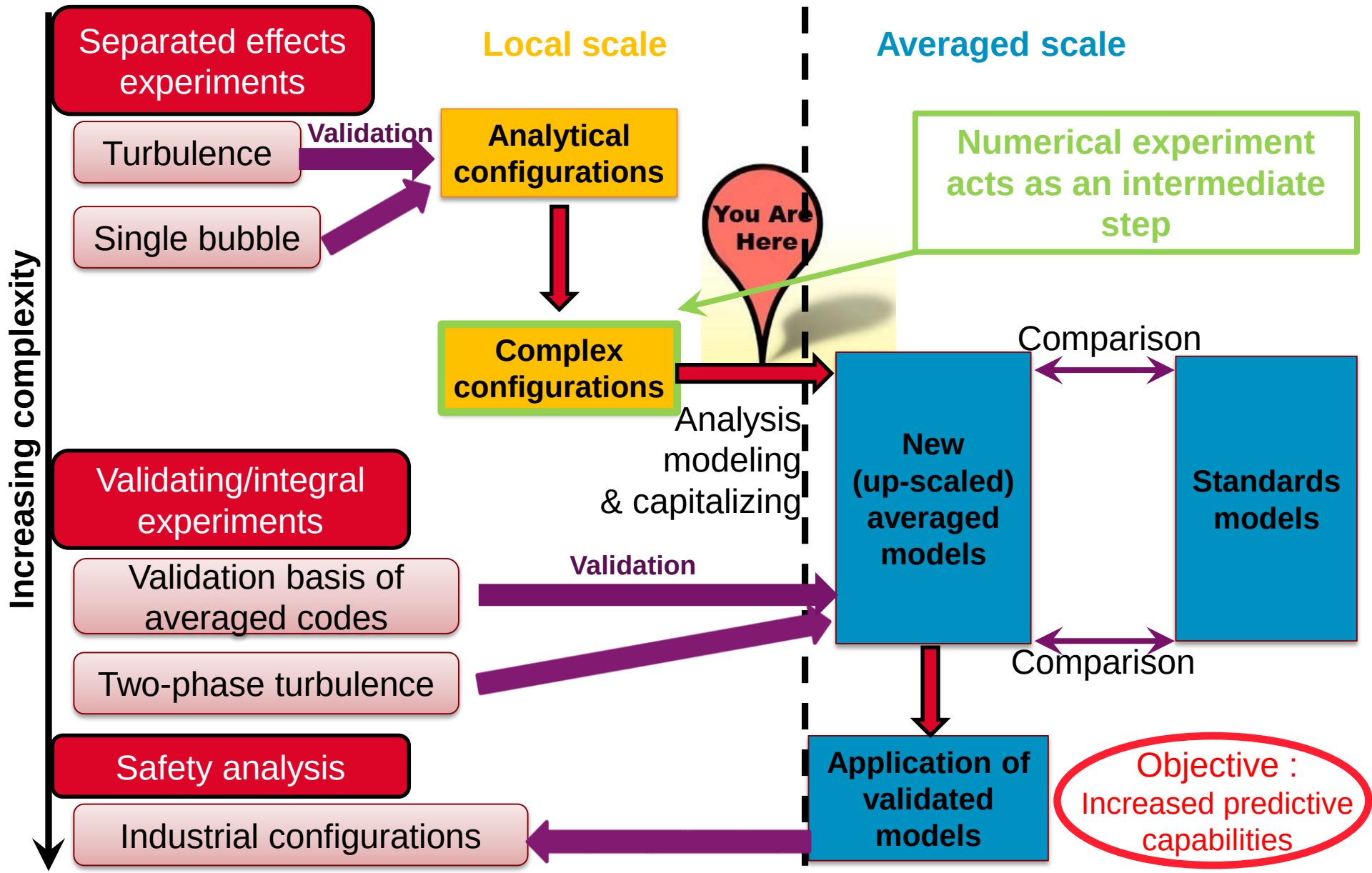
The role of Direct Numerical Simulation



- DNS advantages:
  - To access to ***very local information*** hardly accessible via experiments:
    - Temperature – velocity fluctuations at high pressure;
    - Interfacial transfers…
  - To understand physical mechanism – to decompose phenomena (one-by-one analysis).
- Experiments play a key role in models' validation at any step.

⇨ Up-scaling : extract information/closures for averaged models from local simulations

Global Up-scaling Methodology



The role of Direct Numerical Simulation

- How does DNS work?
  - Resolving all the interfaces;
  - Generally resolving all scales in each phase;
  - We restrict our discussion to continuum fluid mechanics;
  - One still has to model:
    - Wall interactions.
    - Coalescence and break-up.
    - Nucleation and collapse.

- Talk overview:
  1. The numerical method
  2. Quest for up-scaled models

PART 1.
THE NUMERICAL METHOD: FRONT-TRACKING ALGORITHM

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Governing equations

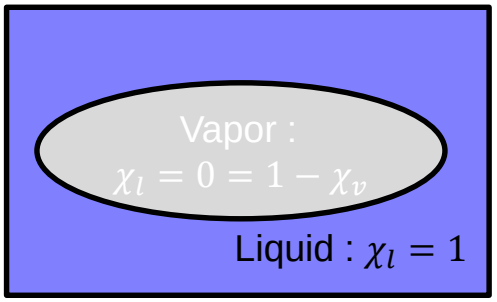
One-fluid formulation (local instantaneous description)

- Local instantaneous description (continuum fluid mechanics)
  - Navier-Stokes equations:

$$\nabla \cdot \boldsymbol{u}_k = 0$$

$$\frac{\partial \rho_k \boldsymbol{u}_k}{\partial t} + \nabla \cdot (\rho_k \boldsymbol{u}_k \boldsymbol{u}_k) = -\nabla p_k + \rho_k \boldsymbol{g} + \nabla \cdot \boldsymbol{\tau}_k \text{ with } \boldsymbol{\tau}_k \widehat{=} \mu_k (\nabla \boldsymbol{u}_k + \nabla^T \boldsymbol{u}_k)$$

  - Interfacial jump conditions:
    - Velocity continuity: $u_1^n = u_2^n$ and $u_1^t = u_2^t$
    - Interfacial normal stress balance: $\sum_k (p_k \boldsymbol{n_k} - \boldsymbol{\tau}_k \cdot \boldsymbol{n}_k) = -\sigma \kappa \boldsymbol{n}$



- Extension to full space
  - Multiply by phase indicator function χ_k: 1 in phase k, 0 otherwise.

$$\frac{\partial \chi_k \rho_k \boldsymbol{u}_k}{\partial t} + \nabla \cdot (\chi_k \rho_k \boldsymbol{u}_k \boldsymbol{u}_k) = -\nabla (\chi_k p_k) + \chi_k \rho_k \boldsymbol{g} + \nabla \cdot [\chi_k \mu_k (\nabla \boldsymbol{u}_k + \nabla^T \boldsymbol{u}_k)] - (p_k \boldsymbol{n_k} - \boldsymbol{\tau}_k \cdot \boldsymbol{n}_k) \cdot \nabla \chi_k$$

- One-fluid formulation
  - Definition of "one-fluid" fields: $\phi \widehat{=} \sum_k \chi_k \phi_k$
  - Adding up and using jump conditions:

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \boldsymbol{u}) = -\nabla p + \nabla \cdot [\mu (\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u})] + \sigma \kappa \boldsymbol{n}\, \delta^i$$

  - Combined "one-fluid" formulation valid at any point in the sense of distributions
  - Phase-indicator function χ_k is advected by the local velocity field (mixed VOF/FT algorithm)

TrioCFD: Front-Tracking algorithm

One-fluid formulation (with phase-change)

1. Mass:
   - Phase incompressibility: $\nabla \cdot \boldsymbol{u} = [\![1/\rho]\!]\dot{m}\delta^i$
   - Interfacial transport: $\frac{\partial \chi}{\partial t} + \boldsymbol{u}^i \cdot \nabla \chi = 0$ with $\boldsymbol{u}^i = \boldsymbol{u} - \frac{1}{\rho}\dot{m}\boldsymbol{n}\delta^i$
2. Momentum: $\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) = -\nabla P + \nabla \cdot (\mu \nabla \boldsymbol{u}) + \rho \boldsymbol{g} + \sigma \kappa \boldsymbol{n}\delta^i$
3. Energy: $\frac{\partial \rho c_p T}{\partial t} + \nabla \cdot (\rho c_p \boldsymbol{u} T) = \nabla \cdot (k \nabla T) + \mathcal{L}^{vap}\dot{m}\delta^i$

- The One-fluid formulation contains the following jump relations…
  1. Mass : $\dot{m}_1\delta^i + \dot{m}_2\delta^i = 0$
  2. Momentum : $(\dot{m}_k \boldsymbol{u}_k + p_k \boldsymbol{n}_k - \boldsymbol{\tau}_k \cdot \boldsymbol{n}_k) \cdot \nabla \chi_k = -\sigma \kappa \boldsymbol{n}\delta^i$
  3. Energy : $k_k \nabla T_k \cdot \nabla \chi_k = \dot{m}\mathcal{L}^{vap}\delta^i$
- …but the interfacial entropy principle must be supplied to complete the description:
  - Interfacial thermo-dynamic equilibrium : $(T - T^{sat})\ \delta^i = 0$
  - Continuity of tangential velocity : $u_1^t = u_2^t$
- The general method implemented in TrioCFD is able to deal with:
  - Coalescence and break-up;
  - Phase change : velocity and temperature gradient discontinuities dealt with Ghost Fluid Method (GFM);
  - Contact lines;
  - But unfortunately, no periodic boundary conditions for interfaces…
- Periodicity has been implemented in a separated module dedicated to structured Cartesian eulerian meshes and parallel efficiency (IJK_FT).

TrioCFD: Front-Tracking algorithm

General algorithm

- Time-stepping:

- Fully coupled fractional time-step algorithm (3rd order, Runge-Kutta low storage)
- For the 3 sub-steps of each time step :

1. Update the marker's position (Interfacial transport): $\boldsymbol{x}^{\star} = f(\boldsymbol{x}^{n}, \boldsymbol{u}^{n}, \Delta t)$
2. Remeshing* and mass preserving* algorithms: $\boldsymbol{x}^{n+1} = g(\boldsymbol{x}^{\star})$
3. Update the new phase indicator function : $\chi^{n+1} = h(\boldsymbol{x}^{n+1})$
4. Update physical properties : $\rho^{n+1} = \rho(\chi^{n+1})$ and $\mu^{n+1} = \mu(\chi^{n+1})$

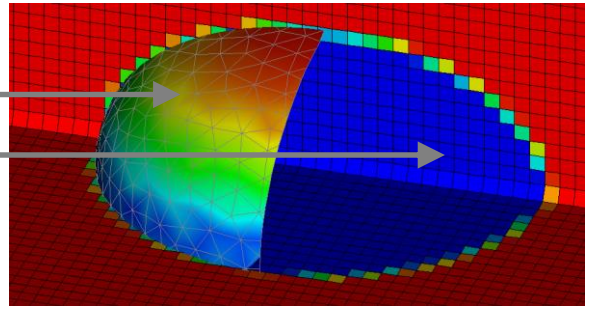
---

5. Velocity prediction : $\frac{\rho^{n+1}\boldsymbol{u}^{\star} - \boldsymbol{\rho}^{\boldsymbol{n}}\boldsymbol{u}^{\mathrm{n}}}{\Delta t} = \boldsymbol{F}^{n}$ $\quad \boldsymbol{F}^{n} = -\nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) + \nabla \cdot (\mu \nabla \boldsymbol{u}) + S^{i}*$
6. Pressure projection : $\nabla \cdot \left(\frac{1}{\rho^{n}} \nabla P^{n+1}\right) = \frac{\nabla \cdot \boldsymbol{u}^{\star}}{\Delta t}$
7. Velocity correction : $\boldsymbol{u}^{n+1} = \boldsymbol{u}^{n} - \frac{1}{\Delta t} \nabla P^{n+1}$

- f and g are the keys of the method. They represent interpolations of the velocity field and all the tricky functions to preserve the mesh qualities, the volumes of each phases…
- We use the MAC discretization and the density and viscosity are interpolated to faces using a simple arithmetic mean.

