"Micro-Macro Modelling and Simulation of Liquid-Vapour Flows"
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A MESH-ADAPTATIVE VARIATIONAL LEVEL SET

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(***)INRIA-Rocquencourt, (****)INRIA-Sophia and Lemma

Advection models for an interface

Characteristic function: $\chi = 0 \ or \ 1$, interface: $\Gamma = \partial\{\chi = 1\}$

$\chi(x, t = 0) = \chi_0(x)$

$\chi_t + \mathbf{V} \cdot \nabla\chi = 0$

$\chi_t + \nabla \cdot (\mathbf{V}\chi) = 0 \qquad (div\mathbf{V} = 0)$

Case 1: $\mathbf{V}$ is C^1: strong solution in the sense of characteristics, deformation, no break up, filaments,

Case 2: $\mathbf{V}$ is not C^1 , but typically piecewise C^1 and globally H^1: weak solution, $\chi = 0 \ or \ 1$, break up can occur,

Case 3: $\mathbf{V}$ is a distribution, the discontinuity can be diffused.

Numerical advection of a discontinuous function

We concentrate on Eulerian discretisations: what accuracy is attainable?

- A long story from first-order linear (Harten-Hyman-Lax) to TVD/ENO: all of them seem of low accuracy on discontinuities.
- However, using adhoc post-processing, even spectral accuracy can be obtained for some "smooth" discontinuity (D.Gottlieb).
- "Non-smooth" interfaces can be addressed by mesh adaptation.

Plan of the talk:

1. Eulerian approximation of interface advection
2. Mesh-adaptative strategies

1. Eulerian approximation of interface advection

Method 1: Solve with a dissipative discontinuity-capturing scheme:

$$\chi_t + \nabla \cdot (\mathbf{V}\chi) = O(\Delta x)\nabla \cdot (\nabla \chi) + ...$$

Numerical discontinuity width increases and L^1-error is $O(\Delta x^{1/2})$ after a given time, according to the spatial scale of the dissipative term. We can equivalently use the standard width estimate $O(n^{1/2})\Delta x$ where n, number of time steps equals $K\Delta x^{-1}$.

Method 2: Solve with a compressive discontinuity-capturing scheme. For example with FCT, or with ACM. Numerical discontinuity remains in a bounded number of cell width in each side of discontinuity. Discontinuity width and L^1-error remains $O(\Delta x)$.

Method 3: Solve with a Level Set method.

Level Set

$\phi(x, t = 0) = \phi_0(x) \quad , \quad \phi_0 \quad smooth, \quad H(\phi_0) = \chi_0$

$\phi_t + \nabla \cdot (\mathbf{V}\phi) = 0$

$\chi = H(\phi)$

- choose a high-order approximation,

- decide if ϕ's interpolation is continuous.
So would be the interface approximation.

Our choice: P_1 = continuous, piecewise linear ϕ.
Galerkin+ adapted dissipation, third-order on cartesian mesh.

Accuracy analysis of Level Set

Case 1: Smooth velocity,
+ smooth interface
+ small time interval:
+ order $\mathbf{k}$ L^∞-convergence of ϕ-advection scheme:

$$\Rightarrow \quad |H(\phi_h) - H(\phi)|_{L^1} \quad \leq \quad \mathbf{k}$$

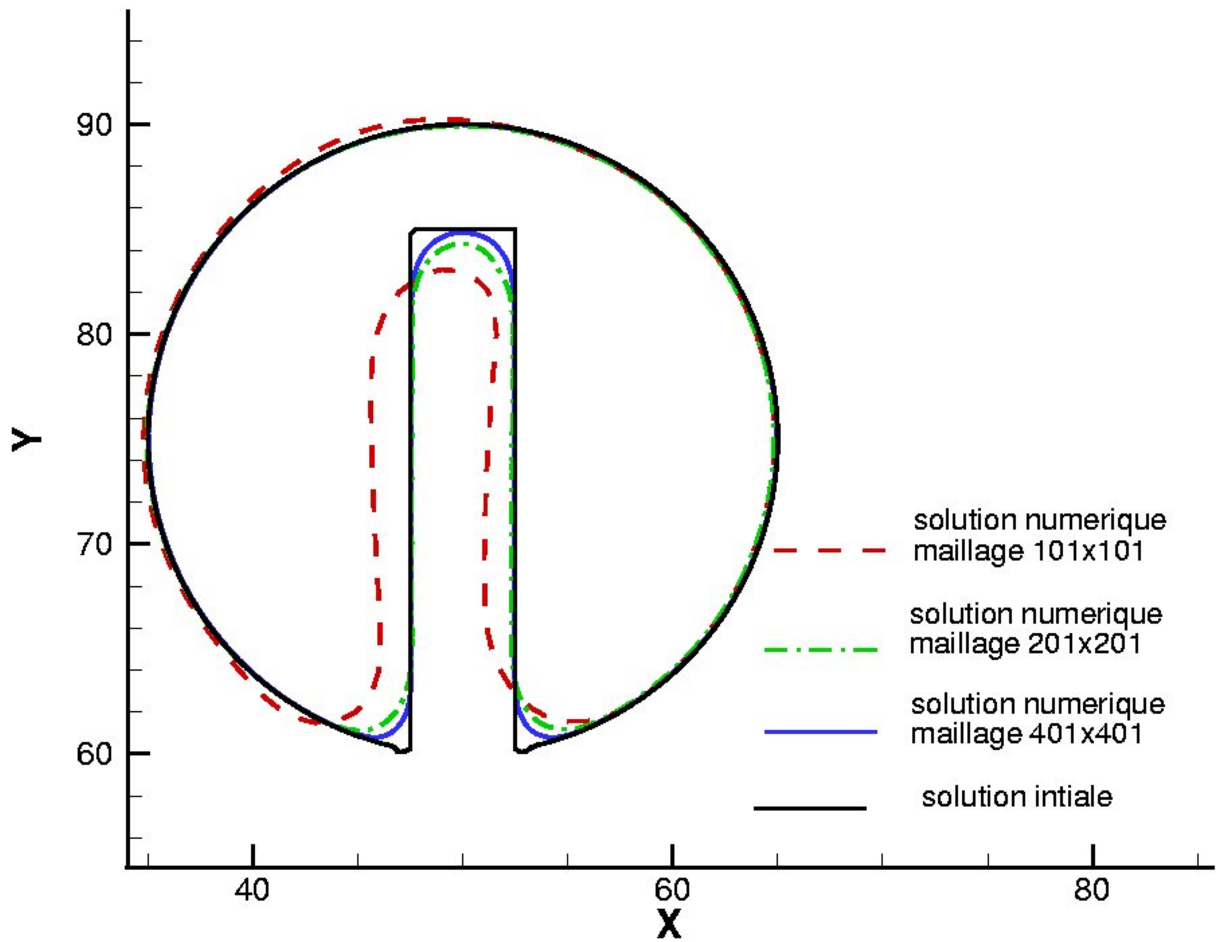
same order $\mathbf{k}$ for $H(\phi)$ as for ϕ

Case 2: Order $\mathbf{k}$ L^p-convergence of ϕ-advection scheme:

$$\Rightarrow \quad |H(\phi_h) - H(\phi)|_{L^1} \quad \leq \quad \mathbf{2k/3}$$

However: Too-small scales may arise ($\Rightarrow$ "order one"):
- discontinuity of normal to interface,
- small filaments/veils,
- break up.

Accuracy benchmark for primal Level Set



Accuracy of primal Level Set

- Disk: $(u,v) = \frac{\pi}{314}(50 - y, x - 50) \quad \phi_0 = ((x-50)^2 + (y-75)^2)^{1/2} - 10$ on $[0, 100]^2$
- Zalesak's notched disk.

Mesh/case	$H(\phi)$: Rel. L_1 error	$H(\phi)$: Numerical order
101x101/disk	99. 10^{-5}	-
201x201/disk	11. 10^{-5}	3.06
401x401/disk	1.5 10^{-5}	2.96
101x101/notched disk	0.158	-
201x201/notched disk	0.0418	1.94
401x401/notched disk	0.0203	1.04

The conservation issue

Assuming $\nabla \cdot \mathbf{V} = 0$ in Ω , $\mathbf{V} = 0$ on $\partial\Omega$, the "total mass"

$$M_{liquid} \; = \; \int_\Omega H(\phi_h) \; d\Omega$$

should be constant.

The advection of ϕ does not give this, neither ϕ reinitialisations applied for avoiding small and large gradients for ϕ.

Global mass correction, replacing ϕ by $\phi + \epsilon$ such that total mass is kept constant

$$\int_\Omega H(\phi_h^{n+1} + \epsilon) + \; d\Omega \;\; = \;\; \int_\Omega H(\phi_h^n) \; d\Omega$$

is useful but not satisfactory.

Dual Level Set

Find $\widehat{\phi}_h \in P_1$ such that:

$$\begin{aligned}&\forall \psi_i \in P_1, \\ &\int_\Omega \psi_i (H(\widehat{\phi}_h))_t dv = \\ &\int_{\partial\Omega} \psi_i H(\widehat{\phi}_h) \mathbf{V} \cdot \mathbf{n} d\Gamma - \int_\Omega H(\widehat{\phi}_h) \mathbf{V} \cdot \nabla \psi_i dv \ (DLS)\end{aligned}$$

Assume that (DLS) holds for a series of cartesian meshes, then:
$\forall\ \psi$ smooth , $\int\int (H(\widehat{\phi}_h) - H(\phi))(-\psi_t - \mathbf{U} \cdot \nabla \psi) dv dt = \mathcal{O}(h^2)$

But in case of small scales, (DLS) has no solution.

