Comments on the stability of collocated finite volume schemes for Lagrangian hydrodynamics

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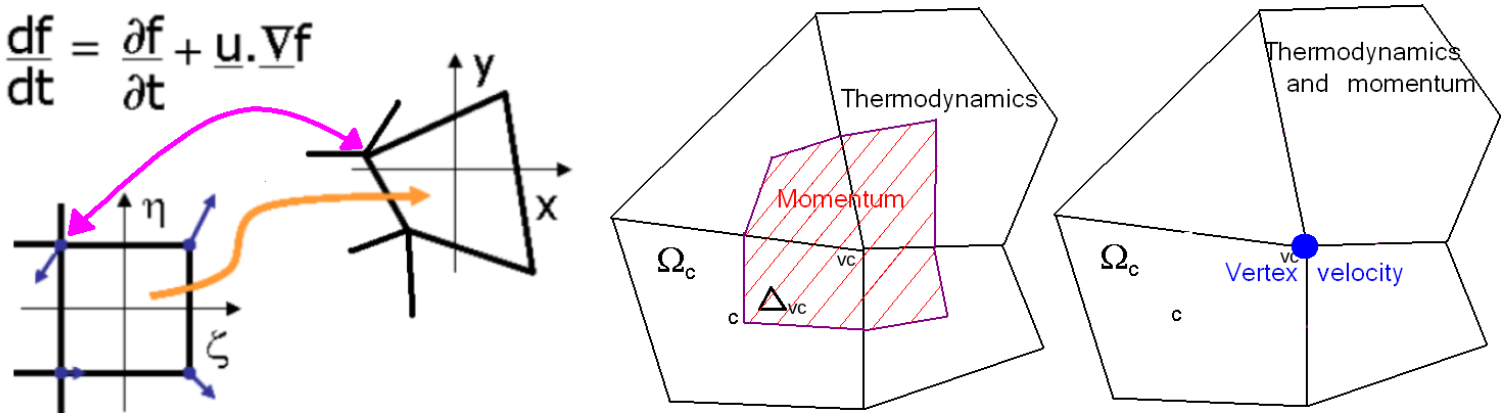
Introduction

Meaning:

- Lagrangian: moving (material motion) unstructured meshes
- Collocated: cell centered variables + Godunov's type resolution
- Staggered: collocated quantities except vertex centered velocities



Lagrange - Staggered and collocated discretisation.

- Collocated: cell-centered momentum, mass, total energy come from conservation laws. Vertex velocity comes from instantaneous Rankine-Hugoniot relations. Conservative form.
- Staggered: both momentum and internal energy updates come from evolution equations. Non conservative form.

Introduction

Two main motivations:

- Need of an alternative framework for common Lagrangian hydro based on staggered schemes (ICF calculations, hypervelocity problems).
- Especially for ALE simulations - well-posed problem wrt Lagrangian boundary conditions - less geometry, simpler.

Historical landmarks:

- Després and Mazeran (D&M) - GLACE scheme 2003 [6].
- Maire and Breil (PHM) - EUCLHYD scheme (CHIC code) 2004 [7].

Conservation laws

Gas dynamics conservation laws in Lagrangian formalism over a control volume $\Omega(t)$ and time t:

$$
(1)\quad
\begin{aligned}
&\frac{d}{dt}\int_{\Omega(t)} \rho dv = 0 && \textit{mass conservation}\\
&\frac{d}{dt}\int_{\Omega(t)} \rho \mathbf{u} dv + \int_{\partial\Omega(t)} p\mathbf{n} ds = 0 && \textit{momentum conservation}\\
&\frac{d}{dt}\int_{\Omega(t)} \rho E dv + \int_{\partial\Omega(t)} p\mathbf{u}.\mathbf{n} ds = 0 && \textit{energy conservation}\\
&\frac{d}{dt}\int_{\Omega(t)} dv - \int_{\partial\Omega(t)} \mathbf{u}.\mathbf{n} ds = 0 && \textit{GCL}
\end{aligned}
$$

Some properties

PE Entropy variation $\Longleftrightarrow$ increase of internal energy.

PA Acceleration and force are colinear.

PS Shear discontinuities may appear.

Conservation laws - Semi discrete form

Assumptions:

- every collocated variables $\in P_0(\Omega_c)$ (Finite Volume),
- $\cup_c \Omega_c$ defines a strict partitionning of the computational domain $\mathcal{D}$,
- no time discretisation.

