QUELQUES APPLICATIONS D'UN SCHEMA SCHEMA MIXTE-ELEMENT-VOLUME A LA LES, A L'ACOUSTIQUE, AUX INTERFACES

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Overview

Ingredients of the Mixed Element Volume (MEV) method:

Finite Element:

P1 exactness,
H1 consistency.

Finite Volume:

conservations,
positivity.

Outline of the talk

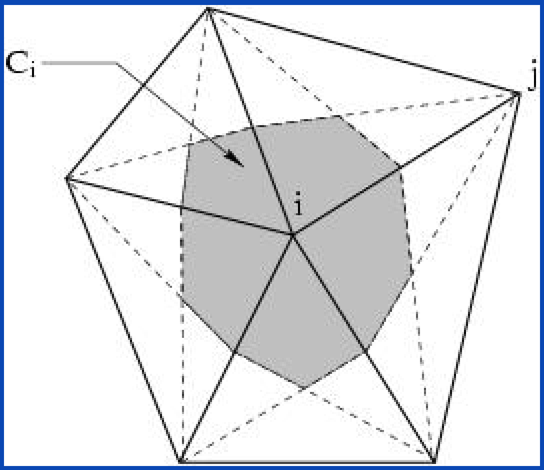
1. Basic options of the numerical method

2. Multiple levels/scales

3. Conservations

4. Positivity

1. BASIC OPTIONS OF THE MEV METHOD



- degrees of freedom at vertices i
- median dual cells C_i
- variational or integral formulation with two types of test functions:

ϕ_i, continuous-P_1, and χ_i, characteristic of C_i.

- Finite-Element evaluation of second derivatives
- Finite-Element/Finite-Volume evaluation of first derivatives

First-order MEV

$$W_t \; + \; div\mathcal{F} \; = \; div\mathcal{R}$$

$$\frac{\mathsf{Vol}(i)}{\Delta t}(W_i^{n+1} \; - \; W_i^n) \quad = \quad \Sigma_{j\in N(i)}\Phi_{ij} \; - \quad \int \nabla\mathcal{R}(W).\nabla\phi_i \;\; dx$$

Upwind numerical integration (Roe):

$$\Phi_{ij} = \frac{1}{2}(\mathcal{F}(W_i).\mathbf{n}_{ij} + \mathcal{F}(W_j).\mathbf{n}_{ij}) \; + \; \frac{1}{2}|A|(W_j - W_i)$$

$$A \quad = \quad \frac{d}{dW}\mathcal{F}(W).\mathbf{n}_{ij}$$

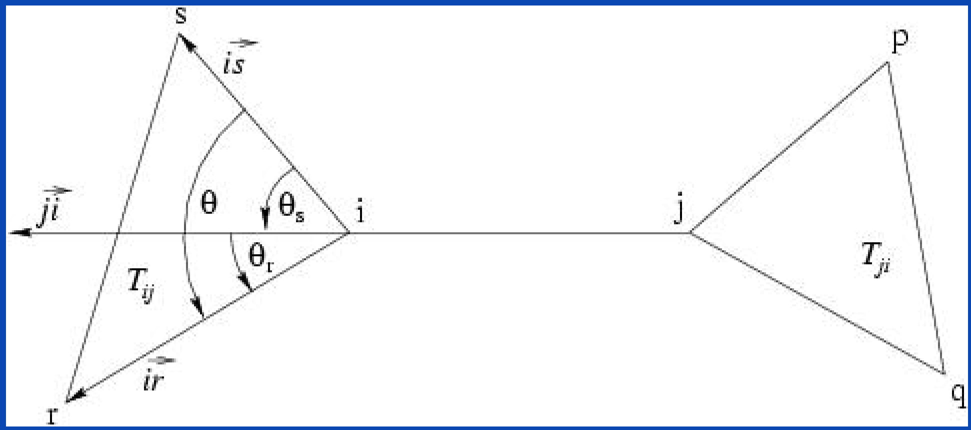
First extension: MUSCL

Edge-based reconstructions using **upwind elements** of each edge.

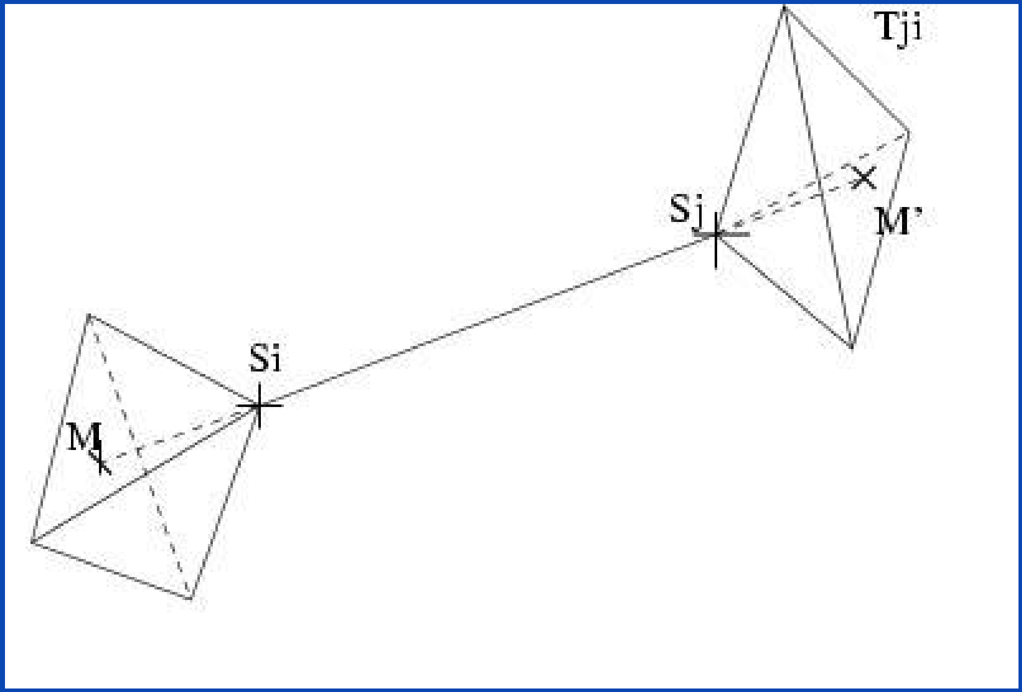
$$(\vec{\nabla} W)_{ij} \; = \; \frac{1}{3}\vec{\nabla} W^{FEM}(T_{ij}) + \frac{2}{3}\vec{\nabla} W^{FEM}(T_{ijk})$$