A primal-dual level set

Find $\widehat{\phi}^{n+1}$ such that $\Psi_i(\widehat{\phi}^{n+1}) = 0 \quad \forall\ i$:

$$\Psi_i(\widehat{\phi}^{n+1}) = \int_\Omega \psi_i H(\widehat{\phi}^{n+1}) dv - b_i$$

$$b_i = \int_\Omega \psi_i H(\phi^n) dv + \Delta t \int_\Omega H(\phi^{n+\frac{1}{2}}) \mathbf{U} \cdot \nabla \psi_i dv - \Delta t \int_{\partial\Omega} \psi_i H(\phi^{n+\frac{1}{2}}) \mathbf{U} \cdot \mathbf{n} d\Gamma$$

Fixed point algorithm:

$$\widehat{\phi}^{(0)} = \phi^{n+1}$$
$$\widehat{\phi}_i^{(\alpha+1)} = \widehat{\phi}_i^{(\alpha)} - \theta^{(\alpha)} \Psi_i(\widehat{\phi}_i^{(\alpha)}) \quad \forall\ i,$$
$$\widehat{\phi}^{n+1} = \widehat{\phi}^{(\infty)}$$

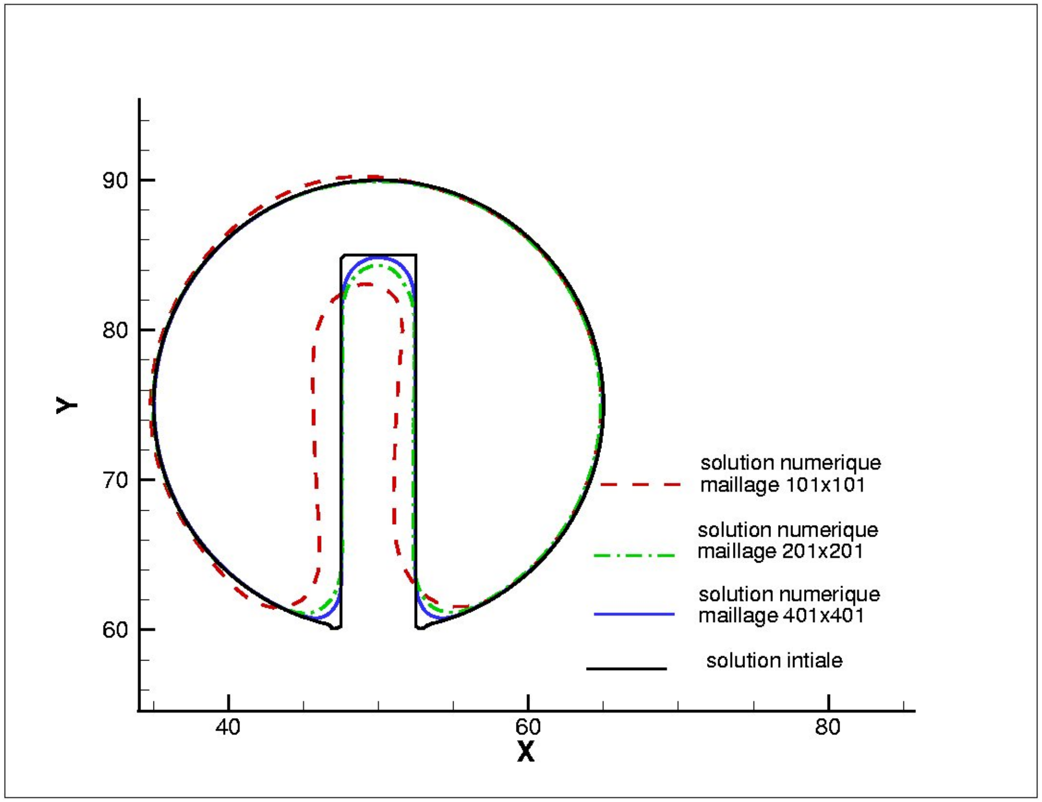
In practice: 1 iteration

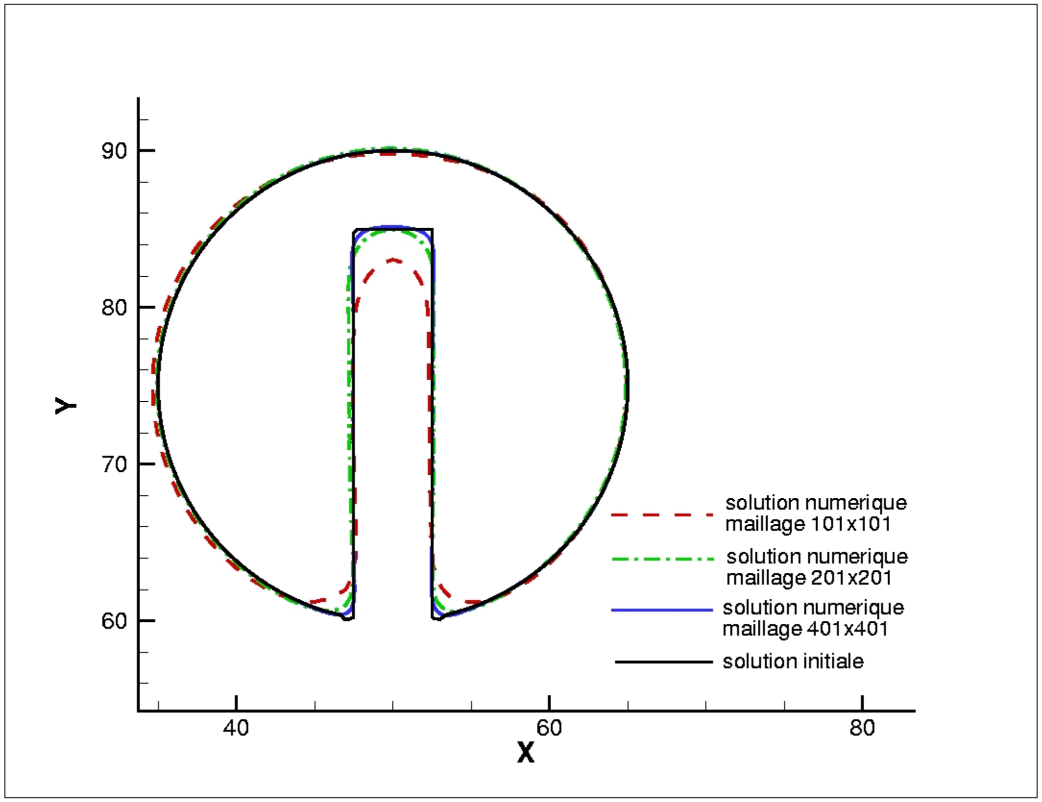
$$\theta^{(0)} : \quad \int_\Omega H(\widehat{\phi}^{(1)}) d\Omega = \int_\Omega H(\phi^n) d\Omega$$

found by a scalar Newton.

A primal-dual level set (2)

- Second-order accurate on smooth disk test case,
- still first-order accurate on notched disk test case,
- error is ten times smaller than without local correction on 401x401 notched disk test case





Coupling within non-homogeneous Navier-Stokes

$\phi,\ \mathbf{U},\ p\ :\ P_1$ approximations

1. Advect ϕ with $\tilde{\mathbf{U}}^n$. $\phi^{n+1} \mapsto \rho^{n+1},\ \mu^{n+1},\ \kappa^{n+1}(*)$

2. Predict velocity: $\bar{\mathbf{U}}^{n+1} = \mathbf{U}^n + \Delta t\ h(\mathbf{U}^n, \phi^{n+1})$

$$h(\mathbf{U}^n, \phi^{n+1}) = -\nabla \cdot (\mathbf{U}^n \times \mathbf{U}^n) + \frac{\mu(\phi^{n+1})\nabla \mathbf{U}^n}{\rho(\phi^{n+1})} + \mathbf{g} - \sigma\kappa(\phi^{n+1})\nabla H(\phi^{n+1})$$

3. Solve pressure equation:

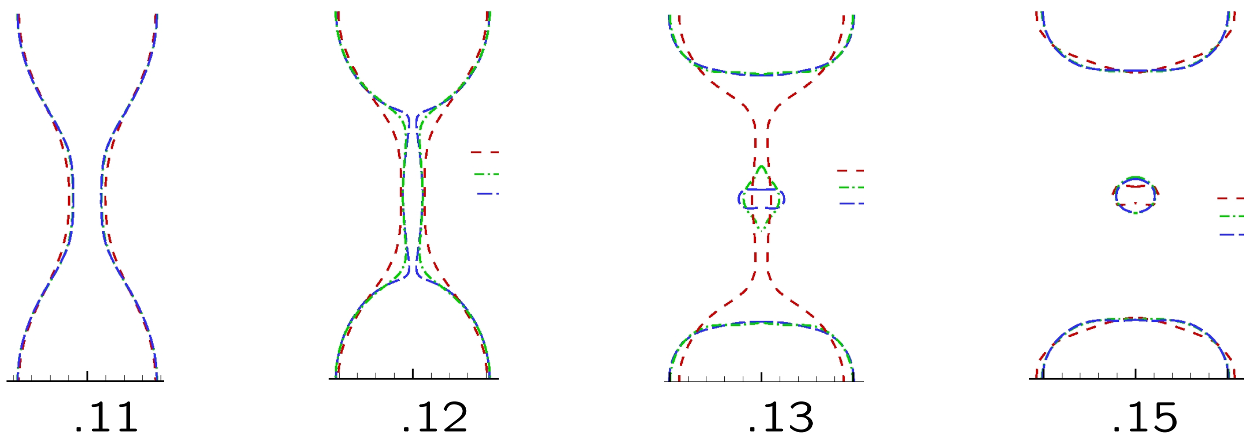
$$\nabla.(\frac{1}{\rho(\phi^{n+1})}\nabla p^{n+1}) = \nabla \cdot (\frac{\bar{\mathbf{U}}^{n+1}}{\Delta t})$$

4. Correct velocity:

$$\mathbf{U}^{n+1} = \bar{\mathbf{U}}^{n+1} - \frac{\Delta t}{\rho(\phi^{n+1})}(\mathcal{P}_{P_0 \mapsto P_1}\nabla p^{n+1})$$
$$\tilde{\mathbf{U}}^n = \mathcal{P}_{P_1 \mapsto P_0}\mathbf{U}^{n-1} + (\mathcal{P}_{P_1 \mapsto P_0}\frac{1}{\rho})\nabla p^n$$