A miracle? $\hookrightarrow$ Semi-discretisation mimics physics

Conservation laws - Semi discrete form

Following the precursors [6], [7], one can write on the whole $\mathcal{D}$ (excerpts):

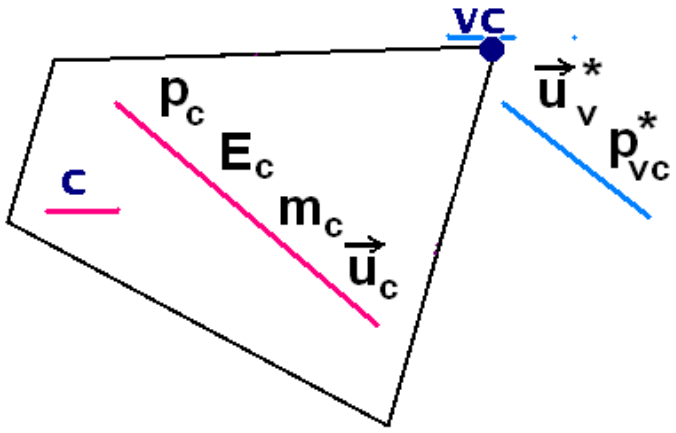
- Momentum conservation: $\dfrac{d}{dt}\left(\sum_c m_c\,\mathbf{u}_c\right) = -\sum_c\sum_{vc} L_{vc}\,\overline{\overline{p}}^*_{vc}\,\mathbf{n}_{vc} = 0$
- Total energy cons.: $\dfrac{d}{dt}\left(\sum_c m_c\,E_c\right) = -\sum_c\sum_{vc} L_{vc}\,\overline{\overline{p}}^*_{vc}\,\mathbf{u}^*_v.\mathbf{n}_{vc} = 0$

Notations

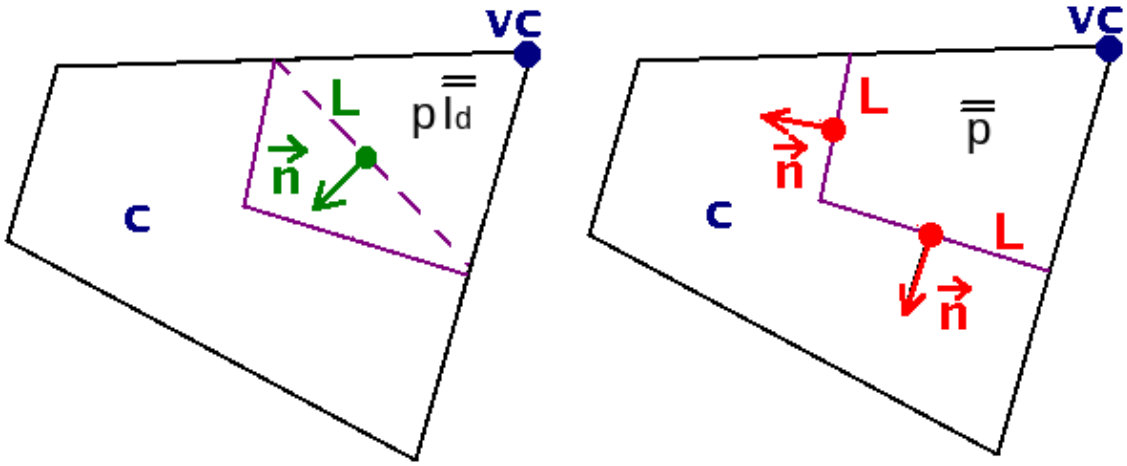
c stands for cell Ω_c,

v for vertex in $\mathcal{D}$,

vc for vertex v seen as node of cell c.



• Tensor pressure $\overline{\overline{p}}_{vc}$ is a consequence of one point (GLACE) or two points (EUCLHYD) quadrature associated to length L and outward normal vector $\mathbf{n}$ associated to node vc.



and:

$$\frac{d}{dt}\left|\Omega_c(t)\right| = \frac{d}{dt}\int_{\Omega_c(t)} dv = \int_{\partial\Omega_c(t)} \mathbf{u}^*.\mathbf{n}d\sigma \qquad (GCL)$$

(2)

$$\frac{d\mathbf{x}}{dt} = \mathbf{u}^*(t,\mathbf{x}) \text{ on } \partial\Omega_c(t) \qquad \textit{vertex motion}$$

But... no respect of property PS, a vertex stays unique

Choice shared by both staggered and collocated scheme.
(see S. Del Pino and Clair talks on slide lines)