$$W_{ij} \; = \; W_i \; + \; (\vec{\nabla} W)_{ij}.\vec{ij}$$

$$\Phi_{ij} \; = \; 0.5(\Phi(W_{ij}) + \Phi(W_{ji})) \; + \; 0.5 \; \delta \; |A|(W_{ji} - (W_{ij}) \; .$$



Upwind-element reconstruction: 3D



Edge-upwind tetrahedra

Arbitrary Lagrangian-Eulerian formulation

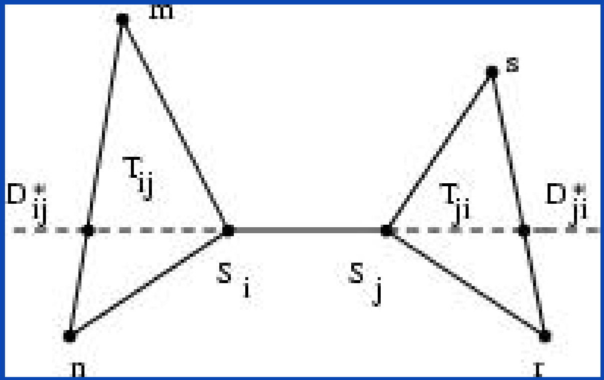
$$\frac{\partial}{\partial t}(V(x,t)w(t)) + F^c(w(t),x,\dot{x}) = R(w(t),x)$$

$$|\Omega_i^{n+1}|W_i^{n+1} \;=\; |\Omega_i^n|W_i^n \;-$$

$$\Delta t \sum_{j\in V(i)} |\partial\bar{\Omega}_{ij}| \;\Phi\left(W_i^{n+1},W_j^{n+1},\bar{\nu}_{ij},\frac{x_{ij}^{n+1}-x_{ij}^n}{\Delta t}\right)$$

$$\Phi(W,W,\nu,\kappa) \;=\; F(W)\;\nu^x \;+\; G(W)\;\nu^y \;+\; H(W)\;\nu^z \;-\kappa W.$$