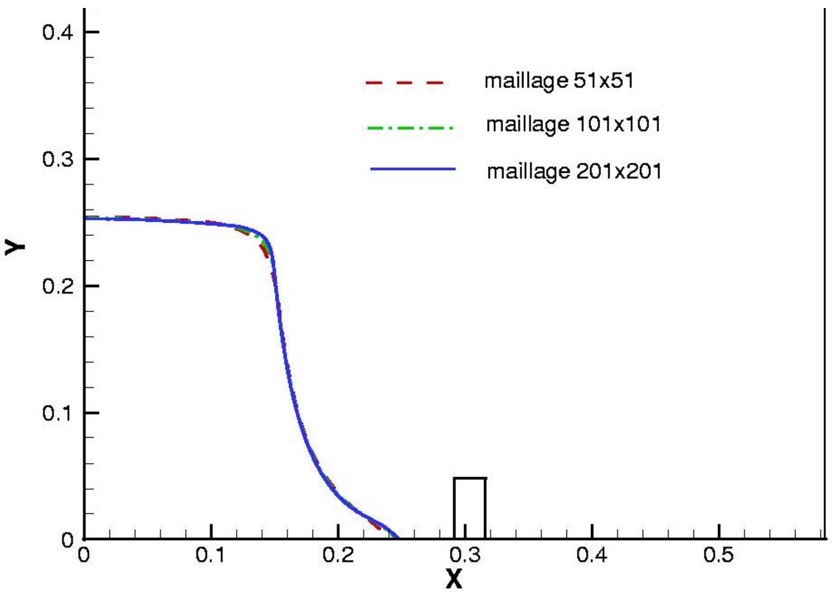
(*) Interface thickening on $3\Delta x$

A first example: Rayleigh capillary instability



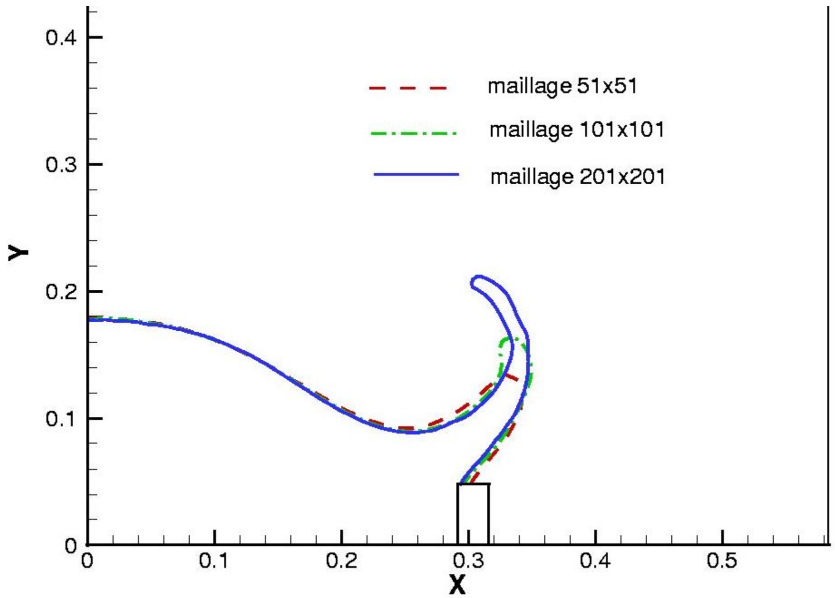
Physical time(s.)	number of nodes	L_1 norm of $\delta H(\phi)$
0.11	902	-
0.11	3402	$2.45461.10^{-6}$
0.11	13202	$3.23397.10^{-7}$
0.11	Numerical order	2.92
0.12	902	-
0.12	3402	$5.515.10^{-6}$
0.12	13202	$1.520.10^{-6}$
0.12	Numerical order	**1.86**
0.13	902	-
0.13	3402	$1.38947.10^{-5}$
0.13	13202	$2.236.10^{-6}$
0.13	Numerical order	2.63

A second example: falling water column

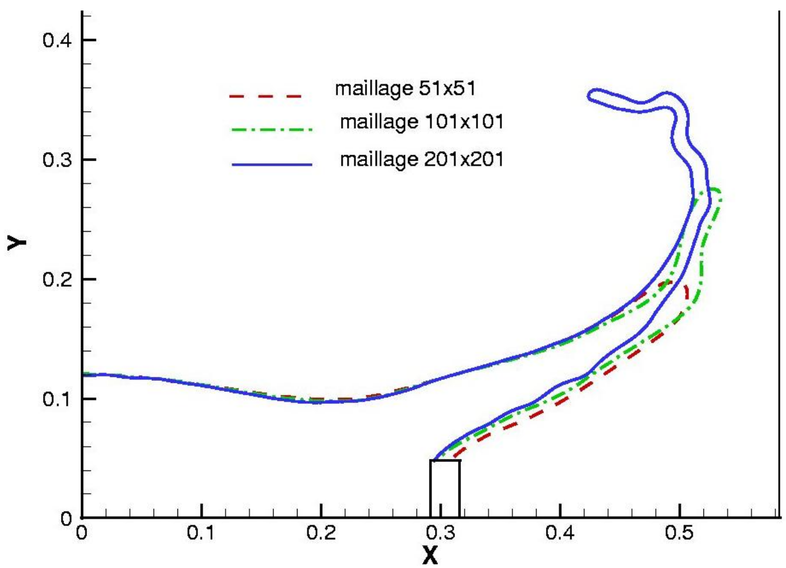


Computations / exp. Koshizuka

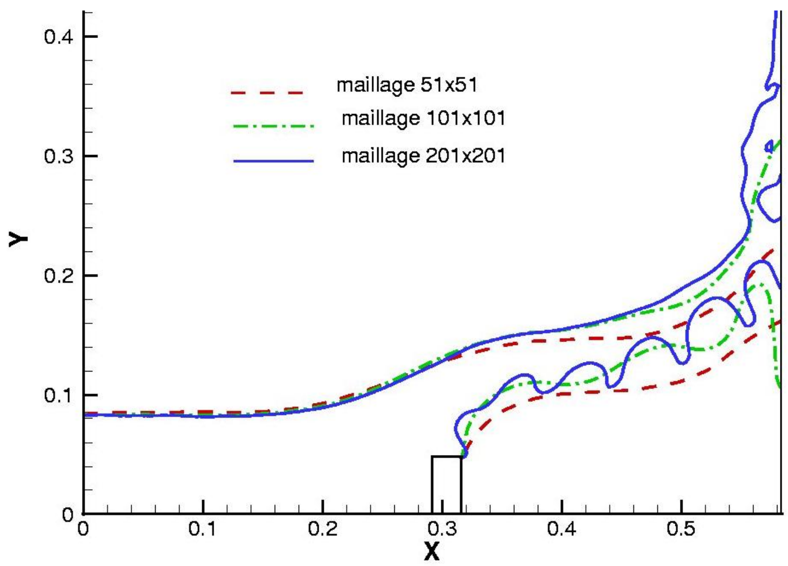
Falling water column (2)

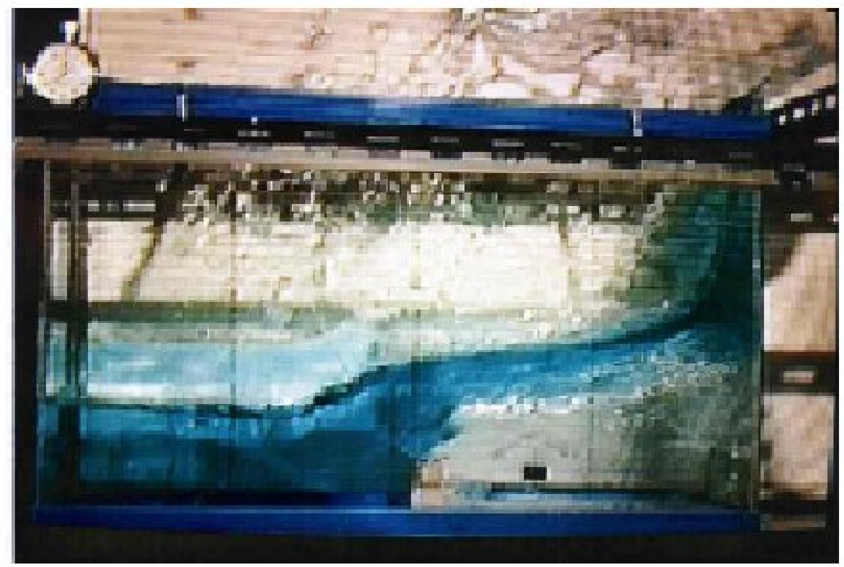


Falling water column (3)

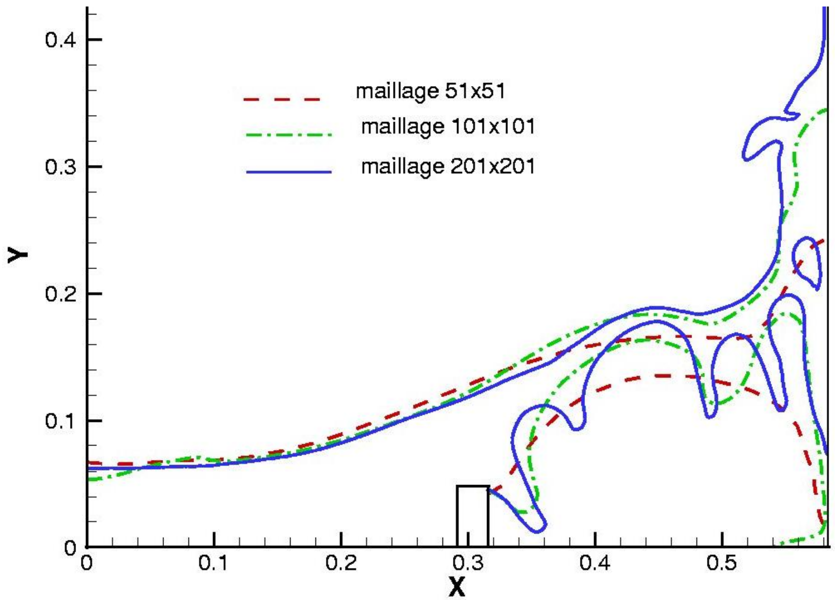


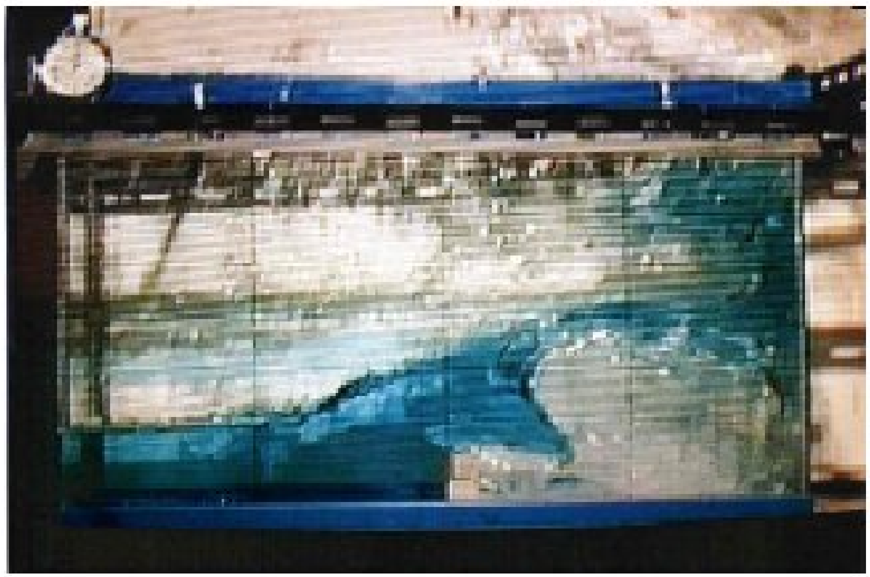
Falling water column (4)





Falling water column (5)





Orientation

Mesh Conv. (uniform reft.)	L^2 Order of Conv.
Shock Cap. Dissip.	1/2
Shock Cap. Compress.	1
Level Set, smooth interface	2+

The Level Set Method is able to master with high-order accuracy all medium scale events of an interface advection.

In the case of a coupled two-fluid model, both
- large-scale instabilities and
- small scales may arise.

The sequel of this talk adresses small-scale approximation:
- small scales in interface representation,
- small scales in velocity.

2. Mesh-adaptative strategies

Purpose: The arising of small scales decrease the numerical convergence and them the efficiency. Mesh adaptation is *expected* to avoid a part of these efficiency loss.

How do we build our expectations?

Which adaptation algorithm can answer to them?

Is it enough to combine discontinuity capturing and mesh adaptation?

Main efficiency evaluator:
Global convergence order α with respect to **number of nodes** N:

$$|u - u_h|_D \quad \leq \quad K \quad N^{-\alpha/d} \qquad\qquad in \quad R^d$$

Steady: D is computational domain N is mesh node number .