Conservation laws - Semi discrete form

Momentum conservation: $\frac{d}{dt}\left(\sum_c m_c\,\mathbf{u}_c\right) = -\sum_{vc}\sum_c L_{vc}\,\overline{\overline{p}}^*_{vc}\,\mathbf{n}_{vc} = 0$ is verified

with the first sufficient condition: $\sum_{c\ni v} L_{vc}\,\overline{\overline{p}}^*_{vc}\,\mathbf{n}_{vc} = 0$, around v given.

i.e. around vertex that vertex v:

$$\boxed{\nabla p^*|_{vc} = 0}$$

We gets on every cell Ω_c:

- Momentum conservation $\quad m_c\,\frac{d}{dt}(\mathbf{u}_c) + \sum_{v\in c} L_{vc}\,\overline{\overline{p}}^*_{vc}\,\mathbf{n}_{vc} = 0$
- Total energy conservation $\quad m_c\,\frac{d}{dt}(E_c) + \sum_{v\in c} L_{vc}\,\overline{\overline{p}}^*_{vc}\,\mathbf{u}^*_v \,.\, \mathbf{n}_{vc} = 0$

Conservation laws - Semi discrete form

and:

- Kinetic energy evolution

$$m_c \frac{d}{dt}\widetilde{k_c} + \sum_{vc} L_{vc}\, \overline{\overline{p}}^*_{vc}\, \mathbf{n}_{vc} \,.\, \widetilde{\mathbf{u_c}} = 0$$

- Internal energy evolution

$$m_c \frac{d}{dt} e_c + \sum_{vc} L_{vc}\, \overline{\overline{p}}^*_{vc}\, \mathbf{n}_{vc} \left(\mathbf{u}^*_v - \widetilde{\mathbf{u_c}}\right) = 0$$

- Entropy variation

$$m_c\, T_c \frac{d}{dt} S_c + \sum_{vc} L_{vc} \underline{\left(\overline{\overline{p}}^*_{vc} - \widetilde{p_c}\right)\ \left(\mathbf{u}^*_v - \widetilde{\mathbf{u}_c}\right)\ \mathbf{n}_{vc}} = 0$$

Miracle?

Semi discretisation $\Longleftrightarrow$

$$\widetilde{\mathbf{u_c}} = \mathbf{u_c}(t^n),\ \widetilde{p_c} = p_c(t^n)\ and\ \widetilde{k_c} = .5 \times \mathbf{u_c}(t^n).\mathbf{u_c}(t^n),\ \varphi^n = \varphi(t^n)$$

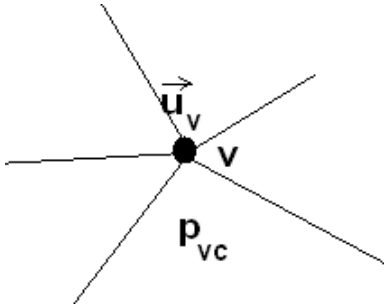
- A Second sufficient condition:

With: $m_c\, T_c\, \dfrac{d}{dt} S_c + \sum_{vc} L_{vc}\ (p^*_{vc} - \widetilde{p_c})\ (\mathbf{u}^*_v - \widetilde{\mathbf{u}_c})\ .\mathbf{n}_{vc} = 0$

Entropy inequality is fulfilled with:

$$\boxed{p^*_{vc} - {p_c}^n = -\rho^n_c s^n_c \left(\mathbf{u}^*_v - {\mathbf{u}_c}^n\right).\mathbf{n}_{vc}}$$

i.e. several subcell pressures are associated to a unique velocity field with the help of a (the) physical jump relation expressed with a characteristic cell centered velocity s_c.



Compatibility relations

In other words, entropy deposition is insured when:

$$\widetilde{\mathbf{u_c}} = \mathbf{u_c}(t^n),\ \widetilde{p_c} = p_c(t^n),\ \widetilde{k_c} = .5 \times \mathbf{u_c}(t^n).\mathbf{u_c}(t^n)$$

i.e. when jump relation is *explicit*.

But for Godunov algorithm, $\widetilde{\mathbf{u_c}} = .5\left[\mathbf{u_c}(t^n) + \mathbf{u_c}(t^{n+1})\right]$, and $\widetilde{p_c} = \ldots$ entropy inequality can be broken especially wrt *admissible* time step value in multidimensional problems... unless implicit discretisation.