Normal, curvature →

Phase indicator, velocity, pressure, temperature (MAC arrangement) →

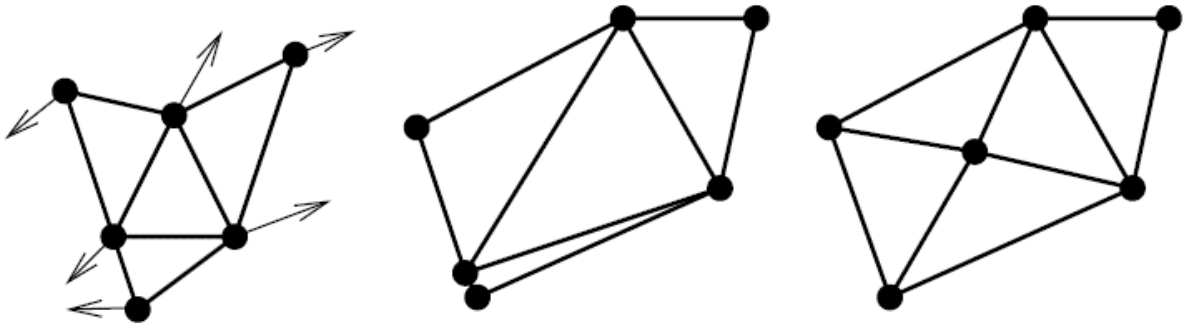


*detailed afterward

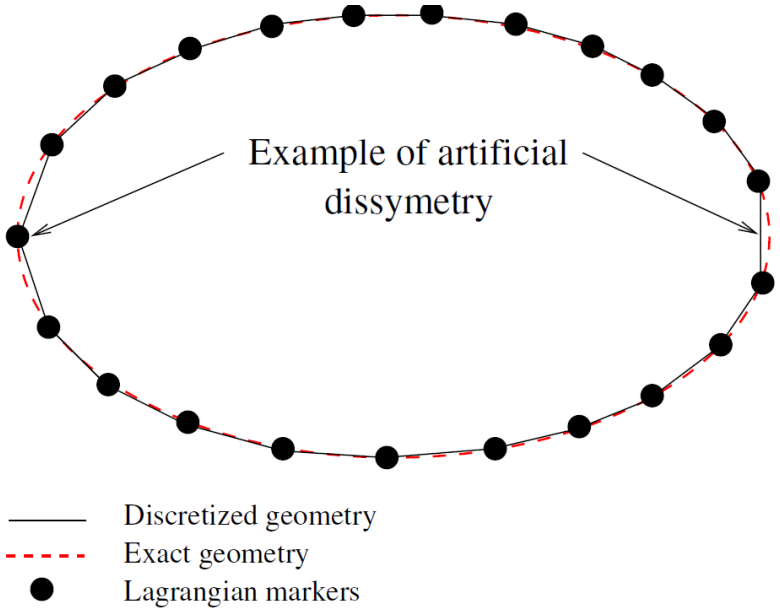
------- actual beginning of a timestep

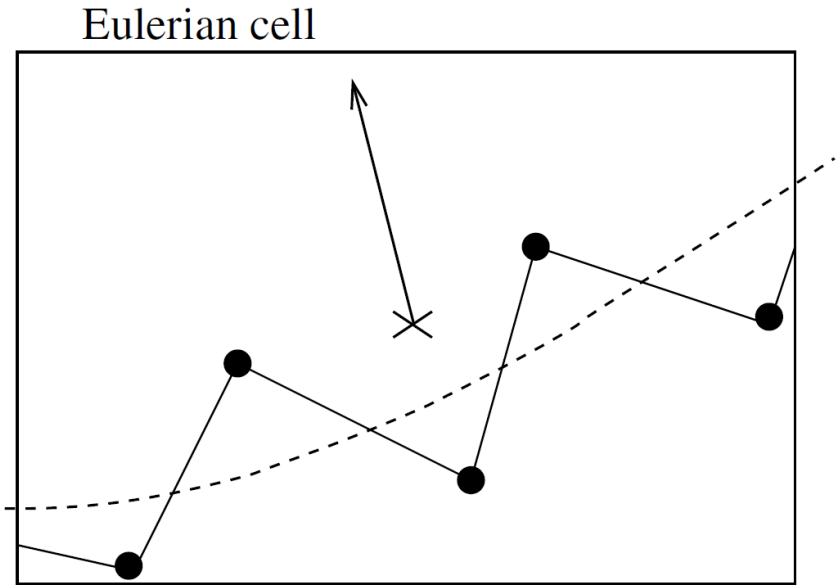
TrioCFD: Front-Tracking algorithm

Remeshing algorithm



- Remeshing is compulsory to keep a good description of the interface;
- Markers' density :
  - High ⇒ accurate prediction of interfacial area, forces…
  - But lower than the eulerian mesh ⇒ unstable if too many dof…
  - … unless interface smoothing FTIS (A. Toutant & al, 2012) is used.

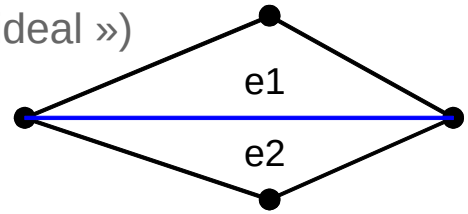


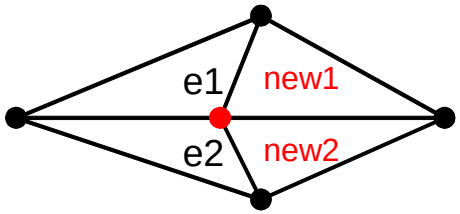


TrioCFD: Front-Tracking algorithm

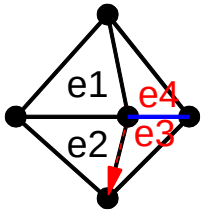
Remeshing algorithm

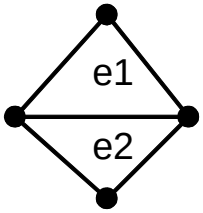
- Size of elements (« facteur_longueur_ideal »)
  - Too long edge (blue)
    / element addition (red):



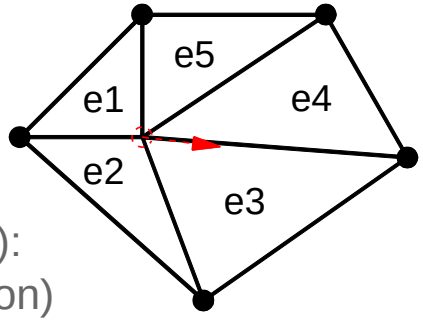


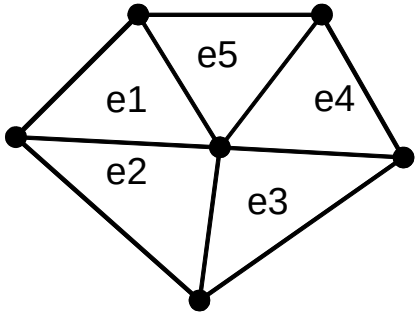
  - Too short edge (blue)
    / element deletion (red):





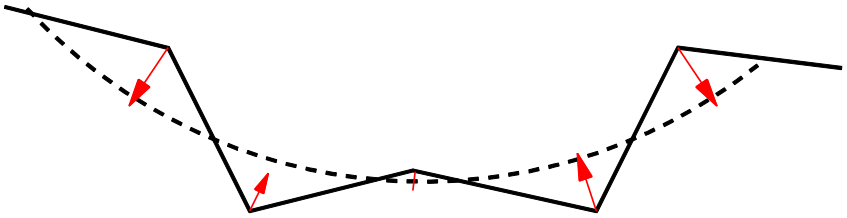
- Rebalancing (« barycentrage »):





- Smoothing of the interface (« lissage »):
  (conservative mass/volume redistribution)
  (equivalent to a 4th order space-filter)

$$\frac{\partial S}{\partial t} = -\alpha \int_{\Gamma} \|\nabla_s \kappa\|^2 \, d\Gamma$$



- Iterative procedure.

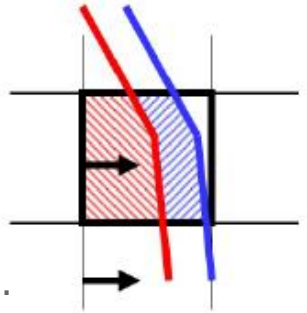
TrioCFD: Front-Tracking algorithm

Semi-local mass conservation

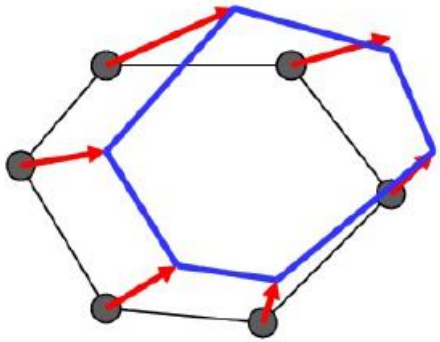
- The density is a function of the markers' positions.
- The advection scheme of the markers is not "consistent" with the equation for mass:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho \boldsymbol{u}) \;\Rightarrow\; \frac{\partial}{\partial t}\int_\Omega \rho dv = \int_{\partial\Omega} \rho \boldsymbol{u} \cdot \boldsymbol{n}\, \mathrm{d}s \text{ (not verified by FT)}$$

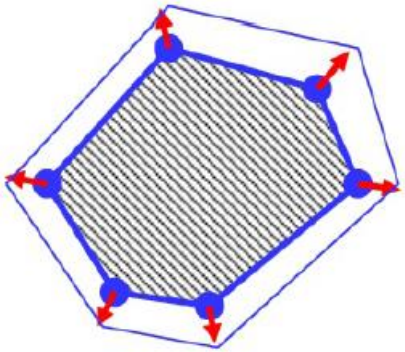
Instead we have: $\frac{\partial}{\partial t}\int_\Omega \rho dv = f\left(\frac{\partial \boldsymbol{x}_i}{\partial t}\right) \neq \int_{\partial\Omega} \rho \boldsymbol{u} \cdot \boldsymbol{n}\, \mathrm{d}s$



- Hence, mass preservation is different from momentum and energy preservation.
- The volume variation through the transport equation is computed for each bubble… (step 1)

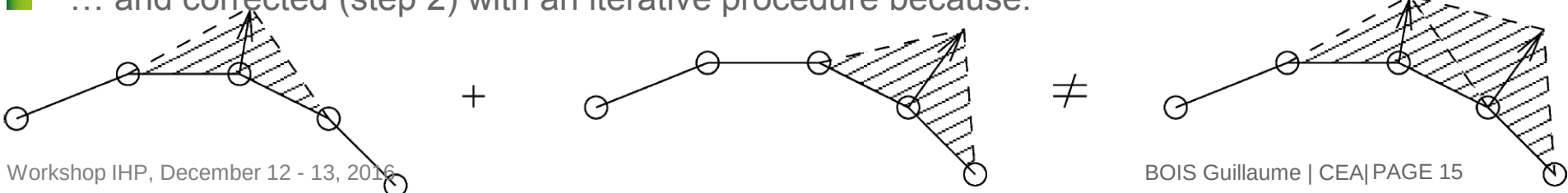


Step 1: Transport by interpolated velocity (not conservative)



Step 2: Correction moving the markers along the normal direction

- … and corrected (step 2) with an iterative procedure because:



TrioCFD: Front-Tracking algorithm

Momentum: Conservation

- There are 2 reasons for the non-conservation of momentum :
  - The volumetric discretization of the surface tension source term is not strictly conservative : $\oint S^i ds \neq 0$
  - The density used in the velocity's prediction and projection steps :
    - Velocity prediction: $\frac{\boldsymbol{u}^\star - \boldsymbol{u}^n}{\Delta t} = \boldsymbol{F}^n \implies \boldsymbol{u}^\star \approx \boldsymbol{u}^n + \Delta t \boldsymbol{F}^n$ with $\boldsymbol{F}^n = -\hat{\rho}^n \nabla \cdot (\boldsymbol{uu})^n + \nabla \cdot (\mu^n \nabla \boldsymbol{u}^n) + S^i$
    - Velocity correction: $\boldsymbol{u}^{n+1} = \boldsymbol{u}^\star - \Delta t \frac{1}{\hat{\rho}^n} \nabla P^{n+1}$

    Where P comes from the pressure projection : $\nabla \cdot \left(\frac{1}{\hat{\rho}^n} \nabla P^{n+1} \right) = \frac{\nabla \cdot \boldsymbol{u}^\star}{\Delta t}$

    Cell-to-face interpolation of the density (discontinuous) is required… not very accurate.