Unsteady: D is *space-time* computational domain. Complexity parameter N is chosen as the mean/maximal spatial mesh node number.

Barrier analysis

Sup bounds for mesh convergence can be deduced (*) from:

- the type of adapted mesh chosen,

- the type of singularity arising.

Mesh adaptation mode: Geometrical context	Isotropic	Anisotropic
Unsteady discontinuity 2D	≤ 1	2
Unsteady capillary breaking 2D	≤ 2	2
Unsteady discontinuity 3D	$\leq 3/4$	2
Unsteady capillary breaking 3D	≤ 2	2

Convergence order α in L^2 for a discontinuous function

(*) steady case: Coudière-Dervieux-Leservoisier-Palmerio, INRIA-RR-4528 2002

Mesh-adaptation, stationary

L^2-optimal metric:

$$\mathcal{M}_{x,y} = \mathcal{R}_{\mathcal{M}}^{-1} \begin{pmatrix} (m_\xi)^{-2} & 0 \\ 0 & (m_\eta)^{-2} \end{pmatrix} \mathcal{R}_{\mathcal{M}}$$

Tranforms any edge of the specified class of mesh into an edge with **unit length**.

$$\mathcal{R}_{\mathcal{M}} \;=\; \mathcal{R}_u \;,\; \mathcal{H}_u = \begin{pmatrix} \frac{\partial^2 u}{\partial x^2} & \frac{\partial^2 u}{\partial x.\partial y} \\ \frac{\partial^2 u}{\partial x.\partial y} & \frac{\partial^2 u}{\partial y^2} \end{pmatrix} = \mathcal{R}_u * \begin{pmatrix} \frac{\partial^2 u}{\partial \xi^2} & 0 \\ 0 & \frac{\partial^2 u}{\partial \eta^2} \end{pmatrix} * \mathcal{R}_u{}^{-1}$$

$$\min_{\mathcal{M}} \int \left(|\frac{\partial^2 u}{\partial \xi^2}|.m_\xi^2 + |\frac{\partial^2 u}{\partial \eta^2}|.m_\eta^2 \right)^2 \, dxdy \qquad \text{with} \int m_\xi{}^{-1} m_\eta{}^{-1} \, dxdy = N, \text{number of nodes.}$$

$$\mathcal{M}_{opt} = N \; C^{-1}(u) \; \mathcal{R}_u^{-1} \begin{pmatrix} |\frac{\partial^2 u}{\partial \eta^2}|^{-5/6} |\frac{\partial^2 u}{\partial \xi^2}|^{1/6} & 0 \\ 0 & |\frac{\partial^2 u}{\partial \xi^2}|^{-5/6} |\frac{\partial^2 u}{\partial \eta^2}|^{1/6} \end{pmatrix} \mathcal{R}_u$$

Fixed point:

- **Prescribe an N.**
- **(a) On current mesh “get u” and compute metric $\mathcal{M}_{opt}$ from u.**
- **(b) Generate a new mesh specified by $\mathcal{M}_{opt}$.**
- **Converge (a)-(b) remeshing process for N.**

Mesh-adaptation accuracy, stationary case

Method: / Mesh adaptation mode:	Isotropic	Anisotropic
Barrier analysis	$\leq$ 1	$\leq$ 2
Optimal Metric Num. exp. (interpolation of u) Heavyside 2D	1	2
Optimal Metric Num. exp. (Euler solution) NACA0012 Mach=1.2	1	2

Convergence order α in L^2 for a discontinuous function

Mesh-adaptation strategy, non-stationary

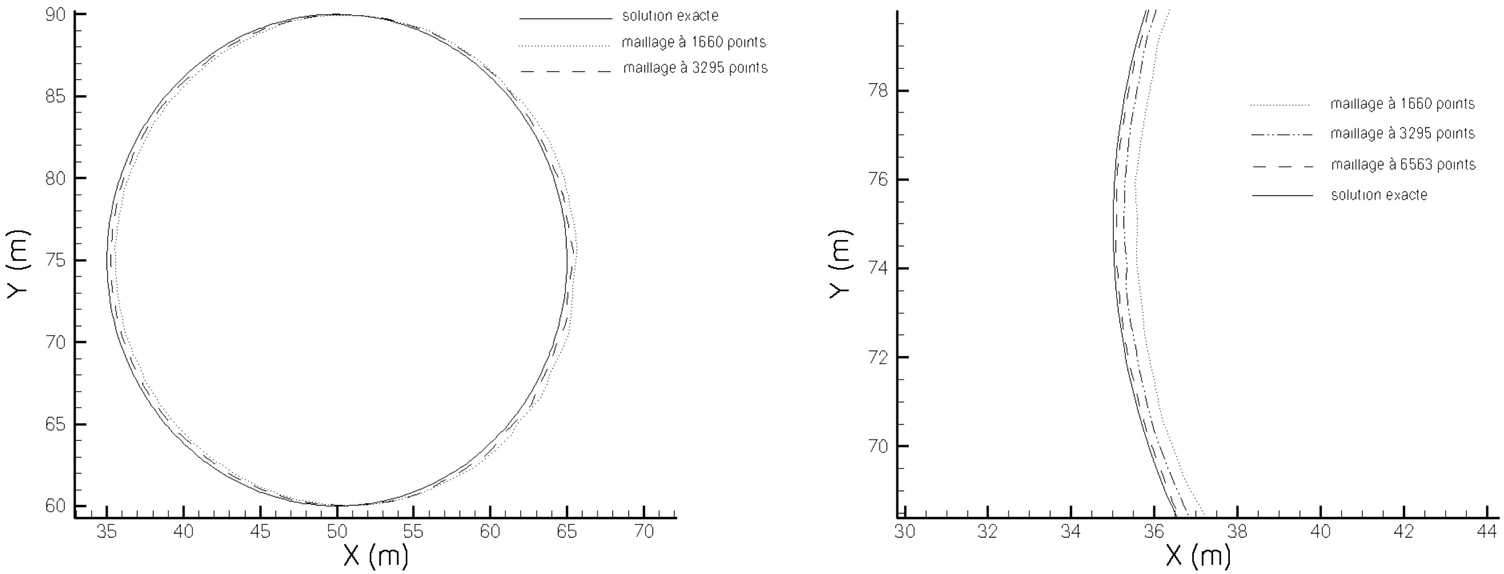
- Time advancing, with **adapted time step** Δt.
  Time step adaptation heuristics: CFL-based

- **Macro time-step** ΔT: time-interval between two remeshings.

- Inside a macro time-step ΔT: metric intersection between time-steps Δt's and **fixed-point** adaptation.
  (Alauzet-George-Mohammadi-Frey-Borouchaki, ECCOMAS2001

- Remeshing: solution interpolation accuracy is paramount.
  (Mehrenberger-Alauzet, canum2006.univ-rennes1.fr)

Mesh-adaptation accuracy, non-stationary(2)