No respect of property PE in the multidimension case

Pb shared by both staggered and collocated schemes.
(see A. Claisse's talk on conservation)

Compatibility relations

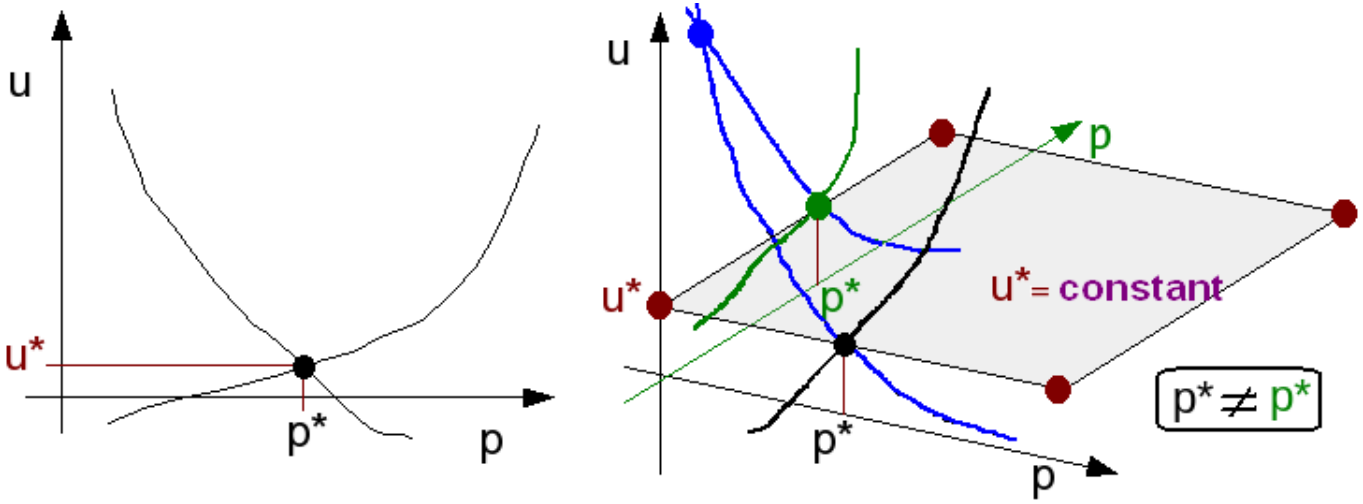
Summary:

- $\mathbf{u}_v^*$ constant $\in \mathbb{R}^2$

$\Longrightarrow$ one stays Lagrangian, $\quad \dfrac{d\mathbf{x}}{dt} = \mathbf{u}^*(t,\mathbf{x})$ *on* $\partial\Omega_c(t)$

- $\boldsymbol{\nabla} p^*|_v = 0$, one keeps *in average* a constant pressure field.

i.e.: the 2D approximated Riemann problem is defined by a strong condition on $\mathbf{u}^*$ and a weaker condition on the pressure p^* that induces a non monotonic distribution of p^* all around a node belonging to more than 3 cells.



Shock polars for a three-cells stencil - two d.o.f for p^*.

Scheme - u^* computation (excerpts)

Multiplying the constitutive relation $p^*_{vc} - p_c = \rho_c s_{vc} \left(\boldsymbol{u}^*_v - \mathbf{u}_c\right).\mathbf{n}_{vc}$
by $\times L_{vc}\mathbf{n}_{vc}$ and summing around a node v:

$$\sum_{vc} L^p_{vc}\overline{\overline{p}}^*_{vc}\mathbf{n}^p_{vc} - \sum_{vc} L^p_{vc}p_c\mathbf{n}^p_{vc} = \sum_{vc} \Lambda_{vc}\left[(\mathbf{u}^*_{vc} - \mathbf{u}_c).\mathbf{n}^p_{vc}\right]\mathbf{n}^p_{vc},\ \Lambda_{vc} = \rho_c s_{vc} L_{vc}$$

With the node constraint $\left(\boldsymbol{\nabla} p^*\right)_v = 0$:

$$\sum_{c \ni v} L_{vc}\left[\overline{\overline{p}}^*_{vc}\mathbf{n}_{vc}\right] = 0 \tag{3}$$

(D&M)-(PHM) get (...) the matrix form for vertex velocities:

$$\boxed{\overline{\overline{M}}^{v}\,\mathbf{u}^*_v = \sum_{c \ni v} \overline{\overline{M^{vc}}}\mathbf{u}_c - \sum_{c \ni v}\left[p_c L_{vc}\mathbf{n}_{vc}\right]}$$

with: $\overline{\overline{M}}^{vc} = \Lambda_{vc}(\mathbf{n}_{vc} \otimes \mathbf{n}_{vc})$ and $\overline{\overline{M}}^{v} = \sum_{c \ni v} \overline{\overline{M}}^{vc}$.