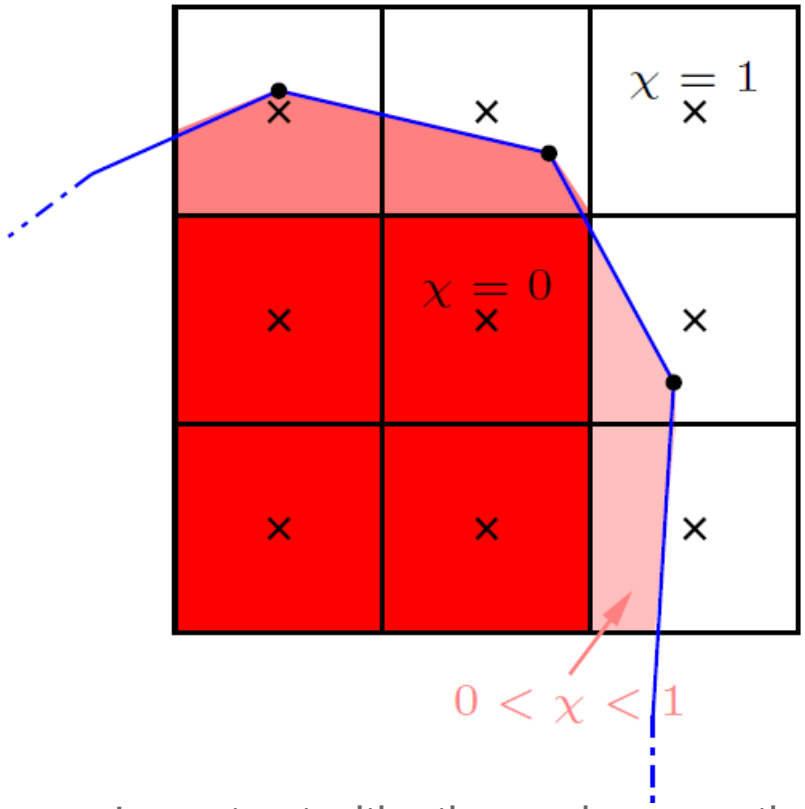
    The density at different timesteps could be used in a conservative formulation of the non-linear term.

- To the best of our knowledge:
  - no LS or FT algorithm preserves momentum to the computer accuracy;
  - There is no clear recommendation in the literature on the best formulation.
- So far, the conservation of momentum has been accurate enough in most cases.

Inter-mesh communication

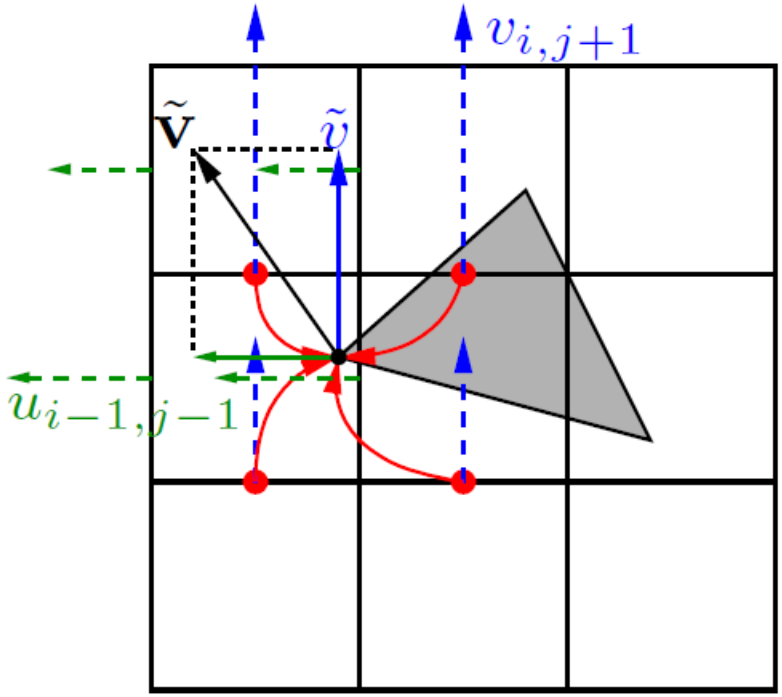
Phase indicator function and velocity interpolation

- Geometric computation of the phase indicator function based on the Front position.



- In contrast with other codes or methods, the sharp phase indicator function is used without smoothing.

- First order interpolation of the MAC velocity;



- The resulting marker velocity is then modified to eliminate the tangential motion of markers (based on the mean velocity of connected markers) in order to limit the need for remeshing algorithms (in particular barycentring)

Inter-mesh communication

Interfacial source term

- The surface tension force is computed along with the gravity as a potential:

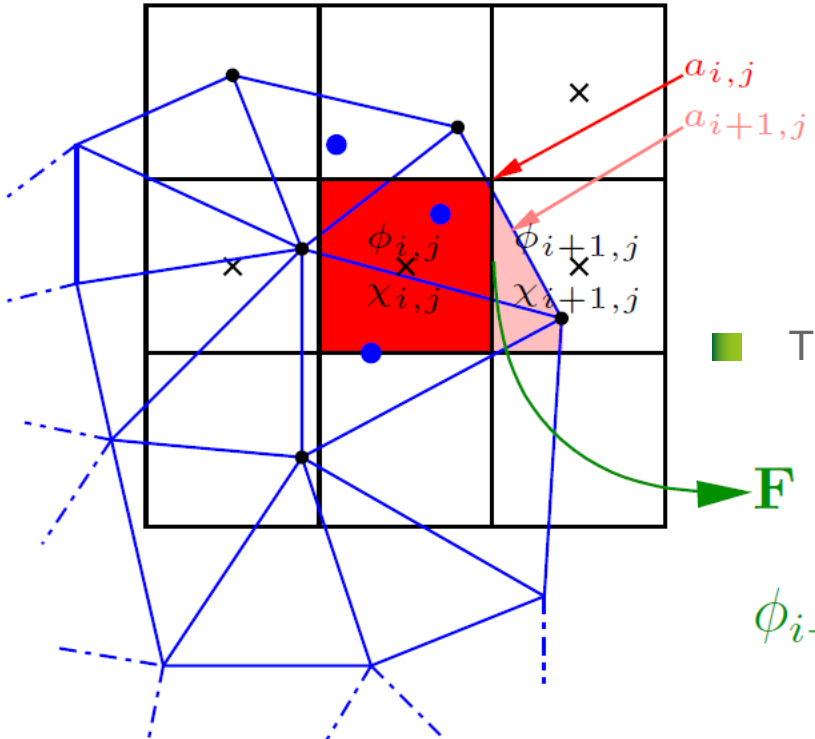
$$-\nabla P + \rho \boldsymbol{g} = -\nabla(P - \rho \boldsymbol{g} \cdot \boldsymbol{x}) - \Delta\rho \boldsymbol{g} \cdot \boldsymbol{x} \nabla\chi$$

The interfacial potential ϕ (computed at the front markers) is defined by:

$$\phi = \sigma\kappa - \Delta\rho \boldsymbol{g} \cdot \boldsymbol{x} - \boldsymbol{\phi_r} \quad \Rightarrow \quad F^i = \phi \nabla \chi_l$$

$$P^{num} = P - \rho \boldsymbol{g} \cdot \boldsymbol{x}$$

- Discrete curvature : surface over volume differential : $\hat{\kappa} = -\frac{\boldsymbol{n}^s \cdot \boldsymbol{n}^v}{\boldsymbol{n}^v \cdot \boldsymbol{n}^v}$ (such that a minimal potential energy can be achieved with a given pressure field and a zero velocity field: no spurious currents).
- The marker position
- A possible repellant potential numerically fitted and computed from the markers from other entities.



- The interfacial force is then computed on the fixed grid:

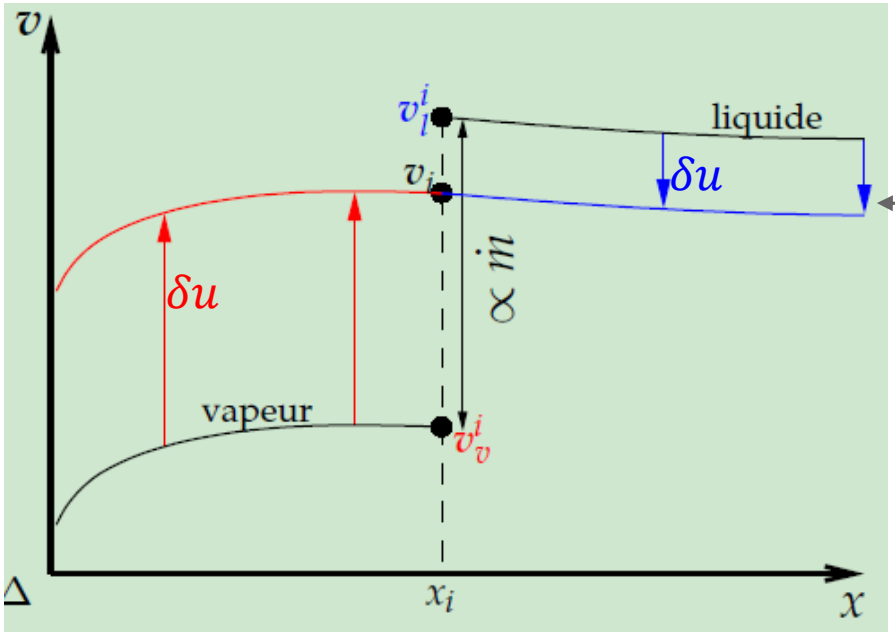
$$\mathbf{F} = (\phi\nabla\chi)_{i+1/2,j} = \phi_{i+1/2,j} \frac{\chi_{i+1,j} - \chi_{i,j}}{\Delta x}$$

$$\phi_{i+1/2,j} = \frac{a_{i+1,j}\chi_{i+1,j} + a_{i,j}\chi_{i,j}}{a_{i+1,j} + a_{i,j}}$$

TrioCFD: Front-Tracking algorithm

Ghost Fluid method (for the interfacial velocity)

- Velocity: build a continuous field for the interfacial velocity (markers' transport).



$$\delta u = \begin{cases} \dfrac{\dot{m}}{\rho_l} & \text{dans le liquide} \\ \dfrac{\dot{m}}{\rho_v} & \text{dans la vapeur} \end{cases}$$