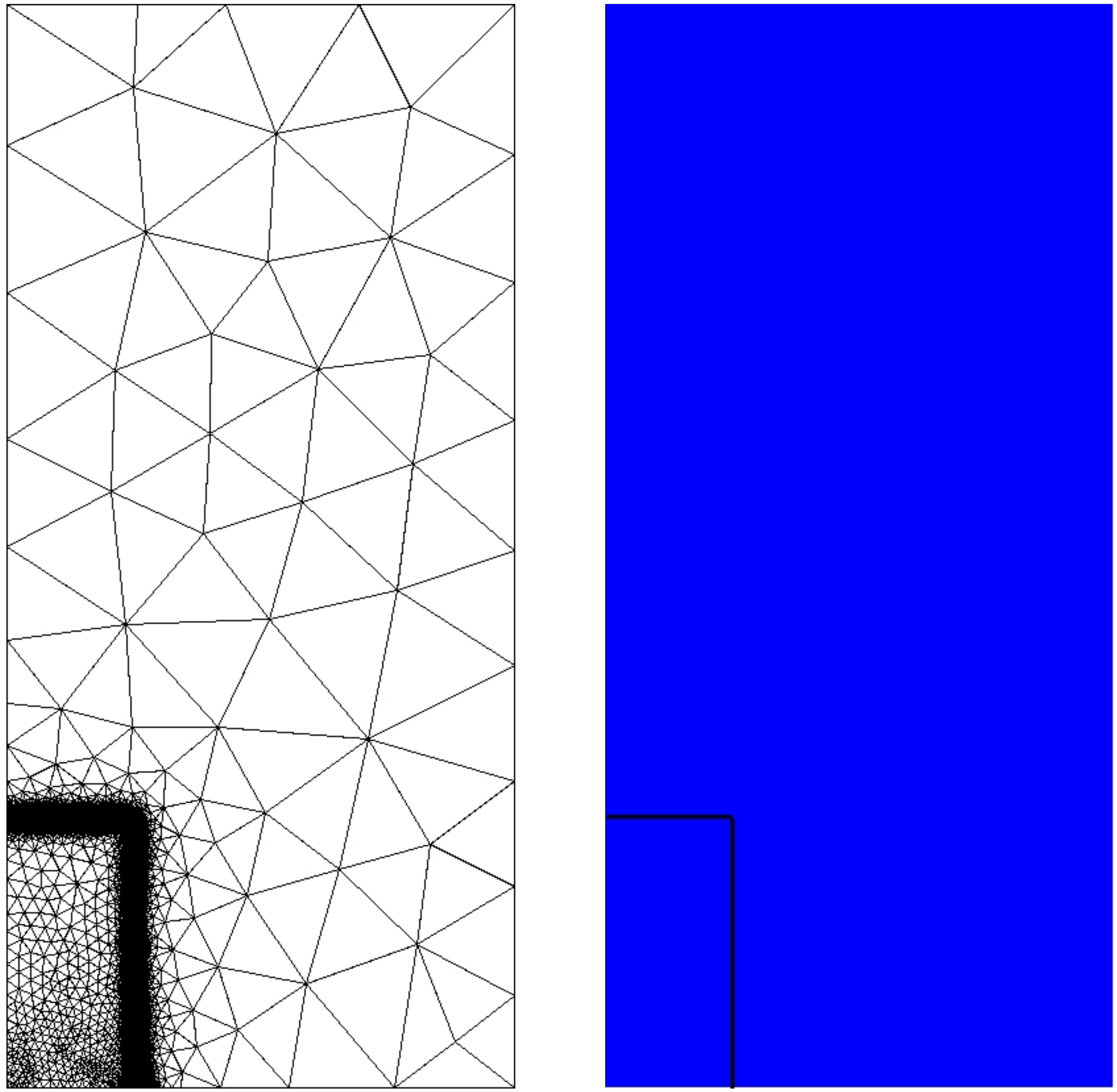


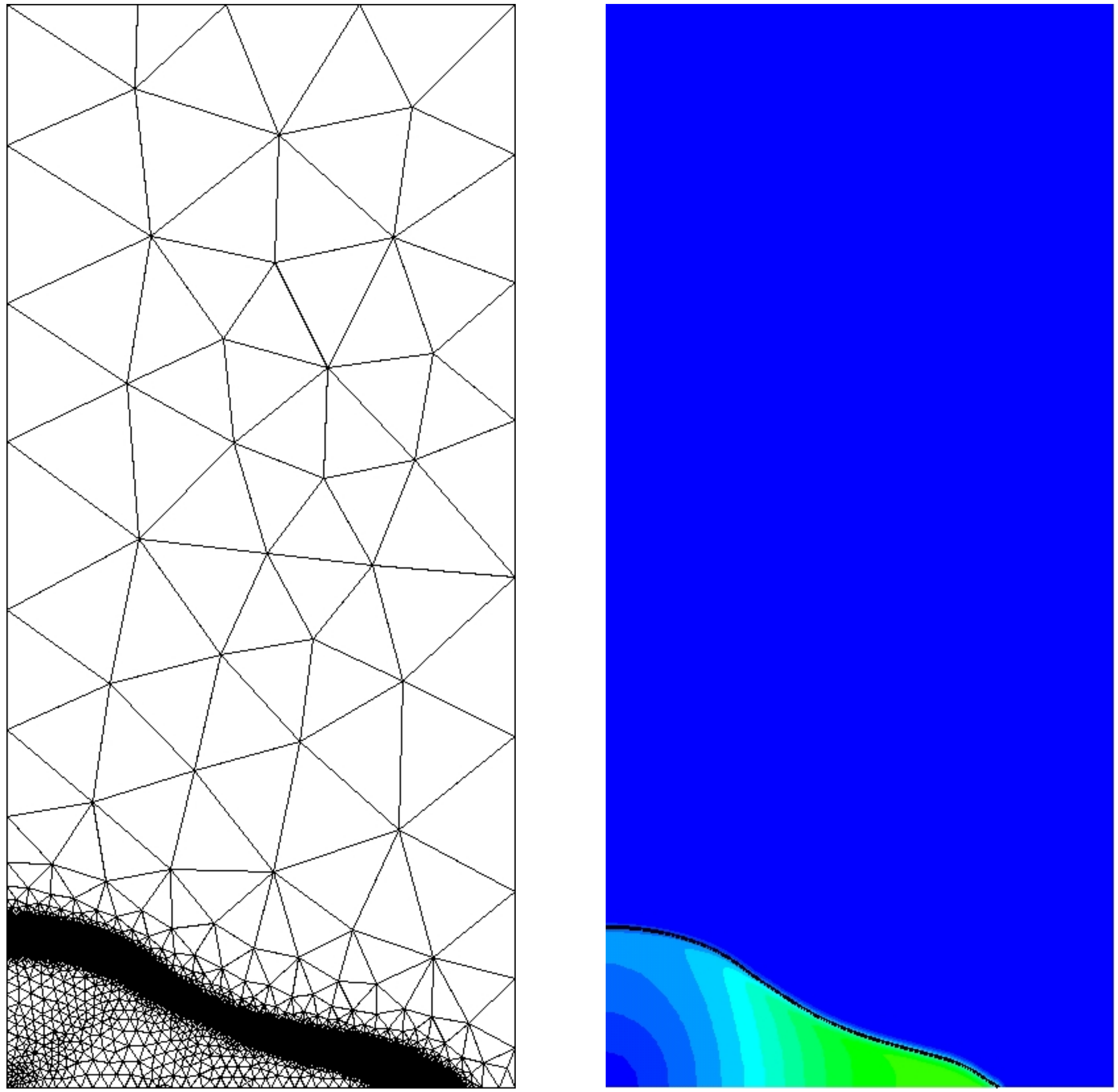
Rotating disk

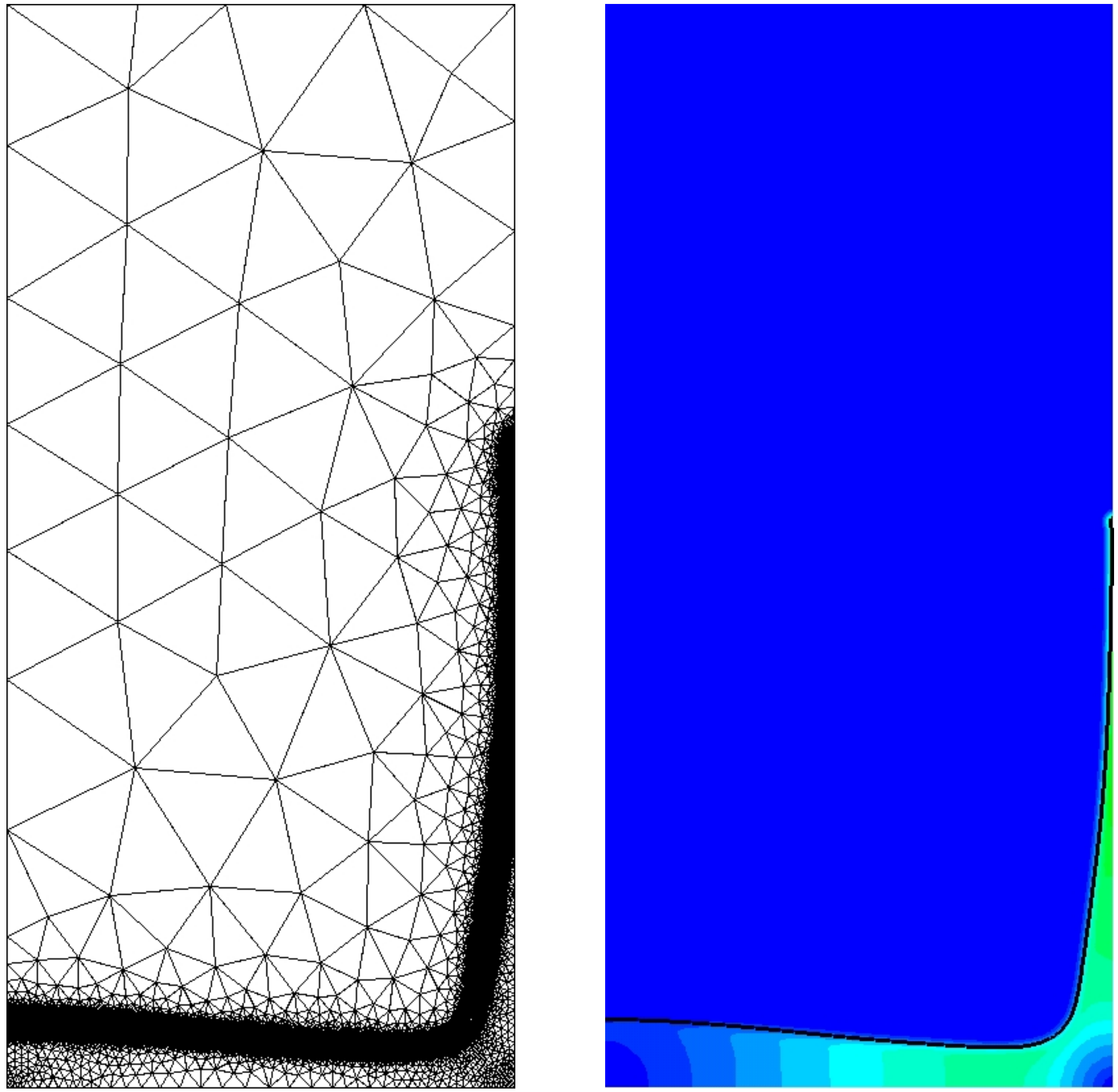
Mesh Conv.	Unif. Conv.	Barrier/iso.	Isotrop.
Shock Capt./Diss.	1/2	1	-
Shock Capt./Compr.	1	1	-
LS, smooth intf.	2+	n.a.	**2-4**