Scheme - u^* computation

- The update of vertex velocity $\mathbf{u}_v^*$ can be written as follows:

$$\mathbf{u}_v^* = \overline{\overline{M^v}}^{-1} \left\{ \sum_{c \ni v} \overline{\overline{M^{vc}}} \mathbf{u}_c \right\} - \overline{\overline{M^v}}^{-1} \mathbf{Grad}(p)$$

equivalent to:

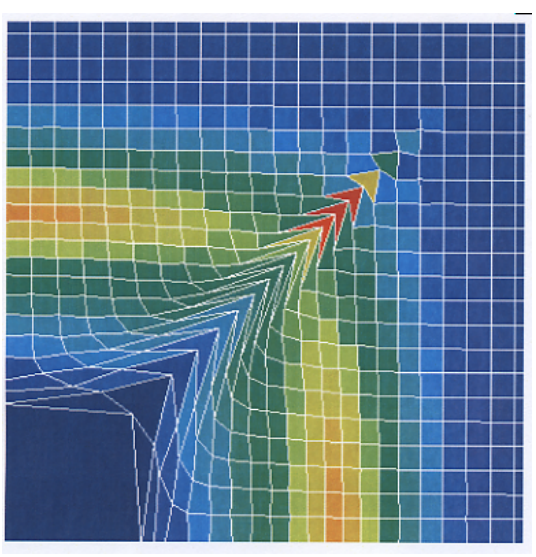
$$\overline{\overline{m}}^{-1} \mathbf{F} = \boldsymbol{\gamma}$$

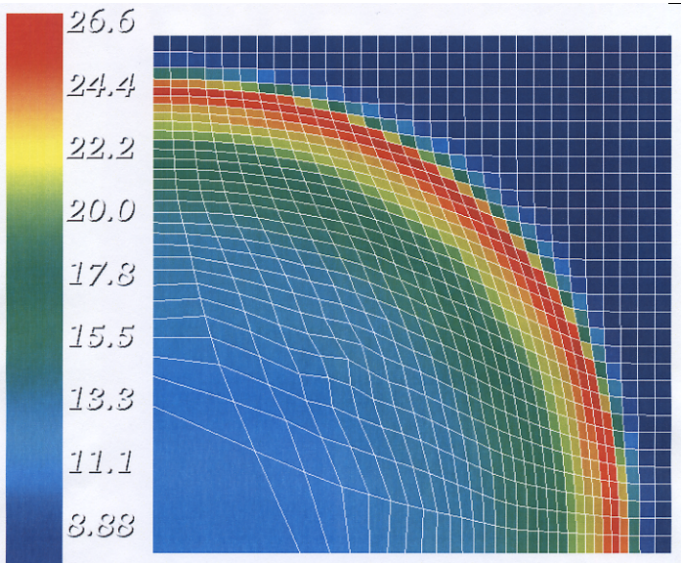
No respect of property PA - Deviation from force direction

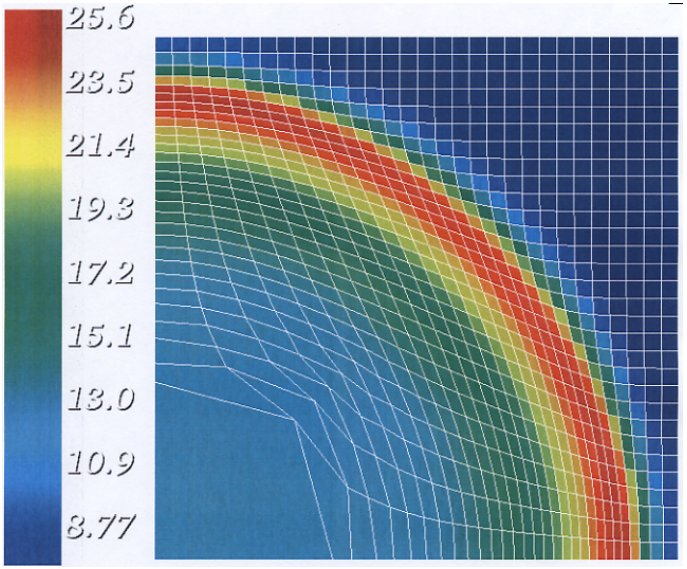
Collocated scheme only (see below).