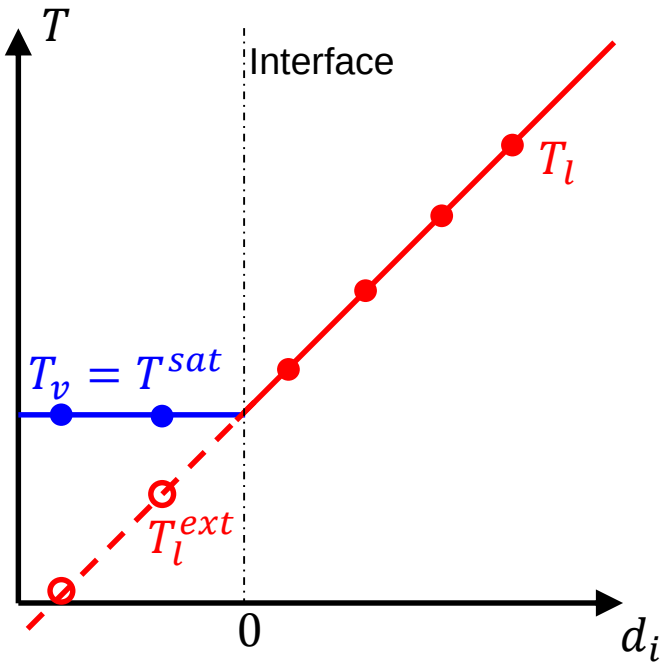
- Extend away from the interface using an eulerian field for the normal to the interface:

$$u - \delta u = \begin{cases} u_l - \dfrac{\dot{m}}{\rho_l} = u^i & \text{dans le liquide} \\ u_v - \dfrac{\dot{m}}{\rho_v} = u^i & \text{dans la vapeur} \end{cases}$$

TrioCFD: Front-Tracking algorithm

Ghost Fluid method (for the temperature)

- Temperature:
  - Continuous extension C^1 of the liquid temperature into the vapor;
  - Ensure $T^i = T^{sat}$;
  - Evaluate the phase-change rate accurately from the gradient of the liquid temperature.
- Algorithm:
  1. Compute the normal liquid temperature gradient at the interface;
  2. Determine the ghost temperature;
  3. Compute the phase-change rate



$$(\boldsymbol{n}\cdot\nabla T)_i = \frac{T_i - T^{sat}}{d_i}\, e^{\kappa\, d_i/2} \simeq \frac{T_i - T^{sat}}{d_i}\left(1 + \kappa\,(d_i/2) + \frac{\kappa\,(d_i/2)^2}{2} + \mathcal{O}(d_i^3)\right)$$

$$T_i = T^{sat} + (\boldsymbol{n}\cdot\nabla T)_i\, \frac{1}{\kappa}\left(1 - e^{-\kappa\, d_i}\right) \simeq T^{sat} + (\boldsymbol{n}\cdot\nabla T)_i\; d_i\left(1 - \frac{\kappa\, d_i}{2} + \frac{\kappa^2\, d_i^2}{6}\right)$$

$$\dot{m}_i = \frac{k\,(\boldsymbol{n}\cdot\nabla T)_i}{\mathcal{L}}$$

TrioCFD: Front-Tracking algorithm

Summary

- Some advantages of the FT:

- Accuracy;
- Capacity to deal with jumps conditions very locally (without smoothing or smearing of density jumps or interfacial forces);
- Control over the coalescence and break-up phenomena (criteria not necessarily equal to one mesh size);
- Capability to deal with surfactants and variable surface tension or saturation temperature (towards more complex physics or more accurate descriptions);
- Offers nice possibilities to introduce sub-grid models.

- Some drawbacks or technical issues:

- Heavy implementation (especially for 3D parallel computations);
- Periodic boundary conditions hard to treat;
- Remeshing & control of lagrangian mesh quality;
- Convergence of the pressure solver for highly discontinuous fluids or high interfacial forces (if no smoothing of forces and properties are used);
- Computational cost? It is generally hard to compare different codes and what is the same accuracy (not necessarily the same resolution).

Some references

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- Toutant, A., *Modélisation physique de l'interaction entre interfaces et turbulence*, PhD thesis, INP-Toulouse, 2006.
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- Toutant, A., Chandesris, M., Jamet, D. and Lebaigue, O., *Jump conditions for filtered quantities at an under-resolved discontinuous interface. Part 2: a priori tests*. Int. J. Multiphase Flow, vol. 35 (12), p.1119-1129, 2009.
- Magdeleine S., *Démonstration de la potentialité des méthodes de SND diphasique à renseigner les modèles moyennés: Application à la colonne à bulles*, PhD thesis, INP-Grenoble, 2009.
- Bois G., *Transferts de masse et d'énergie aux interfaces liquide-vapeur avec changement de phase : proposition de modélisation aux grandes échelles des interfaces*, PhD thesis, INP-Grenoble, 2011.
- Toutant A., Mathieu B. and Lebaigue O., *Volume-conserving mesh smoothing for front-tracking methods*, Computers and Fluids, vol. 67, p. 16-25, 2012.

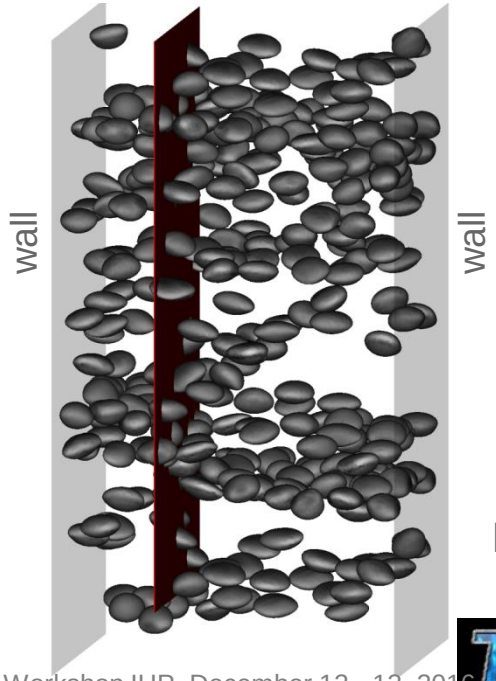
PART 2.
QUEST FOR UP-SCALED MODELS

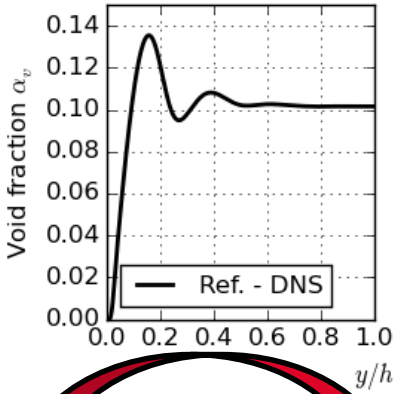
OUTLINE

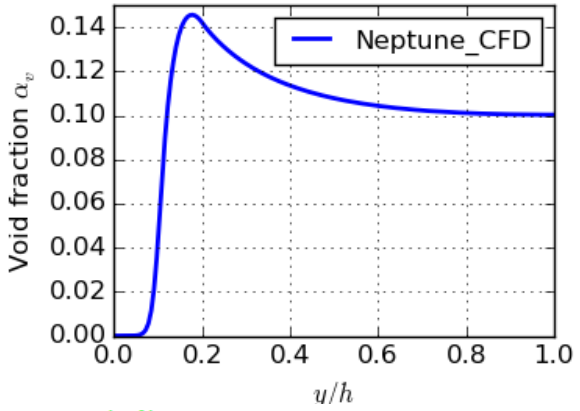
1. Introduction & context
2. Part 1. The numerical method: Front-Tracking algorithm
   - ➢ Governing equations: The One-fluid formulation
   - ➢ General algorithm
     - ✓ Remeshing
     - ✓ Mass & momentum conservation
     - ✓ Sharp discontinuities & interfacial source term
     - ✓ Ghost Fluid Method for phase change
3. Part 2. Quest for up-scaled models
   - ➢ Objectives
   - ➢ Working cases: Bubbly upward turbulent flows
   - ➢ Averaged analysis
     - ✓ Shear stress budget
     - ✓ Void fraction & velocity profiles
   - ➢ Two-fluid Model
     - ✓ Formulation
     - ✓ Closure relations
4. Conclusion & prospects

Objectives

- 2-phase RANS CFD modelling of bubbly flows:
  - The only practical tool able to deal with industrial applications (high Reynolds number, complex geometry);
  - Strong modeling and validation efforts were made;
  - Further progress is now limited by the lack of precise knowledge of local phenomena: interfaces & turbulence interactions… ⇒ Related to limited measurement techniques;
- Our proposal:
  - To use DNS as “numerical experiments” in reactor core conditions;
  - To analyze DNS results to improve modeling of 2-phase RANS CFD.
- Working test case: plane channel – turbulent bubbly flow.



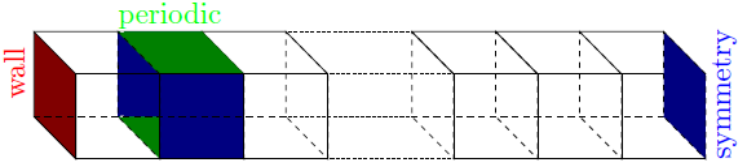




Upscaling

Local scale DNS

Averaged scale 2-phase RANS CFD



TRUST

NEPTUNE

Local scale

Working cases: upward turbulent bubbly flows (1/2)

- Back to the most simple two-phase physics:
  - No phase-change;
  - Constant physical properties;
  - No coalescence.

- Bubbles in a turbulent flow:
  - Study the mechanical equilibrium;
  - Momentum analysis;
  - Interfacial momentum exchange terms.

- Two studies:
  - Water & Steam in PWR conditions (155 bars)

  ⇒ Very high fluctuations, relative velocities and void fraction.

  - Lu & Tryggvason (Physics of Fluids, 20, 2008).

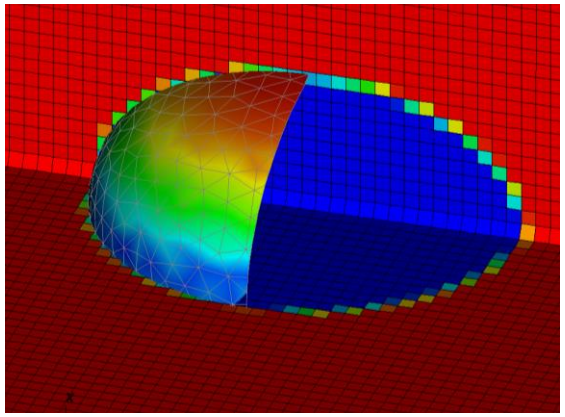
  ⇒ Code benchmark for validation;

  ⇒ Additional statistical analysis.

	WS155	LT2008	
		S	D
$Re_\tau = u_\tau h/\nu_l$	180	127	
$Eo = \rho g d^2/\sigma$	1	0.45	4.5
α_v (%)	10	3	
D_b/h	0.2	0.3	
N_b	936	21	
Size $(/h)$	$2\pi \times 2 \times \pi$	$\pi \times 2 \times \pi/2$	
Resolution (uniform)	$396 \times 1152 \times 192$ $\approx 87.6\text{M}^{\text{ons}}$	$256 \times 192 \times 128$ $\approx 6.2\text{M}^{\text{ons}}$	
Mesh size (in wall-unit) $1\text{w.u.} = h/Re_\tau$	0.3 to 3 w.u.	1.3 to 1.6 w.u.	
Fluid	Pressurized Water & steam	Fictitious	
Gravity	9.81	0.1	
Goal	Push boundaries towards industrial configurations	Validation & tractable computations	

Local scale

Working cases: upward turbulent bubbly flows (2/2)



- **Numerical method:**
  - Mixed Front-Tracking/VOF method implemented in TRUST_IJK;
  - Discretization: 3rd order in time (RK3) and 4th order in space
  - Optimized use of cache memory (Multi-grid solver and high efficiency operators).