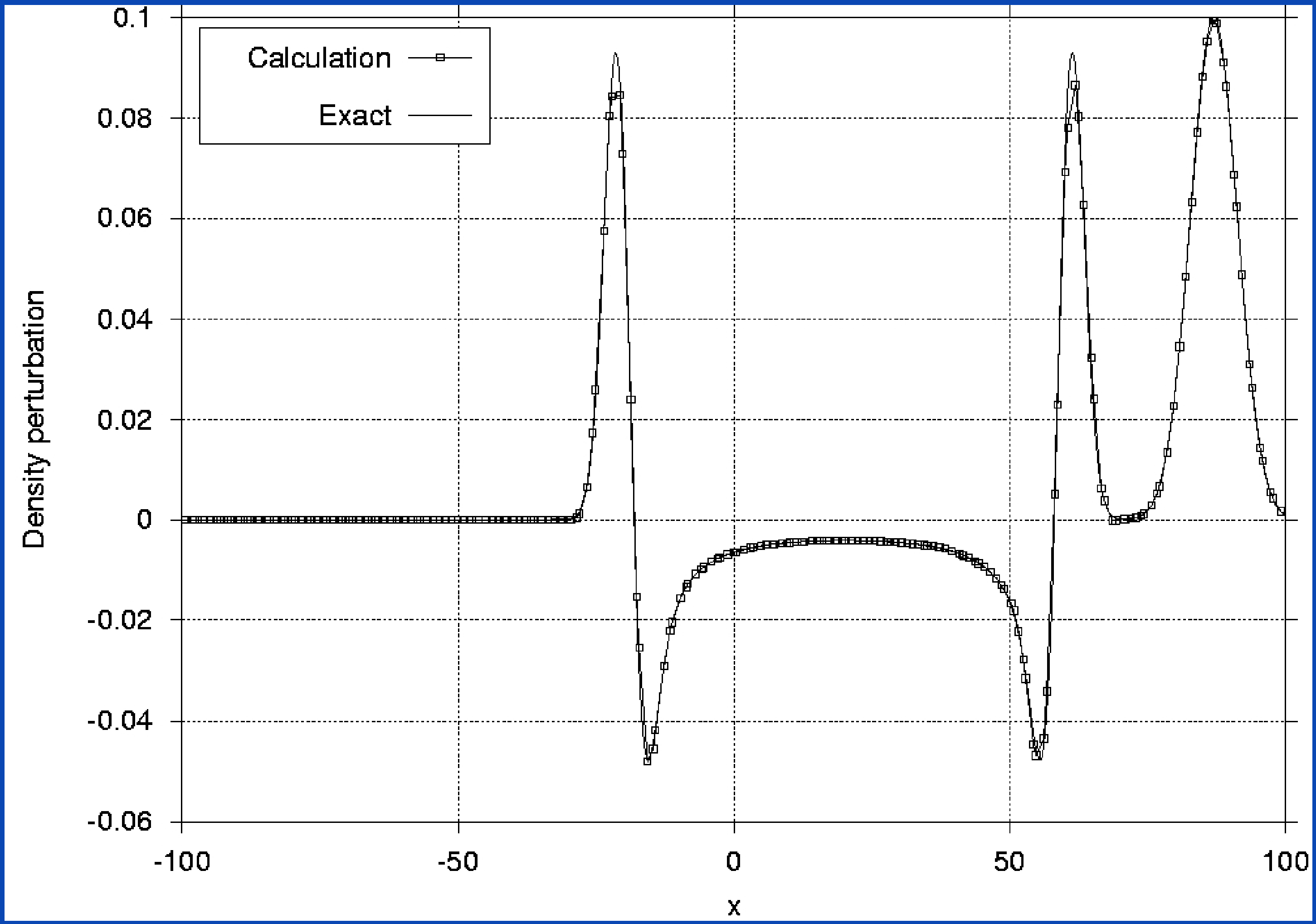
Back to the fluid numerics : V6



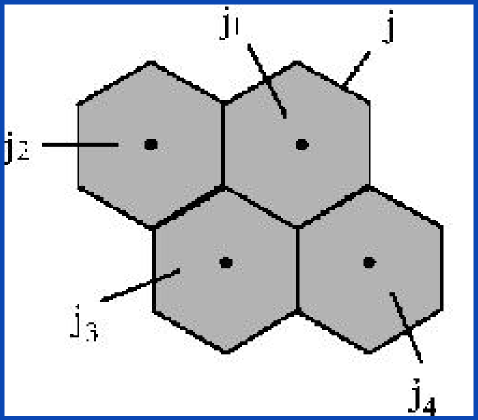
$$(\vec{\nabla} W)^{\mathbf{V6}}_{ij}.\vec{ij} \;=\; \frac{1}{3}(\vec{\nabla} W)_{T_{ij}}.\vec{ij} + \frac{2}{3}(W_j - W_i)$$
$$+\,\xi^a\,(\,(\vec{\nabla} W)_{T_{ij}}.\vec{ij} \;-2(W_j - W_i)\;+(\vec{\nabla} W)_{T_{ji}}.\vec{ij})$$
$$+\,\xi^b\,(\,(\vec{\nabla} W)_{D^*_{ij}}.\vec{ij} \;-\;2\,(\vec{\nabla} W)_i.\vec{ij} \;+\;(\vec{\nabla} W)_j.\vec{ij}\,)$$

$(\vec{\nabla} W)_{D^*_{ij}}$: linear interpolation of **nodal gradients** in nodes m and n.
- **Acoustics**: (Abalakin-Dervieux-Kozubskaya, IJ Acoustics, 3:2,157-180,2004)

V6 : Tam's case for acoustics



2. MULTIPLES LEVELS/SCALES



Agglomeration: several neighboring cells $\Rightarrow$ a coarse one.

$\Rightarrow$ inconsistency for second-order problems.

• Agglomeration MG: corrector terms in the assembly of coarse diffusion terms

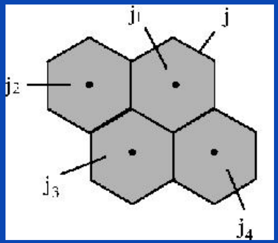
• Additive Multi-Level: smoothed basis functions

• **Variational Multi-Scale (VMS) models**

MEV implementation of Navier-Stokes

$$
\left\{
\begin{array}{l}
\displaystyle \int_\Omega \frac{\partial \rho}{\partial t}\mathcal{X}_i \, d\Omega \; + \; \int_{\partial Supp \mathcal{X}_i} \rho \mathbf{u}.\mathbf{n} \, d\Gamma \; = \; 0 \\[2em]
\displaystyle \int_\Omega \frac{\partial \rho \mathbf{u}}{\partial t}\mathcal{X}_i \, d\Omega \; + \; \int_{\partial Supp \mathcal{X}_i} \rho \, \mathbf{u}\mathbf{u}.\mathbf{n} \, d\Gamma \; + \; \int_{\partial Supp \mathcal{X}_i} P \mathbf{n} \, d\Gamma \\
\displaystyle + \int_\Omega \sigma \nabla \phi_i \, d\Omega \; = \; \mathbf{0} \\[2em]
\displaystyle \int_\Omega \frac{\partial E}{\partial t}\mathcal{X}_i \, d\Omega \; + \; \int_{\partial Supp \mathcal{X}_i} (E+P)\mathbf{u}.\mathbf{n} \, d\Gamma \; + \; \int_\Omega \sigma \mathbf{u}.\nabla \phi_i \, d\Omega \\
\displaystyle + \int_\Omega \lambda \nabla T.\nabla \phi_i \, d\Omega \; = \; 0
\end{array}
\right.
$$

VMS projection



$C^M_{m(k)}$: macro-cell containing the cell C_k.

$$I_k = \{j \ / \ C_j \subset C^M_{m(k)}\}.$$

$$\overline{\phi}_k = \frac{Vol(C_k)}{\sum\limits_{j \in I_k} Vol(C_j)} \sum_{j \in I_k} \phi_j.$$

($Vol(C_j)$: volume of cell C_j)

$$\overline{\mathbf{W}} = \sum_k \overline{\phi}_k \mathbf{W}_k \quad ; \quad \mathbf{W}' = \mathbf{W} - \overline{\mathbf{W}}$$

Smagorinski Large Eddy Simulation model

$S'_{ij} = \frac{1}{2}(\frac{\partial \mathbf{u}'_i}{\partial \mathbf{x}_j} + \frac{\partial \mathbf{u}'_j}{\partial \mathbf{x}_i})$, $\mathbf{u}' = (u'_1, u'_2, u'_3)$, small scale velocity,

$|S'| = \sqrt{2 S'_{ij} S'_{ij}}$, $C'_s = 0.1$, $\Delta'_l = Vol(\mathrm{T}_l)^{\frac{1}{3}}$,.