That induces a specific kind of instabilities that usually spoiles computations.

Instabilities - Sedov like problem







Sedov like problem on an initially square grid. A high temperature initial source is located on one cell.

- *Left: Instabilities associated to* $\overline{\overline{M}}_v$ *with a one-point calculation of shock pressure (GLACE O(Δt,Δx)).*
- *Center: staggered scheme (HEMP O(Δx^2)) with tensor artificial visccosity, instabilities*
- *Right: regular solution obtained with a two-points calculation of shock pressure (EUCLHYD O(Δt,Δx)), some non convex cells.*

Notice: the first run source temperature is 100 $\times$ lesser than for the other runs.

Scheme - u^* computation

- **Goal**: weaken the anisotropic nature of the momentum balance.
- When: a priori (see Després-Labourasse [5] for complementary subcelling by way of subcells entropy deposition).
- Means: modification of the jump condition:
- Velocity-matrix $\overline{\overline{M}}^v = \sum_{c \ni v} \Lambda_{vc} (\mathbf{n}_{vc} \otimes \mathbf{n}_{vc}) = \sum_{c \ni v} \Lambda_{vc} \begin{pmatrix} n_x^2 & n_x n_y \\ n_x n_y & n_y^2 \end{pmatrix}_{vc}$.

being non diagonal,

How to increase the diagonal dominancy?

- Reminder: three basic items

♣ $\mathbf{u}_v^* \in \mathbb{R}^2$.

♡ $\boldsymbol{\nabla} p^*|_v = 0$.

♠ $p^* = \mathcal{R}(\mathbf{u}^*) \longleftrightarrow$ i.e. $p^* - p = \rho s (\mathbf{u}^* - \mathbf{u}).\boldsymbol{\zeta}, \forall \boldsymbol{\zeta}, \ |\boldsymbol{\zeta} = 1.|$

- Choice:

Items ♣ and ♡ are preserved (Lagrange without sliding, GCL). ... but one will *play* with ♠.

Anisotropy

Back to: $$m_c\, T_c\, \frac{d}{dt} S_c + \sum_{vc} L_{vc}\ (p^*_{vc} - \widetilde{p_c})\ (\mathbf{u}^*_v - \widetilde{\mathbf{u}_c})\ .\mathbf{n}_{vc} = 0$$

The standart relation is $$(p^*_{vc} - \widetilde{p_c}) = \rho_c s_c\, (\mathbf{u}^*_v - \widetilde{\mathbf{u}_c})\ .\mathbf{n}_{vc},$$

but $(p^*_{vc} - \widetilde{p_c})\, \mathbf{n}_{vc} = \rho_c s_c\, (\mathbf{u}^*_v - \widetilde{\mathbf{u}_c})$ is also compatible.

It leads (...) to:

$$\mathbf{u}^*_v \left(\sum_{c \ni v} \Lambda_{vc} \right) = \left(\sum_{c \ni v} \Lambda_{vc} \mathbf{u}_c \right) + \left(\sum_{c \ni v} p_c L_{vc} \mathbf{n}_{vc} \right),\ \Lambda_{vc} = \rho_c s_c L_v c$$

i.e. a spherical velocity-matrix.

But because $(p^*_{vc} - \widetilde{p_c})\, \mathbf{n}_{vc}.\mathbf{n}_{vc} = \rho_c s_c\, (\mathbf{u}^*_v - \widetilde{\mathbf{u}_c})\, \mathbf{n}_{vc}$ we get an overdetermined system:

$$\sum_{c \ni v} p_c L_{vc} \mathbf{n}_{vc} = \sum_{c \ni v} \Lambda_{vc}\, [\mathbf{u}^*_v - \mathbf{u}_c] = \sum_{c \ni v} \Lambda_{vc}\, [\mathbf{u}^*_v - \mathbf{u}_c]\, \mathbf{n}_{vc} \otimes \mathbf{n}_{vc}$$

$\Longrightarrow$ need of more complexity: $\boxed{p^*_{vc} \longmapsto \overline{\overline{p^*_{vc}}}}$ (add dof for p^*)

Anisotropy

We set: $\left(\overline{\overline{p^*_{vc}}} - p_c\overline{\overline{I}}\right).\mathbf{n}_{vc} = \Lambda_{vc}\left[\mathbf{u}^*_v - \mathbf{u}_c\right].$