- **Steady-state control:**
  - Flow-rate: fluctuating momentum source term

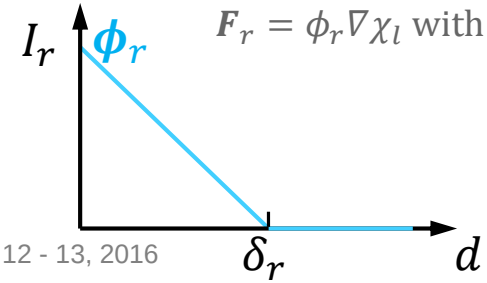
Relaxation parameter

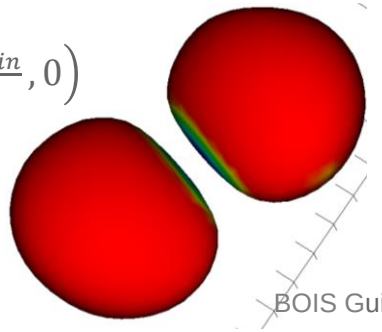
$$\frac{\partial S_x^f}{\partial t} = \frac{\omega_0}{h}\left(\sqrt{\tau_0} - \sqrt{\tau_w}\right) \quad \text{or} \quad S_x^f = \langle\rho\rangle g + \frac{\tau_w}{h} = \text{cste}$$

Wall friction: expected — instantaneous measurement

  - To reach a statistical steady-state, coalescence and wall-contact are not considered
    - Nothing specific was needed for the moderate Reynolds number cases (LT2008);
    - For the higher Reynolds number and strong gravitational case (WS155), small artificial repellant forces were required:

$$\boldsymbol{F}_r = \phi_r \nabla \chi_l \text{ with } \phi_r = \max\left(I_r \frac{\delta_r - d_{min}}{\delta_r}, 0\right)$$

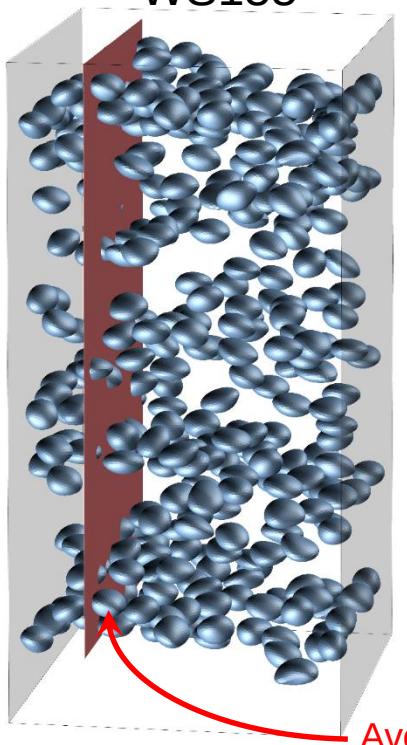




Local scale

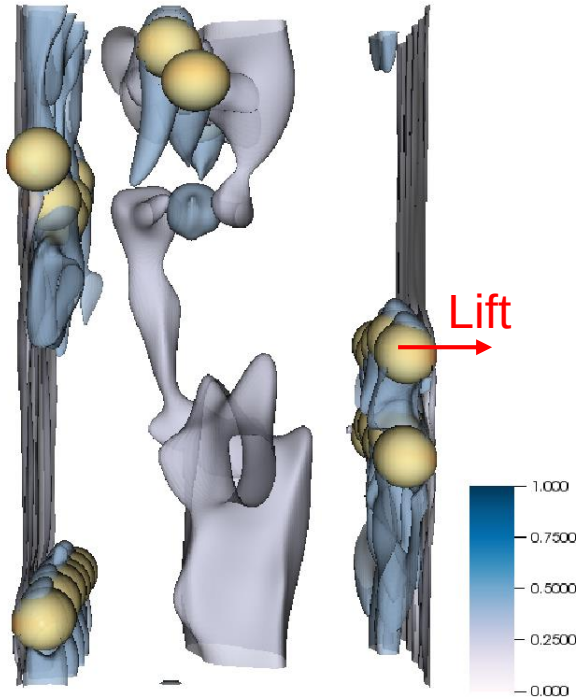
Observations & averaging

WS155



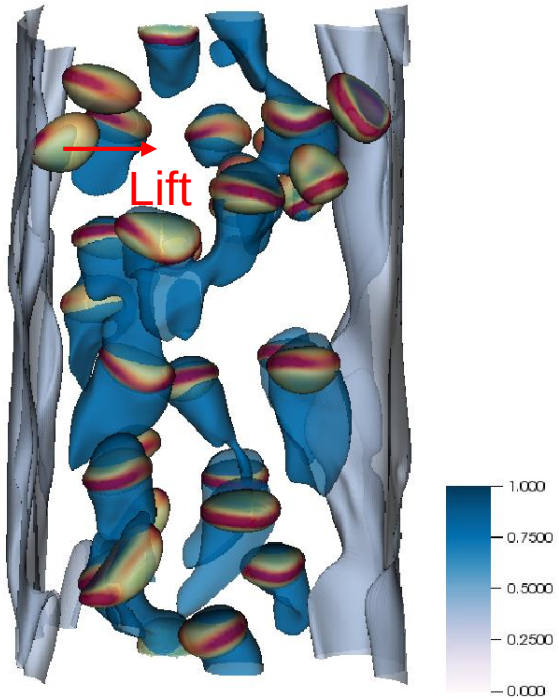
No clear behavior
Very high fluctuations and relative velocities

LT2008_Sphe



Wall-peaking
Horizontal bubble clustering

LT2008_Defo



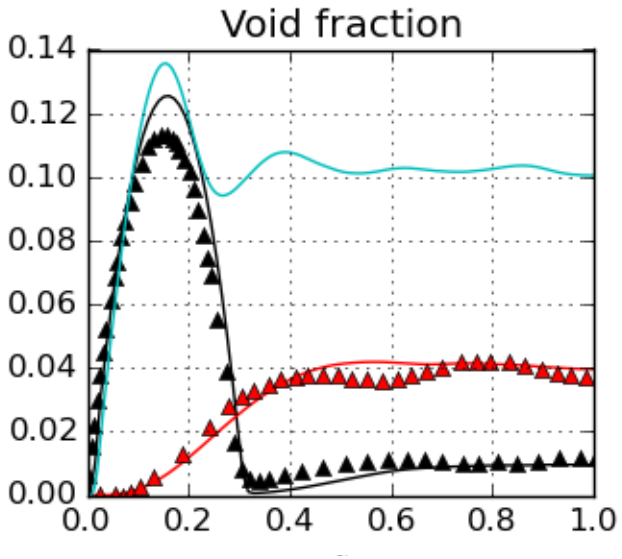
Homogeneous core distribution
Increased pseudo-turbulence

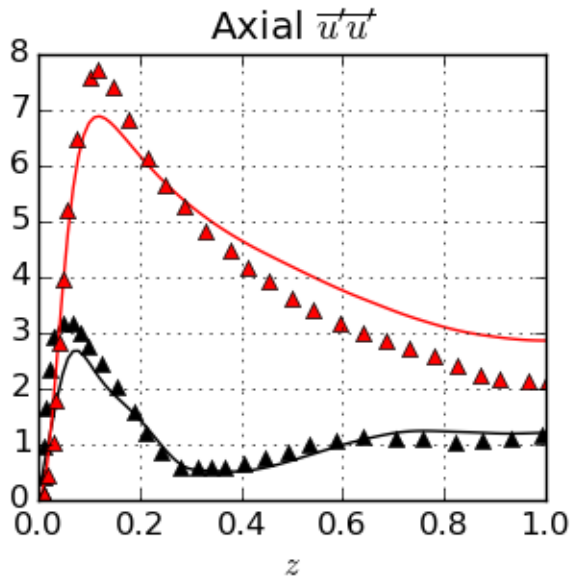
- On-the-fly computation of (xz)-plane (and time) average:
  - void fraction, pressures and velocities;
  - Correlations, interfacial area, mean curvature…

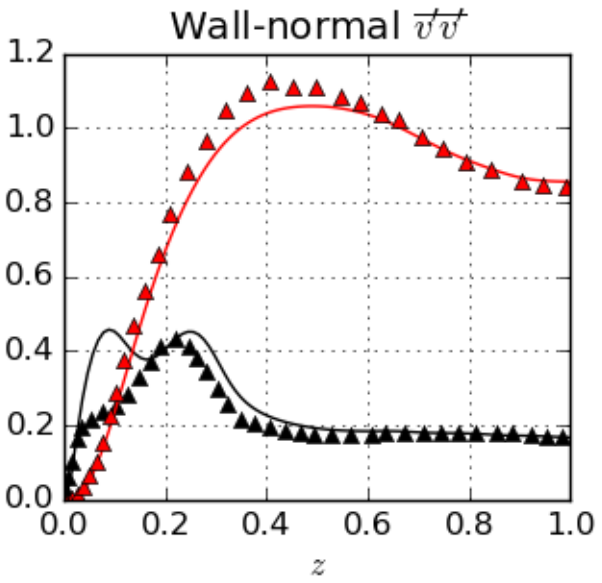
Averaged scale

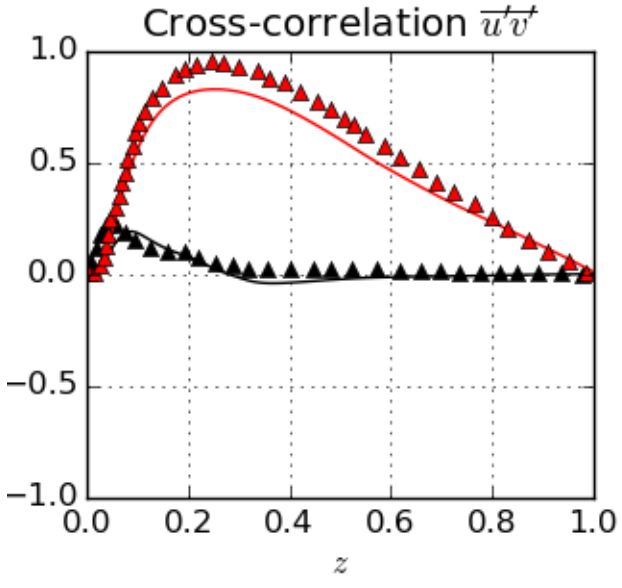
Code validation

- Very good agreements;
- Small discrepancies can reasonably be attributed to:
  - Higher statistical convergence of our results (longer time);
  - Small differences in lagrangian mesh management;
  - Discontinuous properties and sharp interfacial force treatment;
  - Uniform vs. non-uniform eulerian mesh.