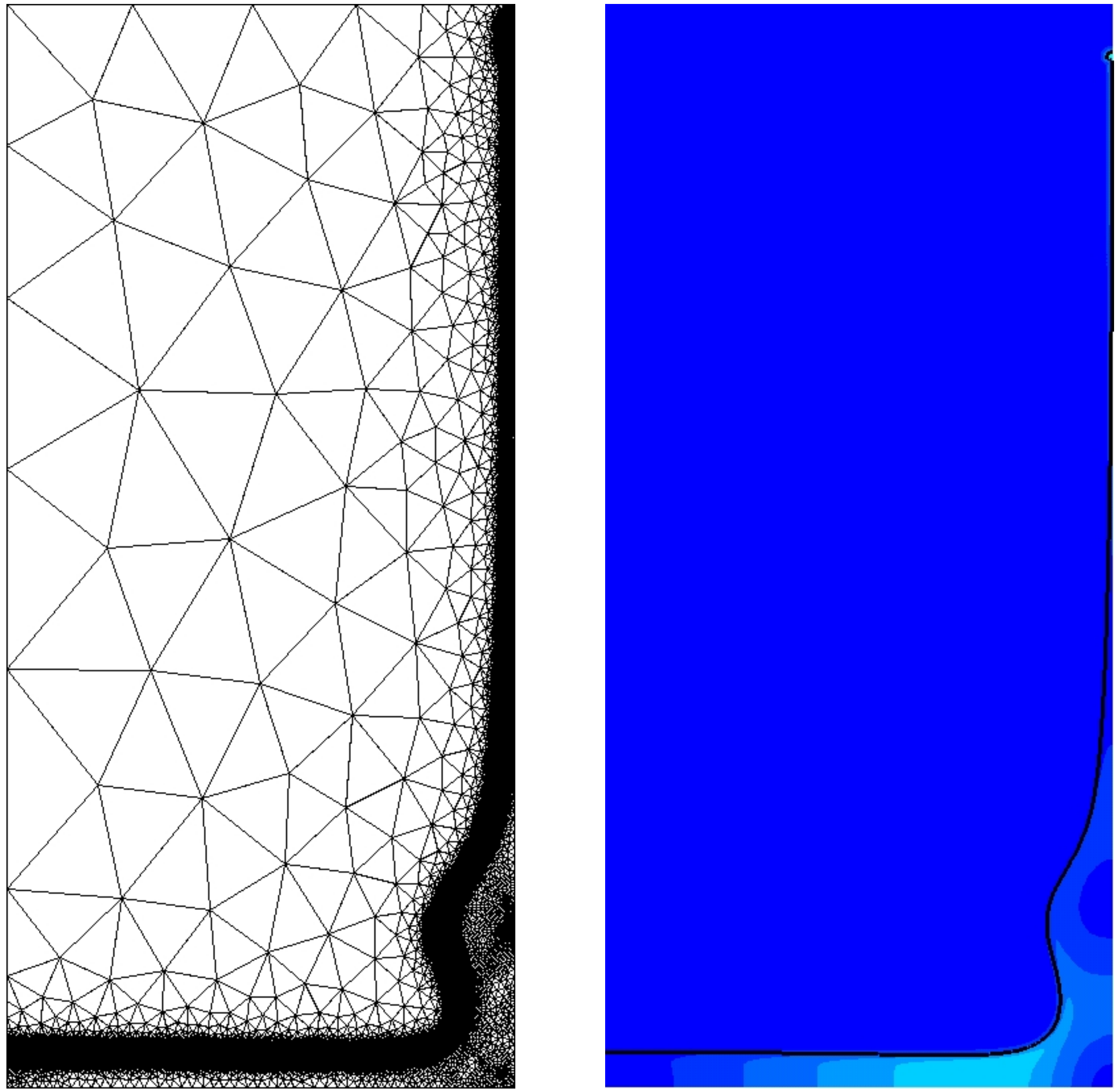
Spatial-oriented analysis, 2D case

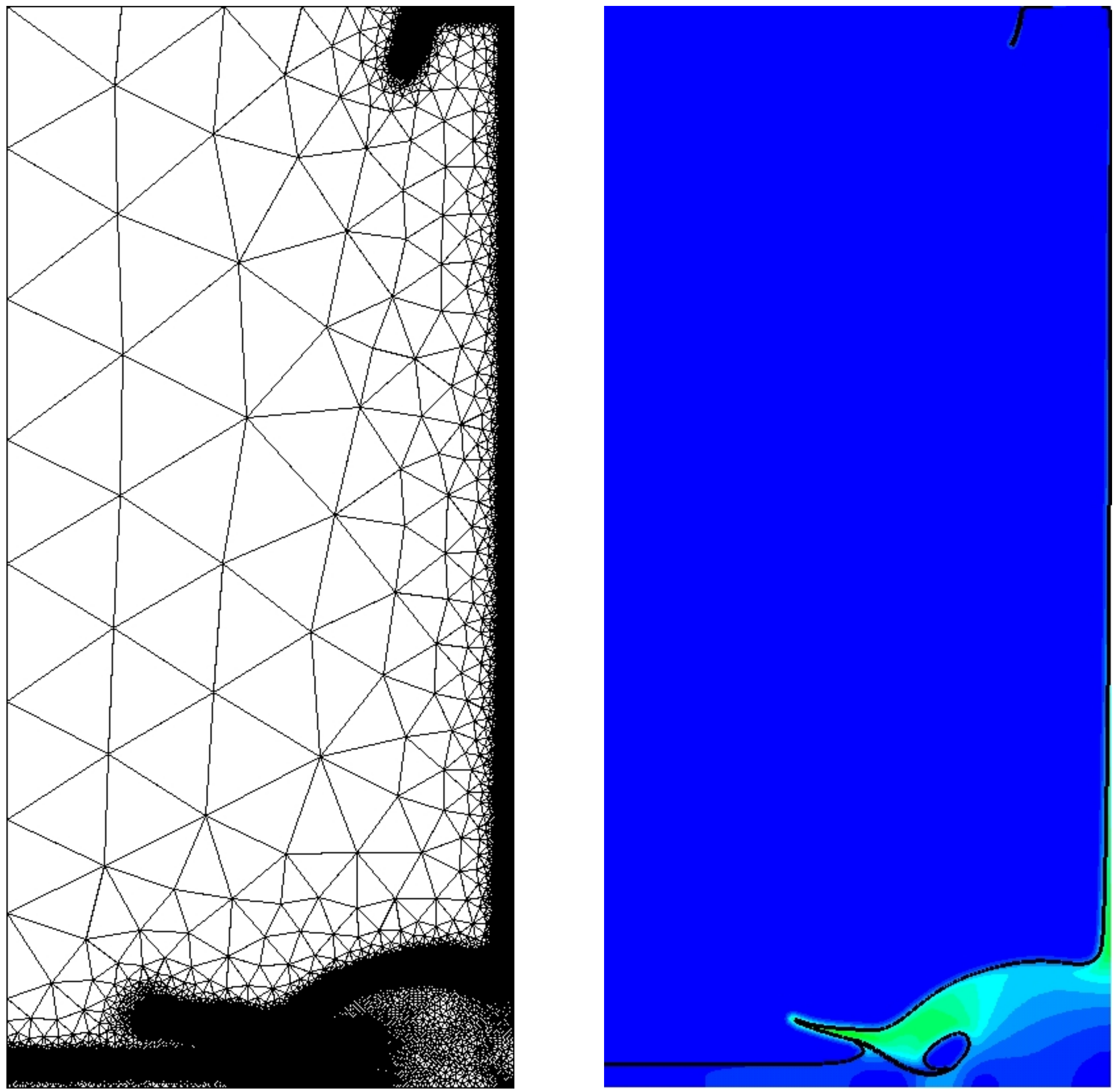
Navier-Stokes- 2D example (3K-130K cells)