But $\forall \mathbf{w},\ \mathbf{w} = (\mathbf{n}.\mathbf{n})\mathbf{w} = (\mathbf{w}\otimes\mathbf{n}).\mathbf{n},\ \forall \mathbf{n},\ |\mathbf{n}| = 1.$

$$\Longrightarrow \qquad \left(\overline{\overline{p^*_{vc}}} - p_c\overline{\overline{I}}\right).\mathbf{n}_{vc} = \Lambda_{vc}\left[(\mathbf{u}^*_v - \mathbf{u}_c)\otimes\mathbf{n}_{vc}\right].\mathbf{n}_{vc}$$

and we choose $\left(\overline{\overline{p^*_{vc}}} - p_c\overline{\overline{I}}\right) = \Lambda_{vc}\left[(\mathbf{u}^*_v - \mathbf{u}_c)\right]\otimes\mathbf{n}_{vc}.$

In order to get a symmetric relation (angular momentum), we write:

$$\left(\overline{\overline{p^*_{vc}}} - p_c\overline{\overline{I}}\right) = \Lambda_{vc}\left\{(\mathbf{u}^*_v - \mathbf{u}_c)\otimes\mathbf{n}_{vc} + \mathbf{n}_{vc}\otimes(\mathbf{u}^*_v - \mathbf{u}_c)\right\} + \overline{\overline{X}}$$

And condition: $\left(\overline{\overline{p^*_{vc}}} - p_c\overline{\overline{I}}\right)\mathbf{n}_{vc} = \Lambda_{vc}\left(\mathbf{u}^*_v - \mathbf{u}_c\right)$

gives $\overline{\overline{X}} = -\Lambda_{vc}\left(\mathbf{u}^*_v - \mathbf{u}_c\right)\left(\mathbf{n}_{vc}.\mathbf{n}_{vc}\right) \qquad \leftarrow \qquad (\mathbf{v}\otimes\mathbf{w}).\mathbf{v} = (\mathbf{v}.\mathbf{v})\mathbf{w}$

Anisotropy

But no more miracle!

You noticed that's only cheap tautology and in practice we must introduce parameters a and b such that:

$$\overline{\overline{p^*_{vc}}} = p_c \overline{\overline{I}} + \Lambda_{vc} \left[a \boldsymbol{\nabla} \left(\mathbf{u}^*_v - \mathbf{u}_c \right) + a \boldsymbol{\nabla}^T \left(\mathbf{u}^*_v - \mathbf{u}_c \right) + c \boldsymbol{\nabla} . \left(\mathbf{u}^*_v - \mathbf{u}_c \right) \overline{\overline{I}} \right]$$

with (1D compatibility): $2a + c = 1$, and with the underlying relations:

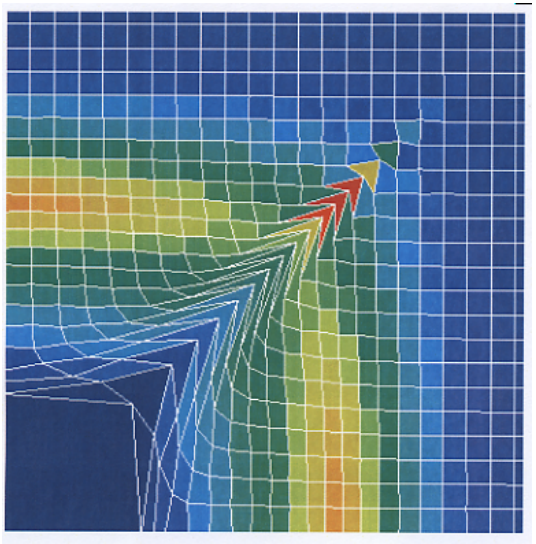
$$\int_\Omega \boldsymbol{\nabla} \mathbf{w} dv = \int_{\partial\Omega} (\mathbf{w} \otimes \mathbf{n}) \, dl, \quad \int_\Omega (\boldsymbol{\nabla} \mathbf{w})^T dv = \int_{\partial\Omega} (\mathbf{n} \otimes \mathbf{w}) \, dl, \quad \int_\Omega \boldsymbol{\nabla} . \mathbf{w} dv = \int_{\partial\Omega} \mathbf{w} . \mathbf{n} dl$$