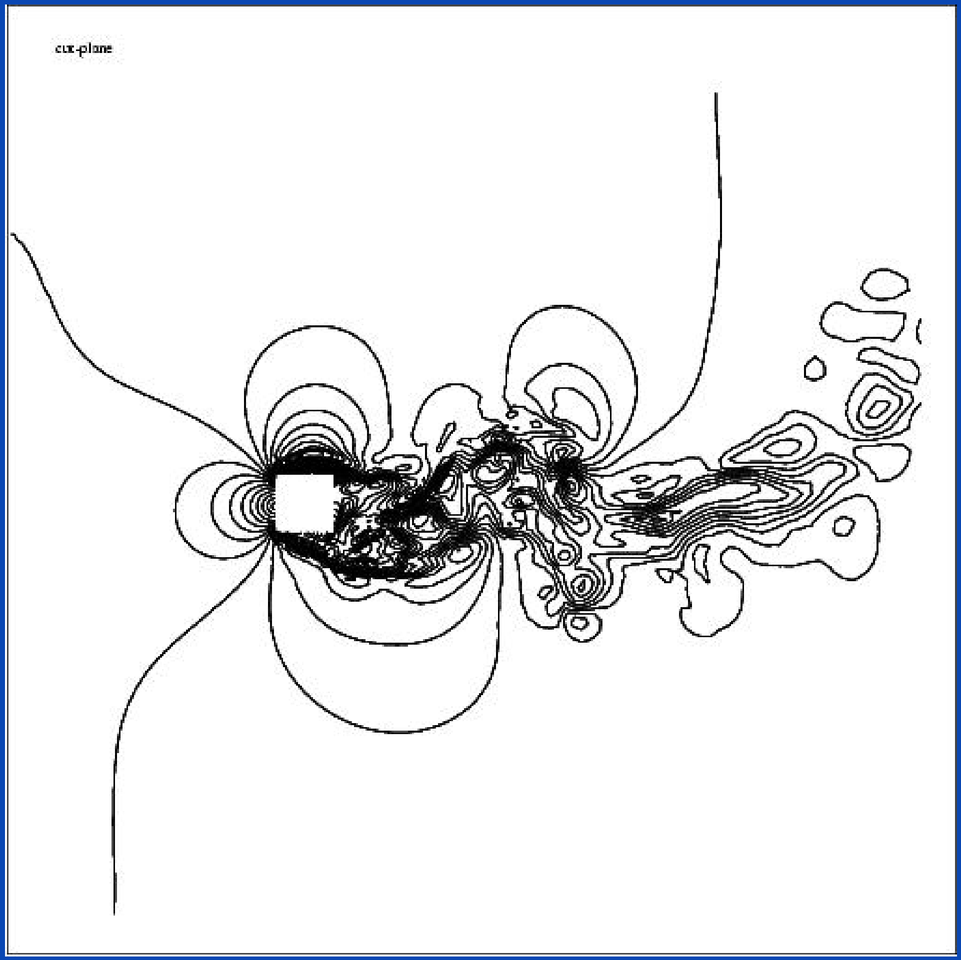
$$\mu'_t \;=\; \overline{\rho}(C'_s \Delta')^2 |S'|,$$

$$\tau'_{ij} \;=\; \mu'_t(2S'_{ij} - \frac{2}{3} S'_{kk}\delta_{ij}).$$

MEV implementation of the VMS LES model (ended)

$$
\left\{
\begin{array}{l}
\displaystyle\int_\Omega \frac{\partial \rho}{\partial t}\mathcal{X}_i \, d\Omega \; + \; \int_{\partial Supp \mathcal{X}_i} \rho \mathbf{u}.\mathbf{n}\mathcal{X}_i \, d\Gamma \; = \; 0 \\[2em]
\displaystyle\int_\Omega \frac{\partial \rho \mathbf{u}}{\partial t}\mathcal{X}_i \, d\Omega \; + \; \int_{\partial Supp \mathcal{X}_i} \rho \, \mathbf{u} \otimes \mathbf{u} \, \mathbf{n}\mathcal{X}_i \, d\Gamma \; + \; \int_{\partial Supp \mathcal{X}_i} P\mathbf{n}\mathcal{X}_i \, d\Gamma \\
\displaystyle + \int_\Omega \sigma \nabla \phi_i \, d\Omega \; + \; \int_\Omega \tau' \nabla \phi'_i \, d\Omega \; = \; \mathbf{0} \\[2em]
\displaystyle\int_\Omega \frac{\partial E}{\partial t}\mathcal{X}_i \, d\Omega \; + \; \int_{\partial Supp \mathcal{X}_i} (E+P)\mathbf{u}.\mathbf{n}\mathcal{X}_i \, d\Gamma \; + \; \int_\Omega \boldsymbol{\sigma}\mathbf{u}.\nabla \phi_i \, d\Omega \\
\displaystyle + \int_\Omega \lambda \nabla T.\nabla \phi_i \, d\Omega \; + \; \int_\Omega \frac{C_p \mu'_t}{Pr_t} \nabla T'.\nabla \phi'_i \, d\Omega \; = \; 0
\end{array}
\right.
$$

Results: flow past a square cylinder



Reynolds=20,000. From Farhat-Koobus, 2003.