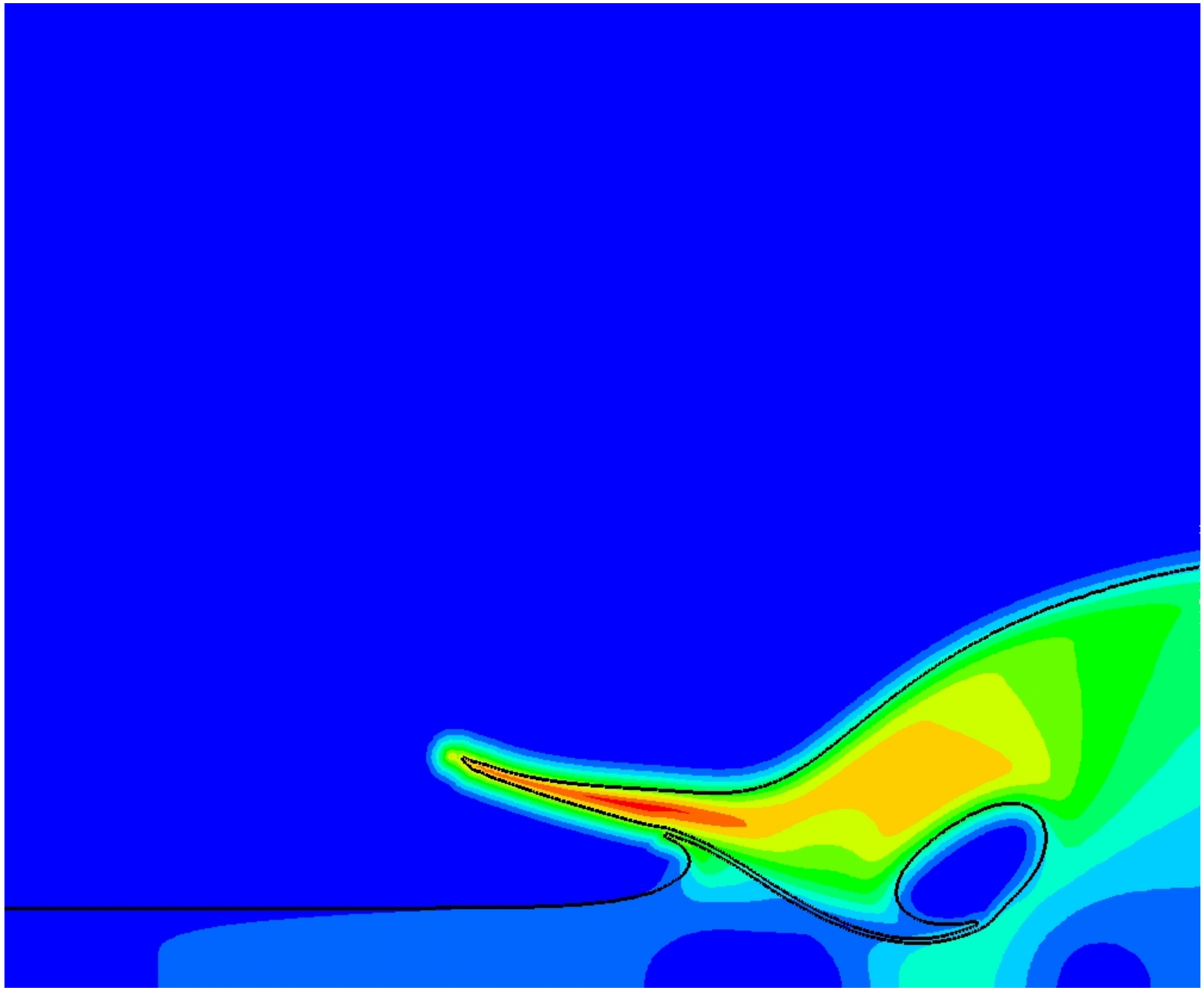


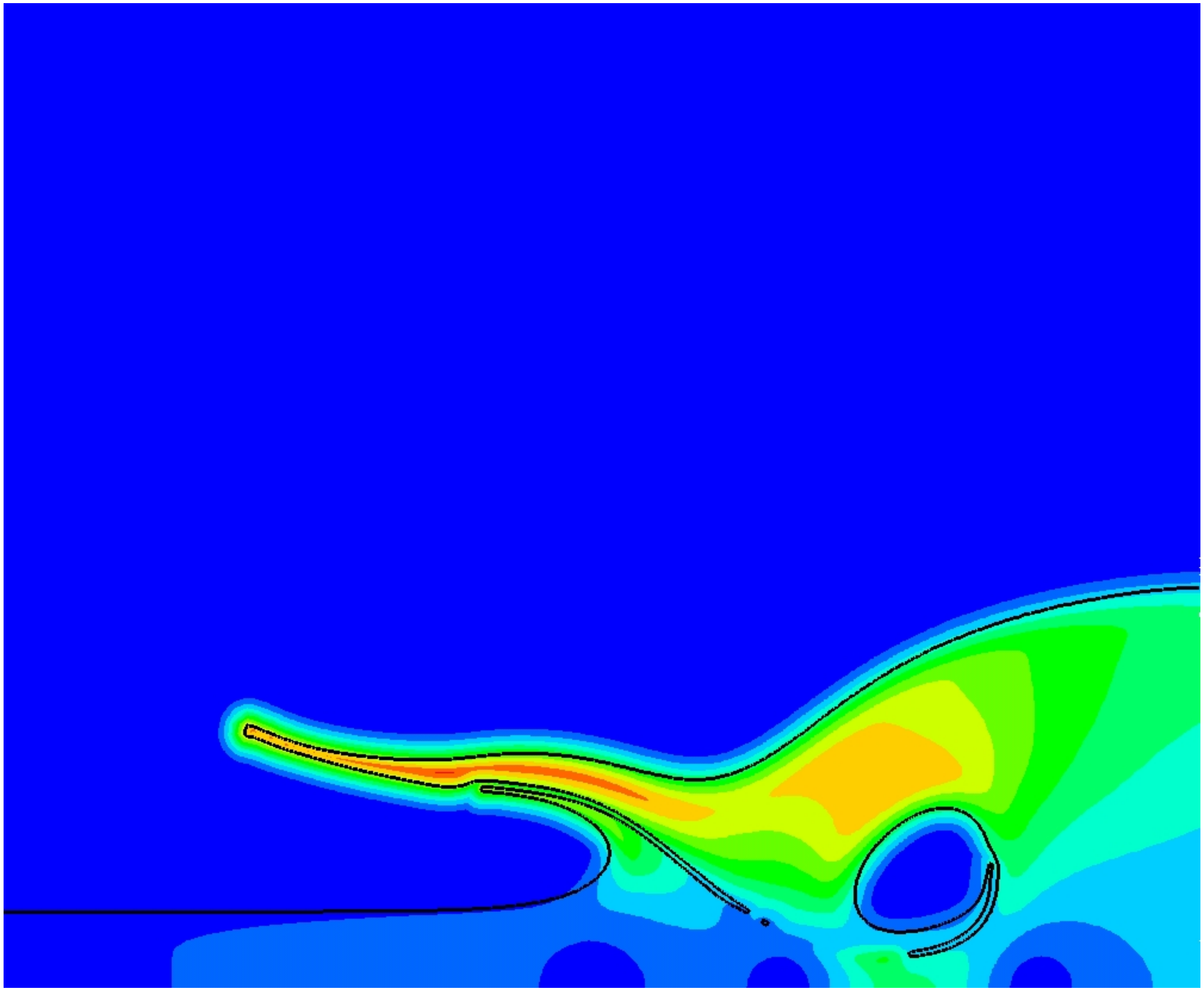


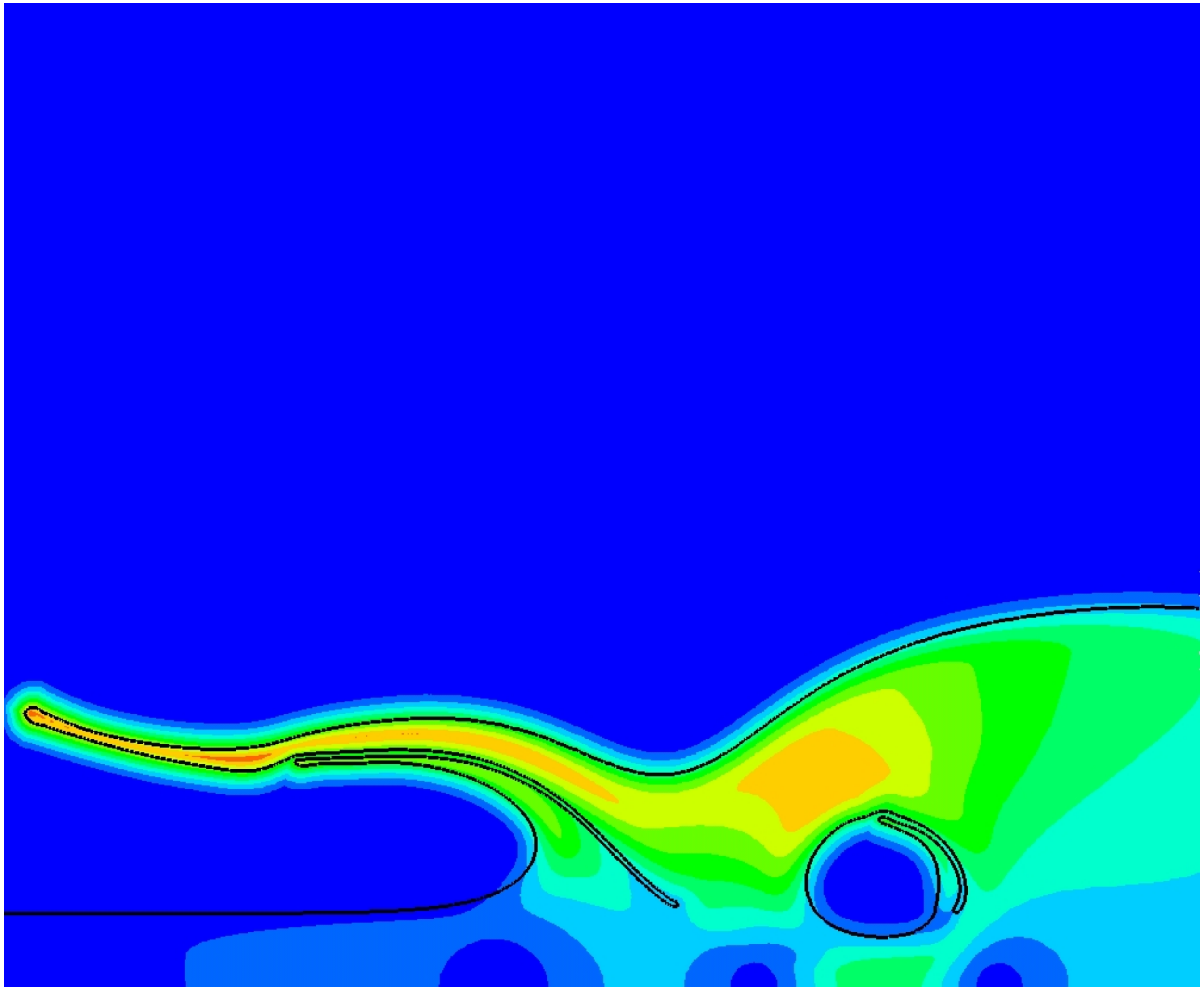




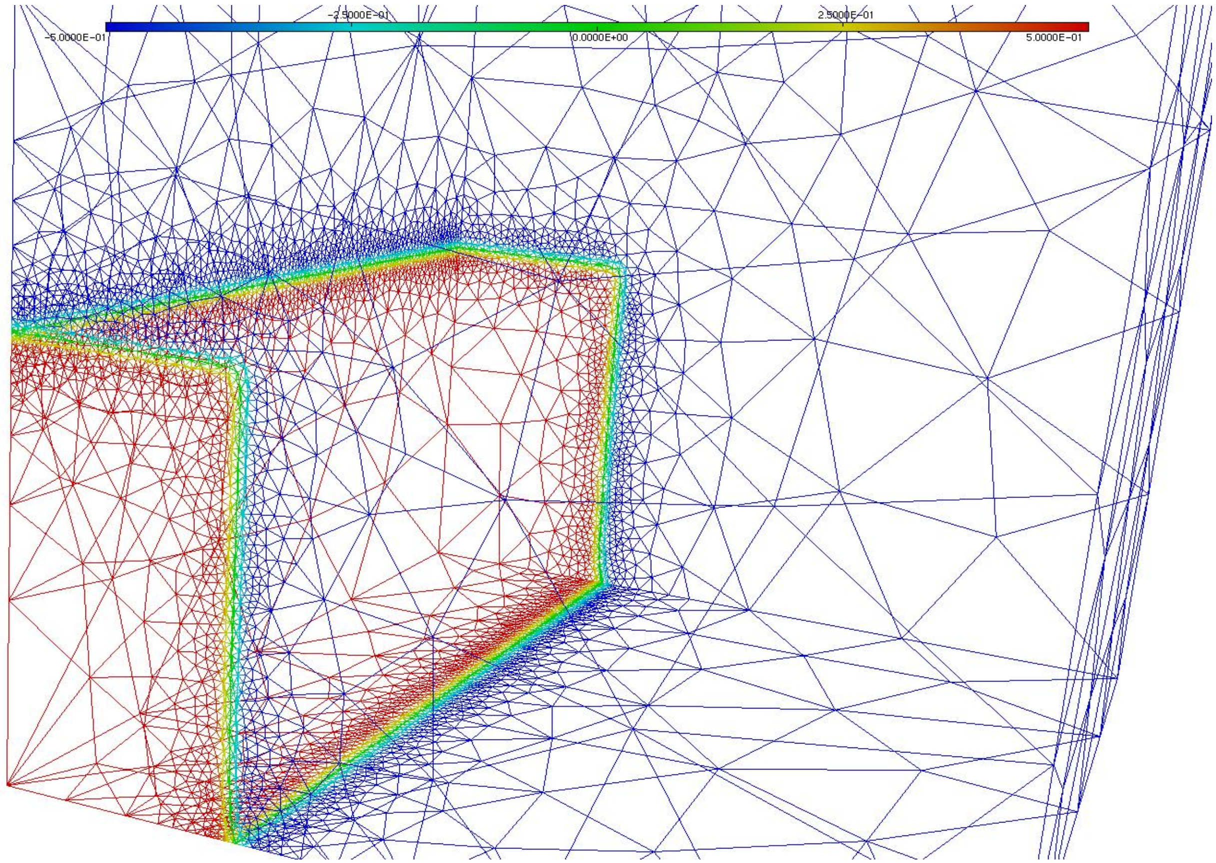


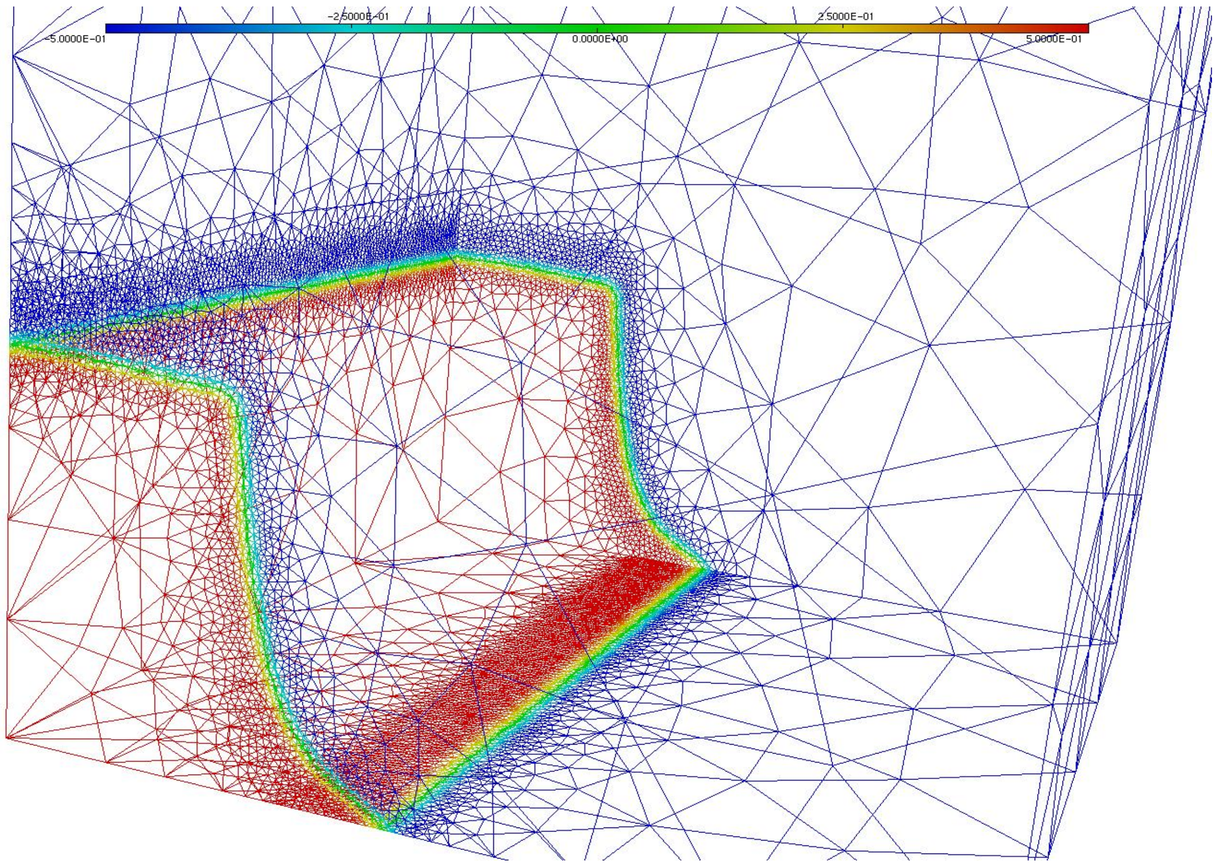






Navier-Stokes- 3D falling water column (20K/200K cells)