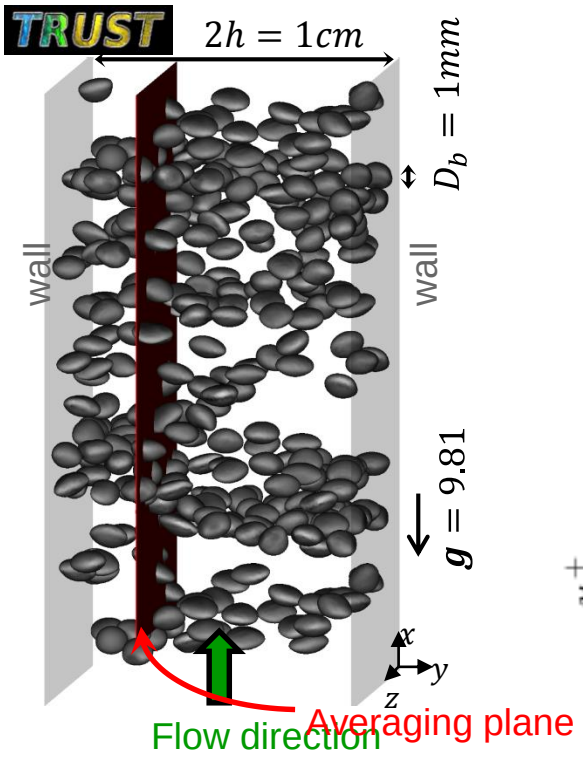




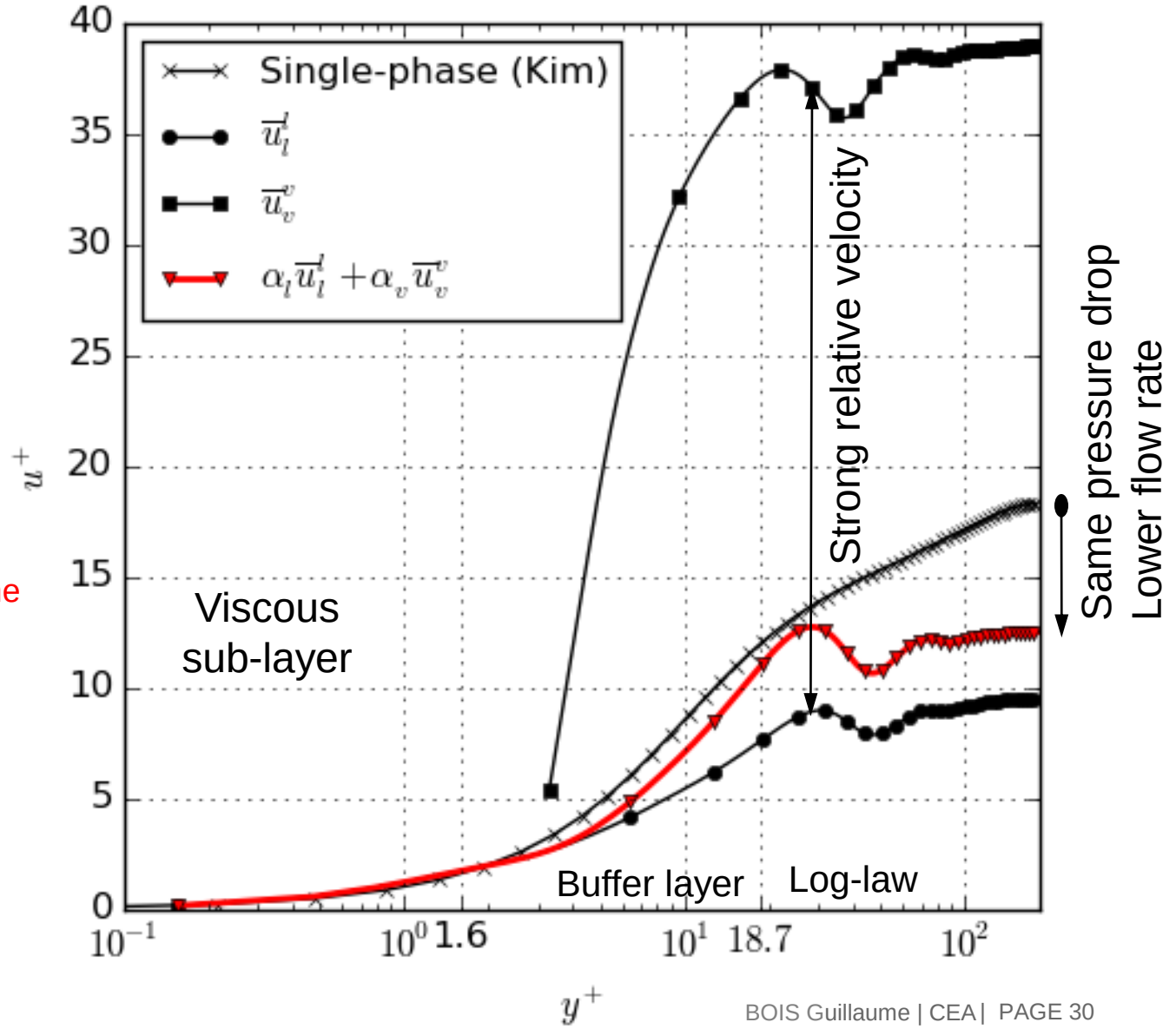


Averaged scale

Velocity profiles



WS155



Averaged scale

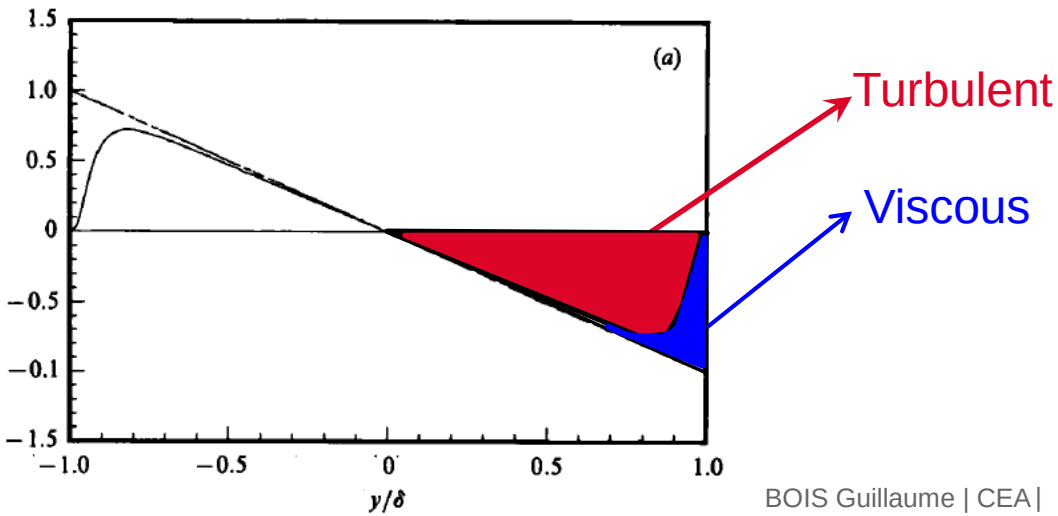
Mechanistic analysis: mixture budget for shear stress (1/2)

- In order to understand the global behavior of the flow, we take the average of the “one-fluid” formulation to assess the balance of forces in the channel;

- Integrating with respect to the wall-normal coordinate, we get the budget for shear-stress.
  - Streamwise:
  $$-\overline{\rho uv} + \overline{\mu \frac{\partial u}{\partial y}} + \int_0^y \overline{\sigma \kappa n_{xv} \delta^i} dy' + \Delta \rho g \int_0^y (\langle \alpha \rangle - \alpha) dy' = \tau_{w0} \left(1 - \frac{y}{h}\right)$$
  - Wall-normal:
  $$-\overline{\rho vv} + \overline{\mu \frac{\partial v}{\partial y}} - \left(\bar{P} - \bar{P}^{wall}\right) + \int_0^y \overline{\sigma \kappa n_{yv} \delta^i} dy' = 0$$

- In incompressible single-phase flow, the streamwise budget for shear-stress simply reduce to the simplified equilibrium between turbulent and laminar shear:

$$-\overline{\rho uv} + \overline{\mu \frac{\partial u}{\partial y}} = \tau_{w0} \left(1 - \frac{y}{h}\right)$$

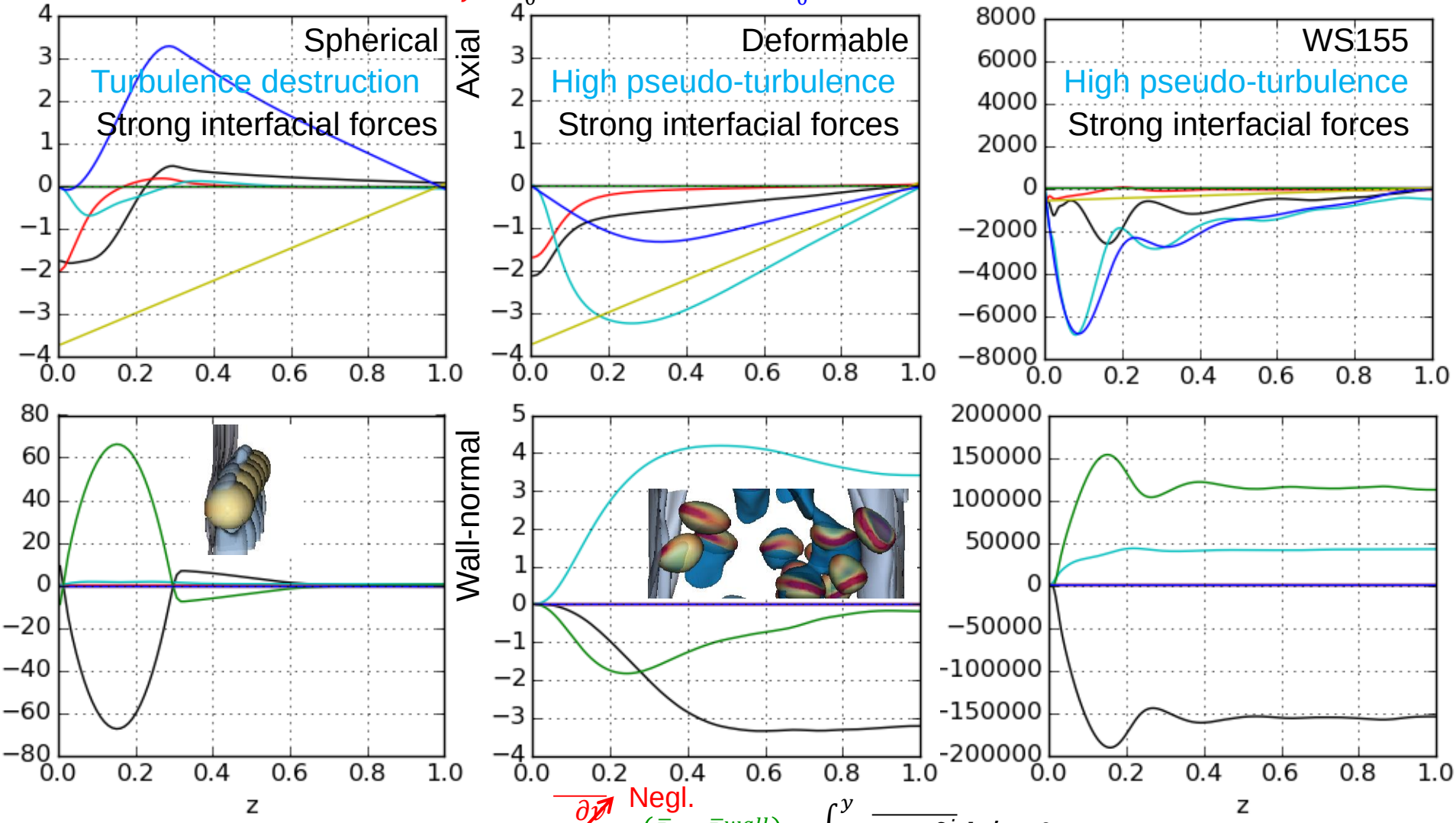


J. Kim, P. Moin, and R. Moser,
J. Fluid Mech. **177**, 133–166 (1987).

Averaged scale

Mechanistic analysis: mixture budget for shear stress (2/2)

$$-\overline{\rho uv} + \overline{\mu \frac{\partial u}{\partial y}} + \int_0^y \overline{\sigma \kappa n_{xv} \delta^i} dy' + \Delta \rho g \int_0^y (\langle \alpha \rangle - \alpha) dy' = \tau_{w0}\left(1 - \frac{y}{h}\right)$$



$$-\overline{\rho vv} + \overline{\mu \frac{\partial v}{\partial y}} - \left(\bar{P} - \bar{P}^{wall}\right) + \int_0^y \overline{\sigma \kappa n_{yv} \delta^i} dy' = 0$$

Negl.