Results: flow past a square cylinder, end'd

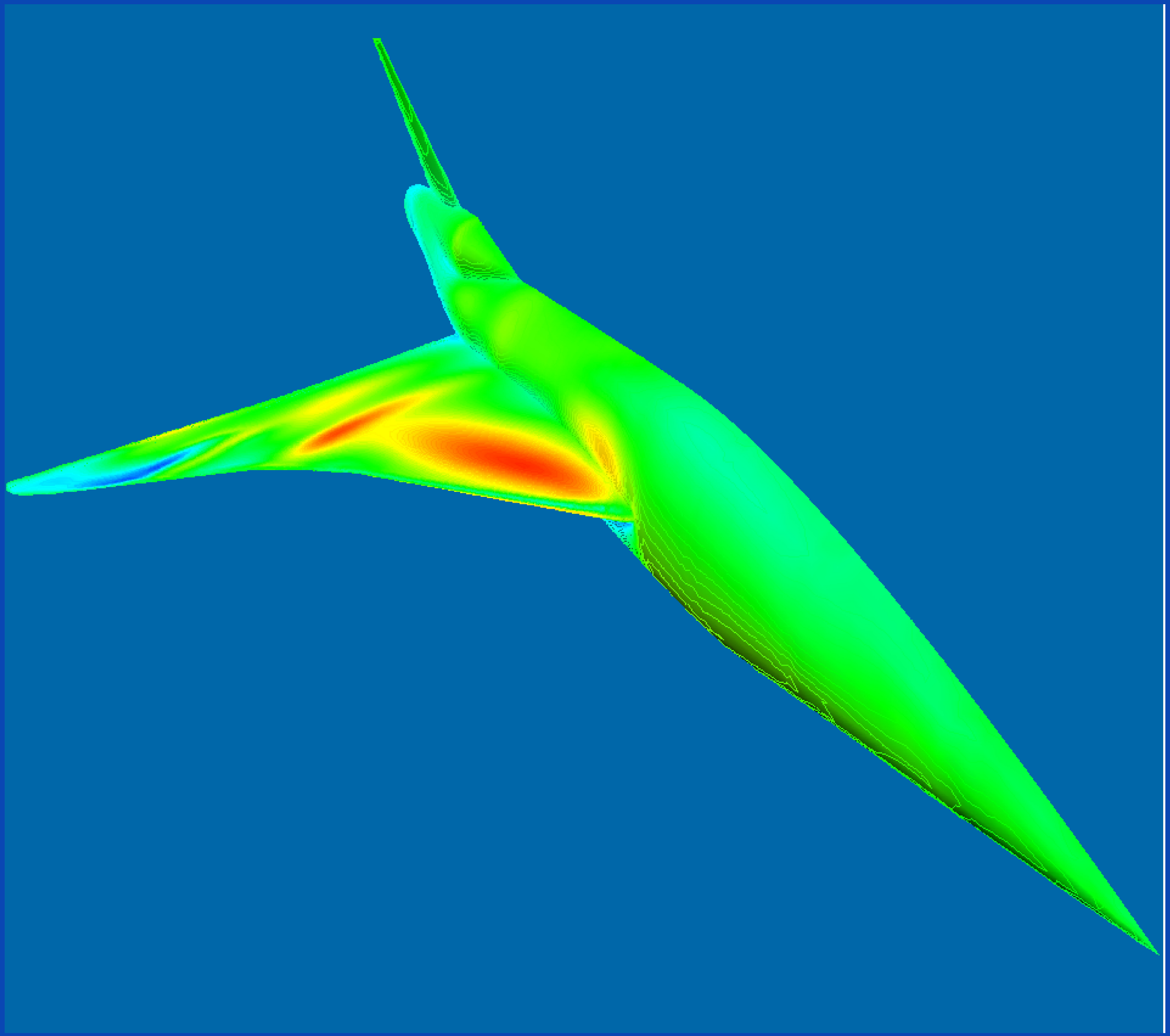
LES	$\overline{C}_d$	C'_d	C'_l	S_t	l_r	$-\overline{C}_{p_b}$
Classical LES	2.00	0.19	1.01	0.136	1.5	1.31
VMS-LES	**2.10**	**0.18**	1.08	0.136	**1.4**	**1.52**

Experiments	$\overline{C}_d$	C'_d	C'_l	S_t	l_r	$-\overline{C}_{p_b}$
Lyn *et al.*	2.10	-	-	0.132	1.4	-
Luo *et al.*	2.21	0.18	1.21	0.13	-	1.52
Bearman *et al.*	2.28	-	1.20	0.13	-	1.60

TAB. 1 – *Bulk coefficients (*): LES simulations and experimental data*

(*) l_r is the recirculation length behind the square cylinder, and $\overline{C}_{p_b}$ is the mean pressure coefficient on rear face at $y = 0$.

AND NEXT...



3. CONSERVATIONS IN ALE FORMULATION

- Conservation of extensive quantities.

- **Geometric Conservation Law (GCL).**

- **Energy budget.**

Geometric Conservation law

"A ALE-GCL scheme computes exactly a uniform flow field"

$$
\begin{aligned}
|\Omega_i^{n+1}|U_i^{n+1} &= |\Omega_i^n|U_i^n \; - \\
& \Delta t \sum_{j\in V(i)} |\partial\bar{\Omega}_{ij}| \; \Phi\left(U_i^{n+1}, U_j^{n+1}, \bar{\nu}_{ij}, \frac{x_{ij}^{n+1} - x_{ij}^n}{\Delta t}\right)
\end{aligned}
$$

$$
\bar{\nu}_{ij} \;=\; 0.5\;\left(\nu_{ij}(x(t_1+\alpha_1(t_2-t_1))) + \nu_{ij}(x(t_1+\alpha_2(t_2-t_1)))\right)
$$

$$
\Rightarrow |\Omega_i^{n+1}| - |\Omega_i^n| \;=\; \int_{\partial\Omega_h(t)} \dot{x}_i\, n_i\, d\Gamma
$$

- Sufficient condition for 1st-order accuracy (Guillard-Farhat).
- Practical stability and accuracy improvements.