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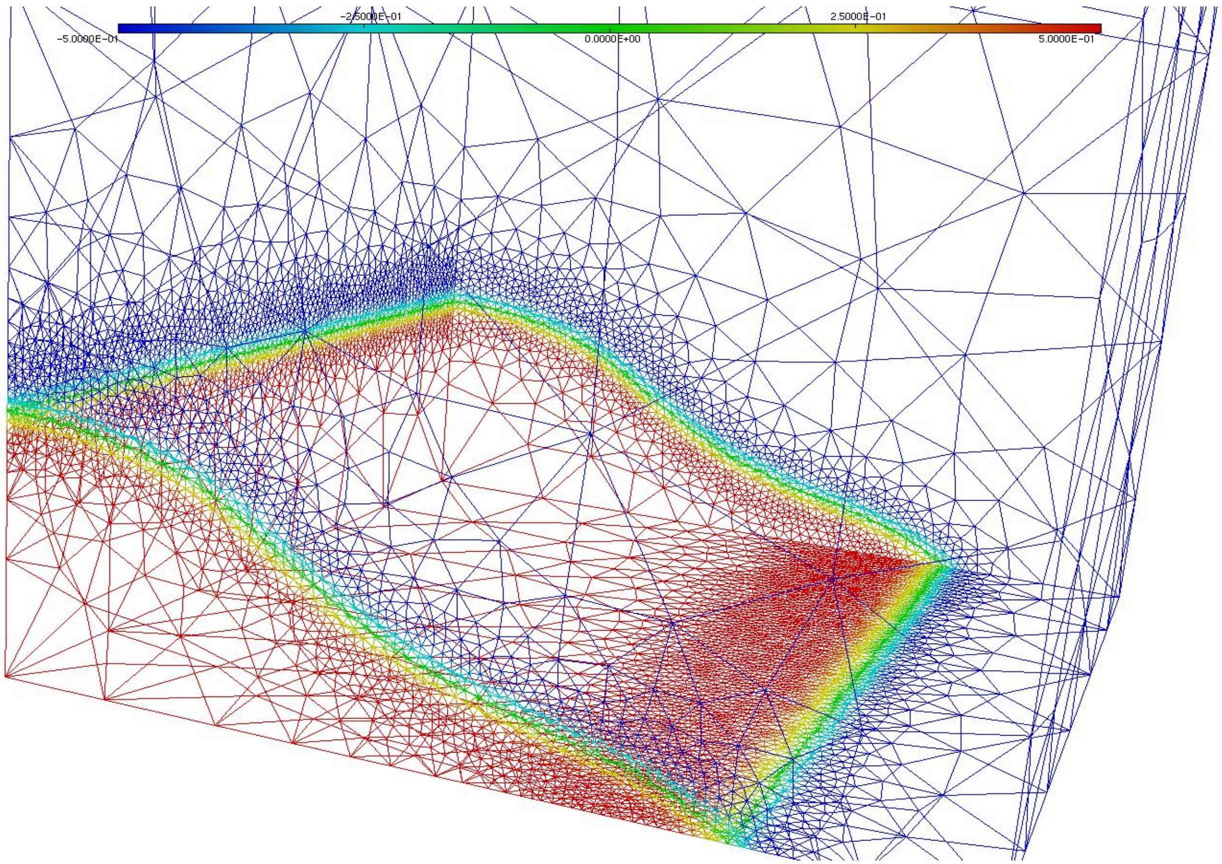
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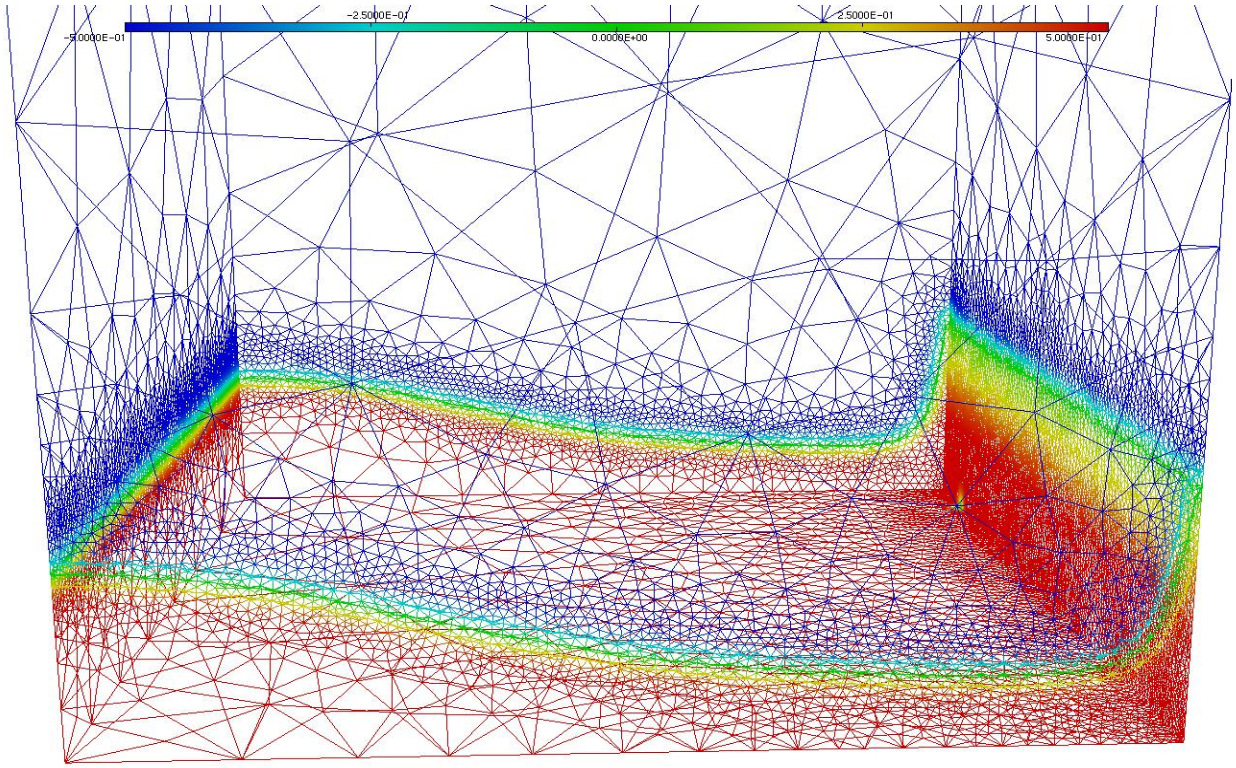

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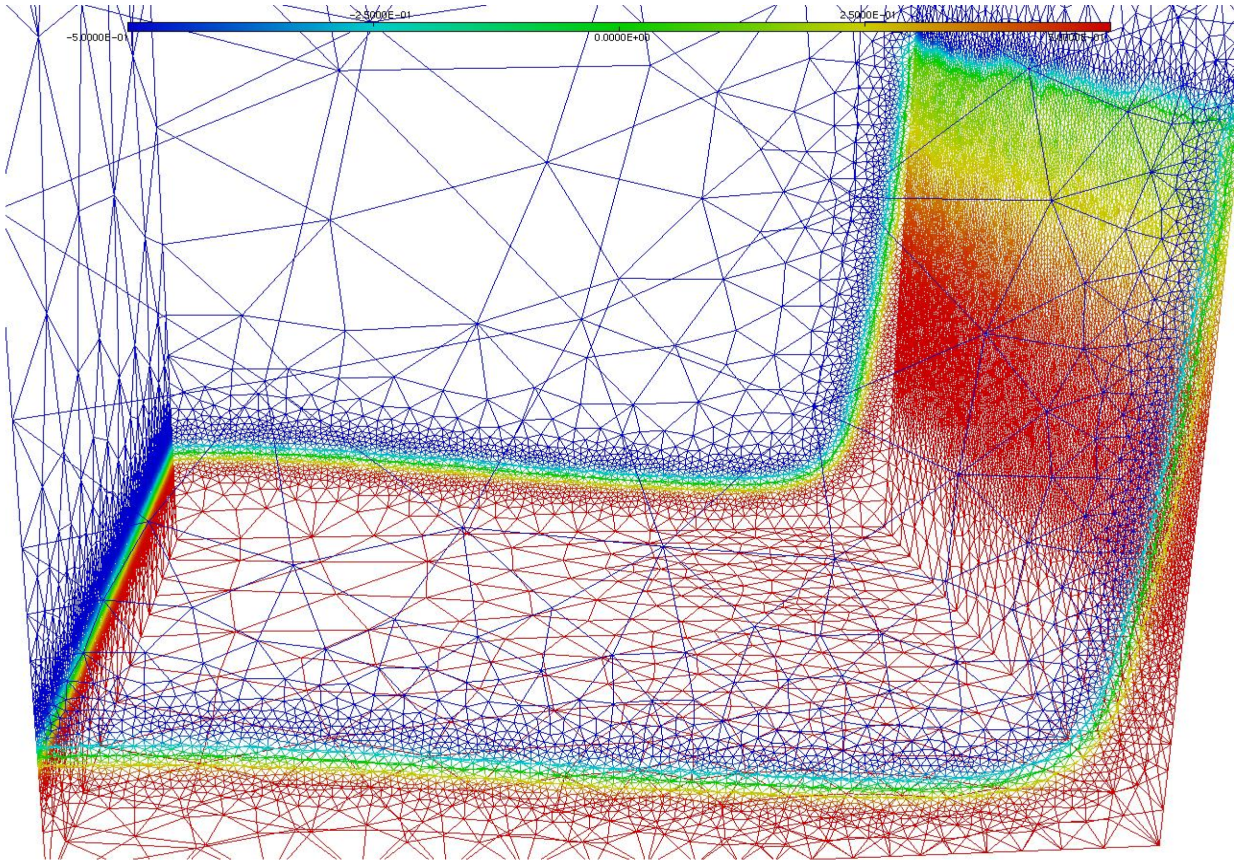
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SOME CONCLUSIONS

We have explored accuracy issues for the Eulerian computation of an interface between non-miscible fluids.

Level Set deals with interface propagation without mixing in a rather accurate manner.

But LS+Navier-Stokes formulation still involves different subgrid events:

- filaments and break up,

- material discontinuities in moment equations.

Both motivate the application of mesh adaptation.

We have analysed and experimented the impact of mesh adaptation on numerics efficiency.

Isotropic mesh adaptation combines well with Level Set.

Anisotropics mesh adaptation is currently examined.