Two-fluid model

Formulation (averaged description) (1/2)

$$\frac{\partial \rho_k \boldsymbol{u}_k}{\partial t} + \nabla \cdot (\rho_k \boldsymbol{u}_k \boldsymbol{u}_k) = -\nabla p_k + \rho_k \boldsymbol{g} + \nabla \cdot \boldsymbol{\tau}_k \text{ with } \boldsymbol{\tau}_k \widehat{=} \mu_k (\nabla \boldsymbol{u}_k + \nabla^T \boldsymbol{u}_k)$$

$\times \chi_k$
+ averaging

Momentum interfacial transfer defined from local fields: $\boldsymbol{M}_l = \boldsymbol{M}_l(\chi, u, p)$

$$\frac{\partial \alpha_k \rho_k \overline{\boldsymbol{u}}_k^k}{\partial t} + \nabla \cdot \left[\alpha_k \rho_k \left(\overline{\boldsymbol{u}}_k^k \overline{\boldsymbol{u}}_k^k + \boldsymbol{R}_{ij}^k\right)\right] = -\nabla\left(\alpha_k \bar{p}_k^k\right) + \alpha_k \rho_k \boldsymbol{g} + \nabla \cdot \left[\alpha_k \bar{\boldsymbol{\tau}}_k^k\right] - \overline{(p_k \boldsymbol{n_k} - \boldsymbol{\tau}_k \cdot \boldsymbol{n}_k) \cdot \nabla \chi_k}$$

Correlation between fluctuations, Reynolds stresses : $\boldsymbol{R}_{ij}^k = \overline{u_i' u_j'}^k$

- "Two-fluid" fields: $\overline{\phi_k}^k \widehat{=} \frac{\overline{\chi_k \phi_k}}{\overline{\chi_k}}$ (weighted average by the phase indicator)
- Void fraction: $\alpha_v = \overline{\chi_v}$
- Fluctuating velocities : $\boldsymbol{u}_k' = \boldsymbol{u}_k - \overline{\boldsymbol{u}}_k^k$

- Constitutive equations on $\boldsymbol{R}_{ij}^k$ and $\boldsymbol{M}_k$ are required to close the system.

- One-fluid versus two-fluid

- One-fluid formulation:
  - Interface tracking method : discontinuous fields;
  - Description of interfacial transfers.
- Two-fluid formulation:
  - RANS models : "interpenetrating media" approach, local coexistence of both phases;
  - Modelling non-linearities: turbulence and interfacial transfer (Generalized drag force).

Two-fluid model

Formulation (averaged description) (2/2)

- $\bar{u}^l$ and $\bar{u}^v$ are solved by two coupled averaged momentum equations (for each $k = \{l, v\}$):
  - Exact: (liquid) $\frac{\partial \rho_l \alpha_l \bar{\boldsymbol{u}}^l}{\partial t} + \text{conv/diff} - \alpha_l \rho_l \boldsymbol{g} = -\alpha_l \nabla \bar{p}^l + \bar{p}^l \nabla \alpha_l + \boldsymbol{M}_l - \nabla \cdot \left(\alpha_l \rho_l \boldsymbol{R}_{ij}^l\right)$
  - Approx.: $\approx -\alpha_l \nabla \bar{p}^l + \left(\bar{p}^l - \bar{p}_{li}^l\right) \nabla \alpha_l + \boldsymbol{I}_{l/v} - \nabla \cdot \left(\alpha_l \rho_l \widetilde{\boldsymbol{R}}_{ij}^l\right)$

Momentum interfacial transfer defined from local fields: $\boldsymbol{M}_l = \boldsymbol{M}_l(\chi, u, p)$

Liquid Reynolds stresses : $\boldsymbol{R}_{ij}^l = \overline{u_i' u_j'}^l$

Exacts

Neglected

Solution of approx. PDEs: $\left(\widetilde{\boldsymbol{R}}_{ij}^l, \varepsilon\right)$

Algebraic relations:
$I_{l/v}$ is a model for: $\boldsymbol{M}_{il} = \bar{p}^l \nabla \alpha_l + \boldsymbol{M}_l$
$\boldsymbol{M}_{il}$: Generalized drag force
(drag, lift, wall lubrication, turbulent dispersion)

- 2 closure relations required (3 if pressure differences are considered).
- Focus on interfacial transfer (dominant, at least in our cases).
- Standard assumption of the one-pressure two-fluid model:
  - Surface tension effects are neglected;
  - Single pressure hypothesis.

⇒ Full transmission of momentum from liquid to vapor (locally and instantaneously):

$$\boldsymbol{M}_{il} + \boldsymbol{M}_{iv} = \boldsymbol{M}_\sigma + \left(\bar{p}_l^l - \bar{p}_v^v\right) \nabla \alpha_l \approx 0$$

Two-fluid model

Closure relations (interfacial momentum transfer)

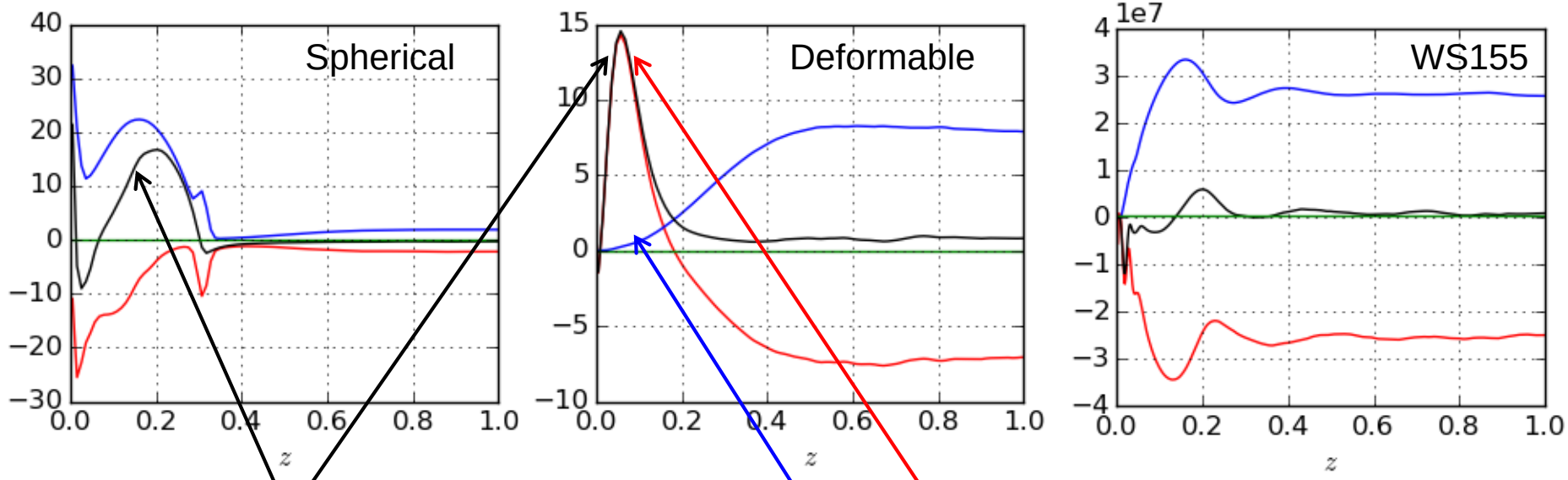
- Standard assumption of the one-pressure two-fluid model:

  ⇒ Full transmission of momentum from liquid to vapor:

$$\boldsymbol{M}_{il} + \boldsymbol{M}_{iv} = \boldsymbol{M}_{\sigma} + \left(\bar{p}_l^l - \bar{p}_v^v\right)\nabla\alpha_l \approx 0 \quad \text{with} \quad \boldsymbol{M}_{ik} = \boldsymbol{M}_k + \bar{p}_k^k \nabla\alpha_k$$

- From the local point-of-view…

$$\underbrace{\frac{\partial \alpha_k \rho_k \bar{\boldsymbol{u}}_k^k}{\partial t} + \nabla\cdot\left[\alpha_k\rho_k\left(\bar{\boldsymbol{u}}_k^k\bar{\boldsymbol{u}}_k^k + \boldsymbol{R}_{ij}^k\right)\right] + \nabla\left(\alpha_k\bar{p}_k^k\right) - \alpha_k\rho_k\boldsymbol{g} - \nabla\cdot\left[\alpha_k\bar{\boldsymbol{\tau}}_k^k\right]}_{\text{Computed from DNS for } k\in\{l,v\}} = \underbrace{-\overline{\left(p_k\boldsymbol{n_k} - \boldsymbol{\tau}_k\cdot\boldsymbol{n}_k\right)\cdot\nabla\chi_k}}_{\boldsymbol{M_k} \text{ deduced from balance}}$$



- Streamwise: $M_{\sigma x}$ is important near the wall where $M_{ivx} \neq -M_{ilx}$ ($\left(\bar{p}_l^l - \bar{p}_v^v\right)\nabla\alpha_l$=0);
- Wall-normal: $M_{\sigma y}$ is the highest followed by M_{ivy} (spherical: $M_{ily} \approx 0$; deformable: $M_{ivy} \approx M_{ily} \approx 0.5\, M_{\sigma y}$ and $\left(\bar{p}_l^l - \bar{p}_v^v\right)\nabla\alpha_l$ negligible)

⇒ Assumption discarded by DNS results: improved modeling of surface tension required

Two-fluid model

Closure relations (interfacial momentum transfer)

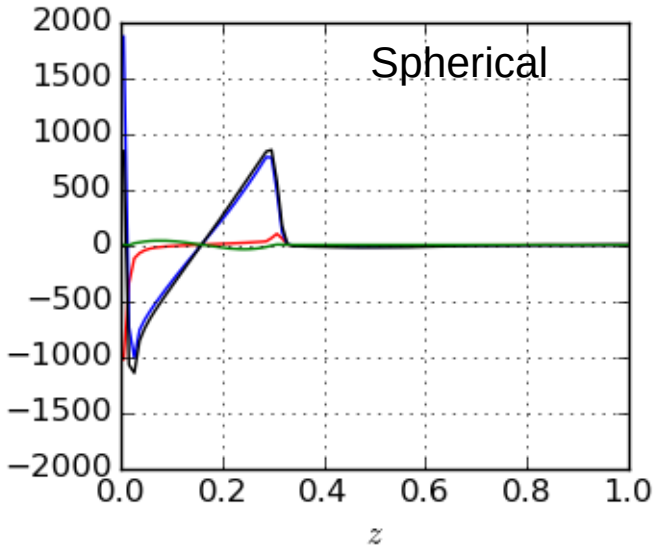
- Standard assumption of the one-pressure two-fluid model:

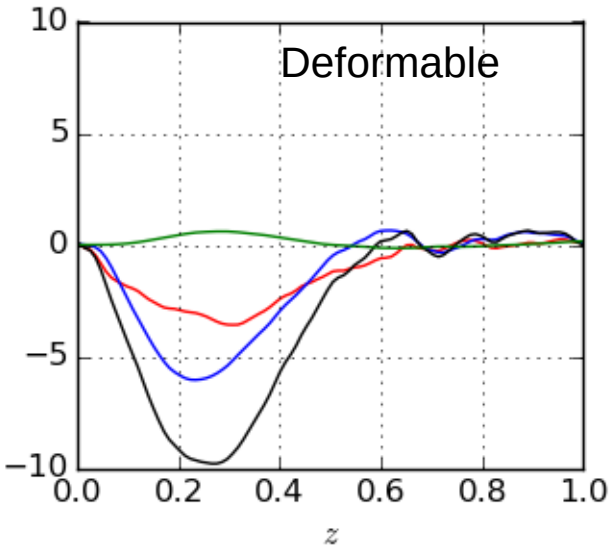
  ⇒ Full transmission of momentum from liquid to vapor:

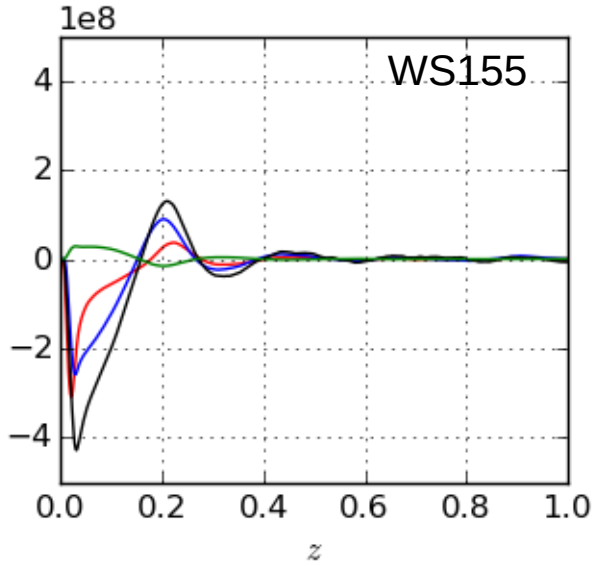
$$\boldsymbol{M}_{il} + \boldsymbol{M}_{iv} = \boldsymbol{M}_{\sigma} + \left(\bar{p}_l^l - \bar{p}_v^v\right)\nabla\alpha_l \approx 0 \quad \text{with} \quad \boldsymbol{M}_{ik} = \boldsymbol{M}_k + \bar{p}_k^k \nabla\alpha_k$$

- From the local point-of-view…

$$\underbrace{\frac{\partial \alpha_k \rho_k \bar{\boldsymbol{u}}_k^k}{\partial t} + \nabla\cdot\left[\alpha_k\rho_k\left(\bar{\boldsymbol{u}}_k^k\bar{\boldsymbol{u}}_k^k + \boldsymbol{R}_{ij}^k\right)\right] + \nabla\left(\alpha_k\bar{p}_k^k\right) - \alpha_k\rho_k\boldsymbol{g} - \nabla\cdot\left[\alpha_k\bar{\boldsymbol{\tau}}_k^k\right]}_{\text{Computed from DNS for } k\in\{l,v\}} = \underbrace{-\overline{\left(p_k\boldsymbol{n_k} - \boldsymbol{\tau}_k\cdot\boldsymbol{n}_k\right)\cdot\nabla\chi_k}}_{\boldsymbol{M_k} \text{ deduced from balance}}$$







- Streamwise: $M_{\sigma x}$ is important near the wall where $M_{ivx} \neq -M_{ilx}$ ($\left(\bar{p}_l^l - \bar{p}_v^v\right)\nabla\alpha_l$=0);
- Wall-normal: $M_{\sigma y}$ is the highest followed by M_{ivy} (spherical: $M_{ily} \approx 0$; deformable: $M_{ivy} \approx M_{ily} \approx 0.5\, M_{\sigma y}$ and $\left(\bar{p}_l^l - \bar{p}_v^v\right)\nabla\alpha_l$ negligible)

⇒ Assumption discarded by DNS results: improved modeling of surface tension required

Conclusion & Prospects

Conclusion

- Validation of code capabilities by a benchmark with the renown work of Lu & Tryggvason.
- DNS of bubbly flow in conditions close to reactor core was achieved;
- Upscaling process to 2-phase RANS CFD model;
- Main findings:
  - Dominant role of the interfacial forces on the flow (models for momentum transfers) over turbulence closure;
  - Some basic assumptions questioned:
    - Surface tension and pressure jump are assumed negligible;
    - A new model seems necessary;

Prospects

- Look for means of introducing surface tension (and pressure difference) in averaged descriptions (a sort of macroscopic Young-Laplace equation and a transport equation);
- Evaluate the impact of modified models on averaged to 2-phase RANS CFD calculations.

- Other flow conditions (parametric studies on Reynolds number, void fraction and bubble size);
- Heavy computational resources required ⇒ work on LES modeling and its validation;

  ISS : Interfaces and Subgrid Scales model,

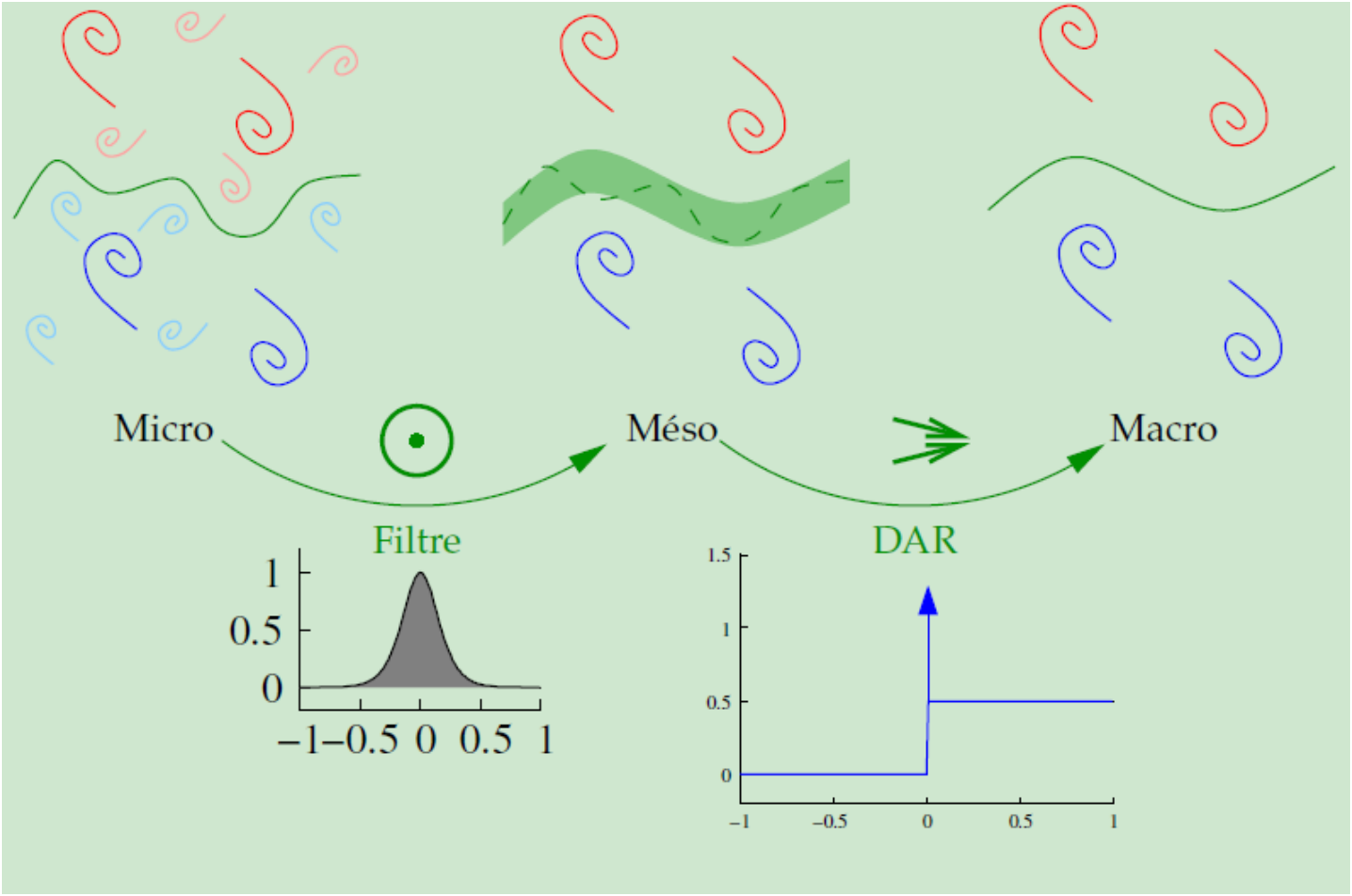
  A. Toutant et al., International Journal of Multiphase Flow 35 (2009) 1100–1118

Prospects

Interfaces and Sub-grid Scale modeling

- DNS is too expensive to be used in parametric studies or at high Reynolds numbers;
- Single-phase LES has been very useful but what should be done close to interfaces?

⇨ Interfaces and Subgrid Scale modeling (ISS, Toutant 2006, Bois 2011)



Acknowledgments

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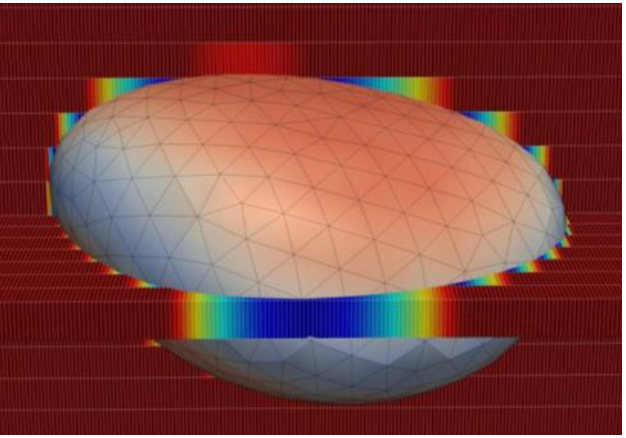
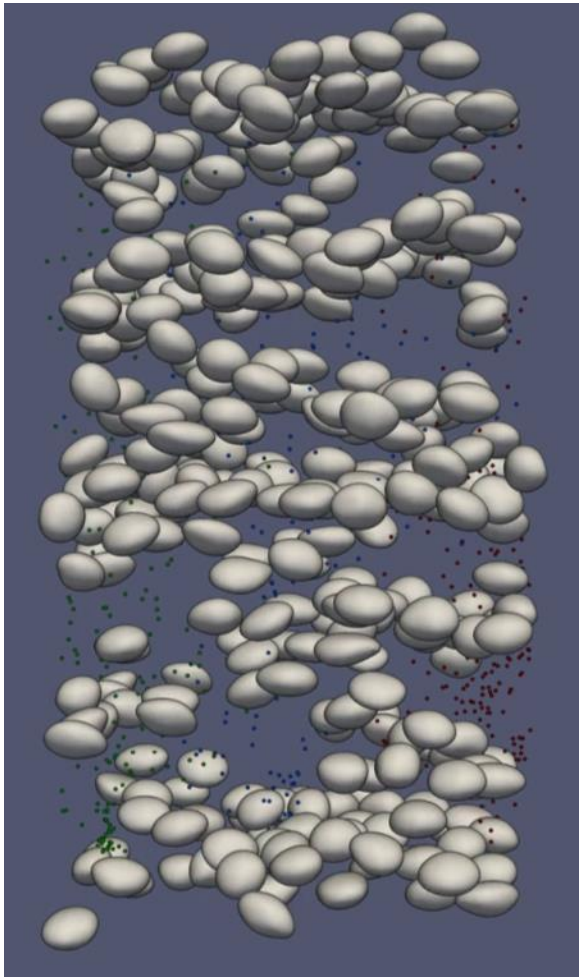
- This work was granted access to the HPC resources of TGCC under the allocations 20XX-20142b7239 and x20162b7712 made by GENCI.

Questions?

Thank you for your attention
Questions?



- 85 Mons hexahedral elements
- Total of 456 000 h.CPU
- 33 runs of 24 hours
  on 576 processors
  on the Curie supercomputer
- Grant GENCI :
  20XX- t20142b7239
  x20162b7712



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