Energy budget of a deforming fluid (1)

Work transfers : pressure work in moment equation:

$$\Delta \mathbf{M}\Big|_{t_1}^{t_2} \,.\, (\mathbf{x}_{ij}^{n+1} - \mathbf{x}_{ij}^{n}) \;=$$

$$\Delta t \sum_{i \in \partial\Omega_h} |\partial\bar{\Omega}_{h,i}| \; \Phi_{\partial\Omega}^{M} \left(W_i^{n+1}, \bar{\nu}_{ij}, \frac{x_{ij}^{n+1} - x_{ij}^{n}}{\Delta t} \right) \,.\, (\mathbf{x}_{ij}^{n+1} - \mathbf{x}_{ij}^{n})$$

$$\Delta Work\Big|_{t_1}^{t_2} \;=\; \Delta t \sum_{i \in \partial\Omega_h} |\partial\bar{\Omega}_{h,i}| \; p_i \; \bar{\nu}_i \,.\, (\mathbf{x}_{ij}^{n+1} - \mathbf{x}_{ij}^{n})$$

Energy budget of a deforming fluid (2)

The energy equation **must** satisfy the Geometric Conservation Law and this is obtained by an adhoc time integration:

$$|\Omega_i^{n+1}|\ E_i^{n+1} \quad =$$

$$|\Omega_i^n| E_i^n - \Delta t \sum_{j \in V(i)} |\partial\bar{\Omega}_{ij}|\ \Phi^E\left(U_i^{n+1}, U_j^{n+1}, \bar{\nu}_{ij}, \frac{x_{ij}^{n+1} - x_{ij}^n}{\Delta t}\right)$$

$|\partial\bar{\Omega}_{ij}|$ and $\bar{\nu}_{ij}$ specified by GCL.

Energy budget of a deforming fluid (3)

Total energy variation:

$$\Delta E\Big|_{t_1}^{t_2} \;=\; -\;\Delta t \sum_{i\in\partial\Omega_h} |\partial\bar{\Omega}_{h,i}|\;\Phi^E_{\partial\Omega}\left(W_i^{n+1},\bar{\nu}_{ij},\frac{x_{ij}^{n+1}-x_{ij}^{n}}{\Delta t}\right)$$

Slip condition:

$$\Delta E\Big|_{t_1}^{t_2} \;=\; -\;\Delta t \sum_{i\in\partial\Omega_h} |\partial\bar{\Omega}_{h,i}|\;\left(\int_{\partial\Omega_{h,i}} (p\mathbf{u})_i\;.\;\bar{\nu}_i\,d\Gamma\right)$$

Energy budget of a deforming fluid (4)

A way of integrating the above is:

$$\Delta E\Big|_{t_1}^{t_2} = \Delta t \sum_{i \in \partial\Omega_h} |\partial\bar{\Omega}_{h,i}| \; p_i \; \bar{\nu}_i \; . \; (\mathbf{x}_{ij}^{n+1} - \mathbf{x}_{ij}^{n})$$

Lemma: *By replacing the energy flux by a product of boundary pressure times the GCL-preserving integration of mesh motion, we can derive a scheme that is conservative, satisfies GCL and have an exact energy budget:*

Work of pressure = Loss of total energy.

Vàzquez-Koobus-Dervieux-Farhat, Spatial discretization issues for the energy conservation in compressible flow problems on moving grids, INRIA-RR4742

4. POSITIVITY

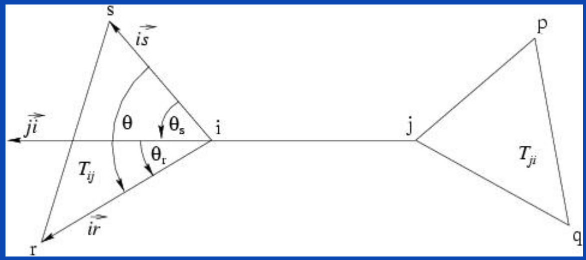
$$\frac{\partial}{\partial t}(V(x,t)U(t)) + F^c(w(t),x,\dot{x}) = 0$$

$$\frac{a_i^{n+1}U_i^{n+1} - a_i^n U_i^n}{\Delta t} + \sum_{j\in\mathcal{N}(i)} \phi(U_{ij}^n,U_{ji}^n,\nu_{ij},\kappa_{ij}) \;=\; 0\,.$$

$$\Phi(u,u,\nu,\kappa) \;=\; F(u)\;\nu^x \;+\; G(u)\;\nu^y \;+\; H(u)\;\nu^z \;-\kappa u.$$

with $\phi(u,v,\nu,\kappa)$ monotone: $\phi'_u \geq 0$ and $\phi'_v \leq 0$.

Limiters



$$\Delta^{-}U_{ij} \;=\; \vec{\nabla}W^{FEM}(T_{ij}).\vec{ij}\ ;\ \Delta^{0}U_{ij} \;=\; \vec{\nabla}W^{FEM}(T_{ijk}).\vec{ij}$$

$$(\vec{\nabla}U)_{ij}.\vec{ij} = L(\Delta^{-}U_{ij}\,,\Delta^{0}U_{ij}\,,\Delta^{\text{higher}}U_{ij})$$

From usual conditions on limiteurs, and from the position of "upwind-elements" :

$$U_{ij} \;=\; \Sigma p_k(U_i - U_k)\ \ ;\ \ U_{ij} \;=\; p_j(U_j - U_i)$$

where all p's are positive.

POSITIVITY, cont'd

$$\frac{a_i^{n+1}U_i^{n+1} - a_i^n U_i^n}{\Delta t} + \sum_{j \in \mathcal{N}(i)} \phi_{ij}(U_{ij}^n, U_{ji}^n, \bar{\nu}_{ij}, \bar{\kappa}_{ij}) \ = \ 0\,.$$

$$\frac{a_i^{n+1}U_i^{n+1} - a_i^n U_i^n}{\Delta t} = \ e_i \ + \ \sum_{j \in \mathcal{N}(i)} g_{ij}(U_{ji}^n - U_i^n) \ + \ h_{ij}(U_{ij}^n - U_i^n)$$

POSITIVITY, cont'd

$$g_{ij} \quad = \quad \frac{\Delta t}{a_i} \, \frac{\phi_{ij}(U_{ij}^n, U_{ji}^n, \nu_{ij}, \bar{\kappa}_{ij}) \;-\; \phi_{ij}(U_{ij}^n, U_i^n, \nu_{ij}, \bar{\kappa}_{ij})}{U_{ji}^n - U_i^n}$$

$$h_{ij} \quad = \quad - \, \frac{\Delta t}{a_i} \, \frac{\phi_{ij}(U_{ij}^n, U_i^n, \nu_{ij}, \bar{\kappa}_{ij}) \;-\; \phi_{ij}(U_i^n, U_i^n, \nu_{ij}, \bar{\kappa}_{ij})}{U_{ij}^n - U_i^n}$$

$$e_i \quad = \quad \left(\frac{a_i^n - a_i^{n+1}}{a_i^n} + \frac{\Delta}{a_i^{n+1}} \sum_{j \in \mathcal{N}(i)} |\partial \bar{\Omega}_{ij}| \bar{\kappa}_{ij} \right)$$

POSITIVITY, cont'd

Lemma: *Assuming the discrete GCL condition and usual limiter properties, under a CFL condition, the above scheme satisfies the maximum/minimum principle.*

Cournde-Koobus-Dervieux, soumis Revue EEF, 2005
Farhat-Geuzaine-Grandmont, JCP 2001

POSITIVITY, cont'd

$$U = (\rho, \rho u, \rho v, \rho w, e, \rho Y), \quad \frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} + \frac{\partial H(U)}{\partial z} = 0$$

$$F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho uw \\ (e+P)u \\ \rho uY \end{pmatrix} \quad G(U) = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ \rho vw \\ (e+P)v \\ \rho vY \end{pmatrix} \quad H(U) = \begin{pmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + P \\ (e+P)w \\ \rho wY \end{pmatrix}$$

$$P = (\gamma - 1)\left(e - \frac{1}{2}(u^2 + v^2 + w^2)\right)$$

Lemma: *Assume that the Riemann solver is ρ-positive, then under a CFL condition, the limited ALE-MEV scheme preserves ρ-positivity and satisfies the maximum/minimum principle for $Y = \rho Y/\rho$.*

Courndé-Koobus-Dervieux, soumis Revue EEF, 2005

Application to a two-phase flow

Five-equation quasi conservative reduced model

$$
\begin{aligned}
\frac{\partial}{\partial t}\alpha_k\rho_k + \mathrm{div}(\alpha_k\rho_k\boldsymbol{u}) &= 0 \\
\frac{\partial}{\partial t}\rho\boldsymbol{u} + \mathrm{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u}) + \nabla p &= 0 \\
\frac{\partial}{\partial t}\rho e + \mathrm{div}(\rho e + p)\boldsymbol{u} &= 0 \\
\frac{\partial}{\partial t}\alpha_2 + \boldsymbol{u}.\nabla\alpha_2 &= \alpha_1\alpha_2\frac{\rho_1 a_1^2 - \rho_2 a_2^2}{\sum_{k=1}^{2}\alpha_{k'}\rho_k a_k^2}\mathrm{div}\boldsymbol{u}
\end{aligned}
$$

with $e = \varepsilon + u^2/2$ and $\rho\varepsilon = \sum_{k=1}^{2}\alpha_k\rho_k\varepsilon_k(p,\rho_k)$.

NUMERICS FOR TWO-PHASE FLOW

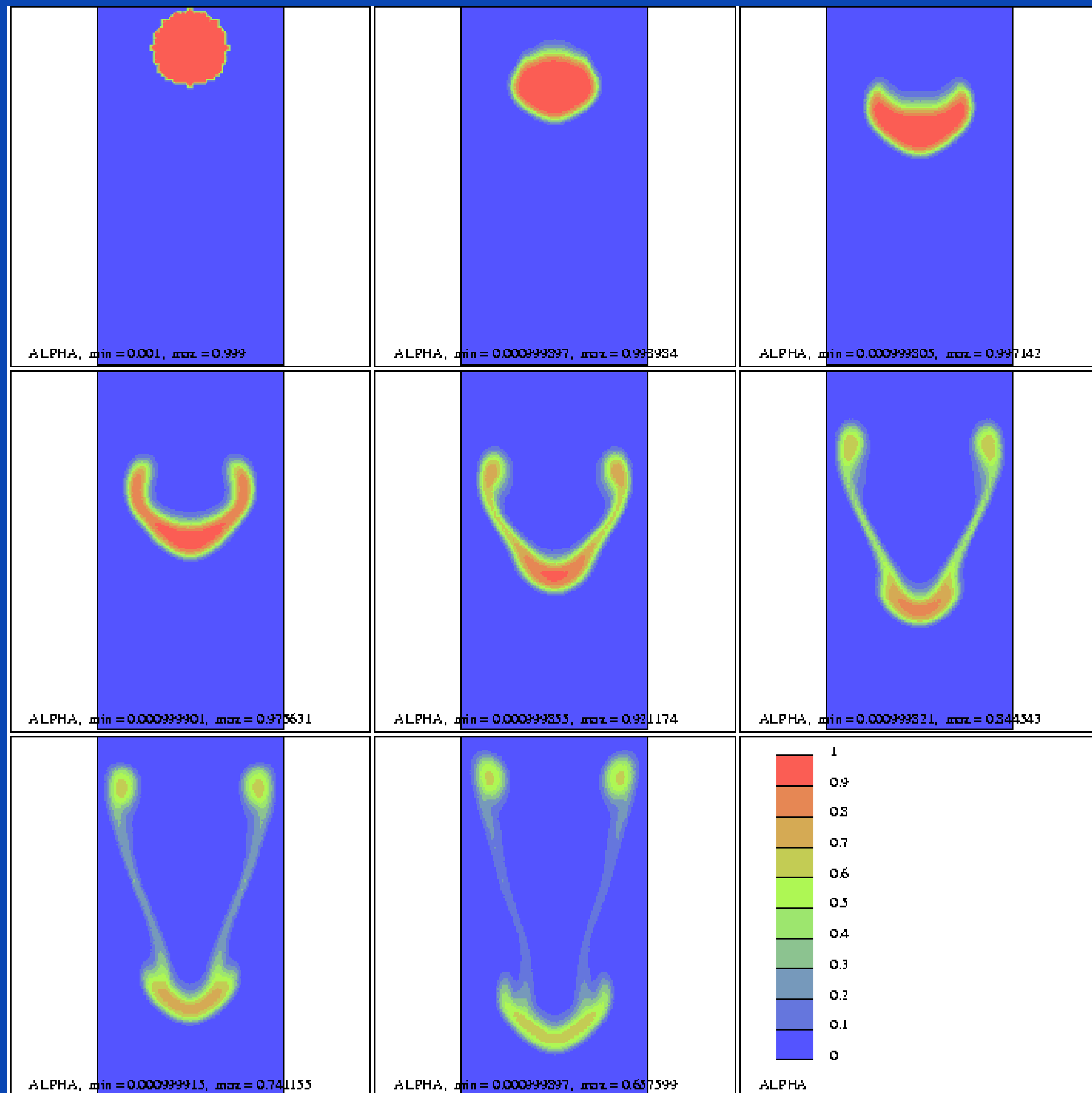
- Acoustic Riemann solver (Murrone-Guillard, Comp.Fluids 2003, JCP 2004))

- Second order limited MEV.

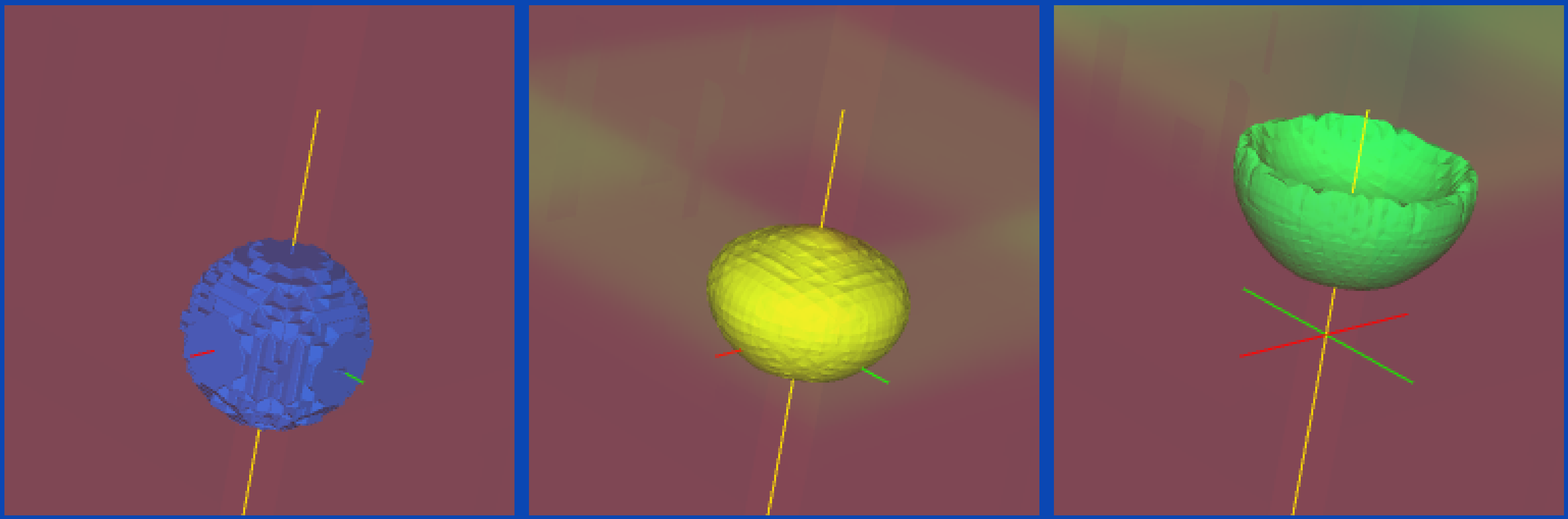
- Source term: upwind integration of $div\mathbf{u}$.

- 3D parallel extension with MEV (Wornom et al.)

Falling drop (2D)



Shock on a drop (3D)



Conclusions

The choice of a very simple scheme permits the proof of a very large set of properties:

- many conservation statements can be made exactly satisfied,

- Maximum principle and positivity, including the moving mesh case.

Today's challenge are:
- showing positivity statements for the new techniques of thick interfaces.
- showing the above properties for new schemes.