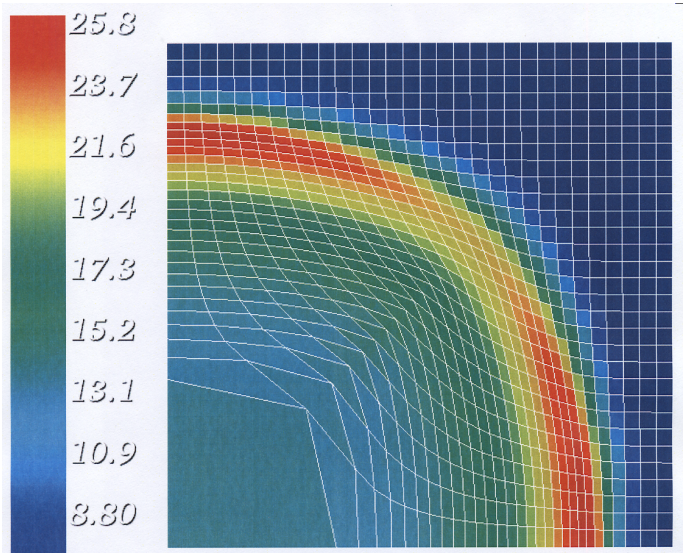
The ratio $r = \dfrac{a}{c}$ measures how the extra-diagonal terms are important.

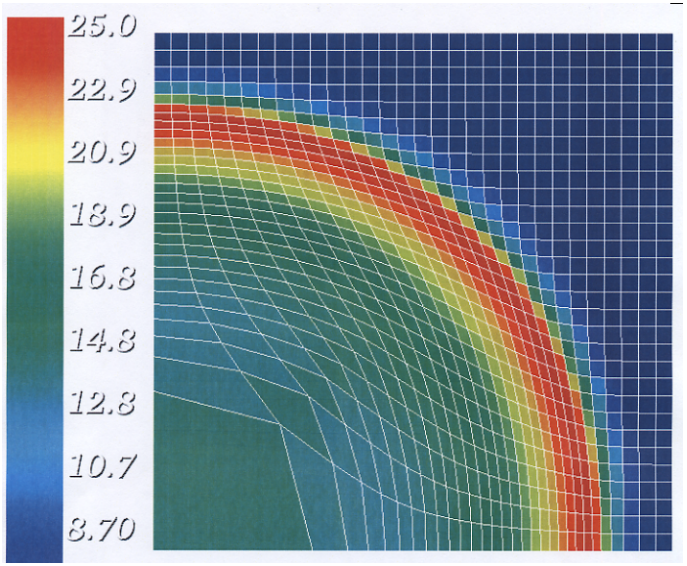
In pactice a value of $r = 10^{-2}$ can be sufficient.

... no more spherical velocity matrix but at least extra diag terms are weakened.

Consequences - Sedov like problem





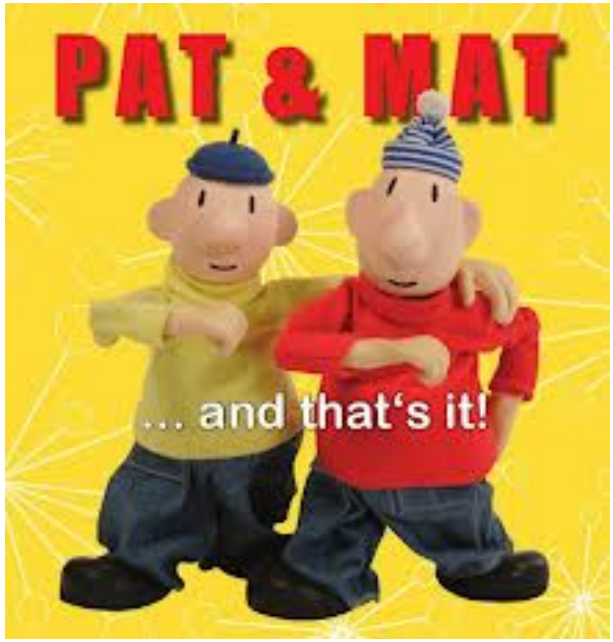


- *Sedov like problem on an initially square grid. A high temperature initial source is located on one cell.*
- *Left: Instabilities associated to* $\overline{\overline{M}}_v$ *with a one-point calculation of shock pressure (GLACE O(Δx)).*
- *Center: No diagonal term.*
- *Right: regular solution obtained with a two-points calculation of shock pressure (EUCLHYD O(Δx)).*

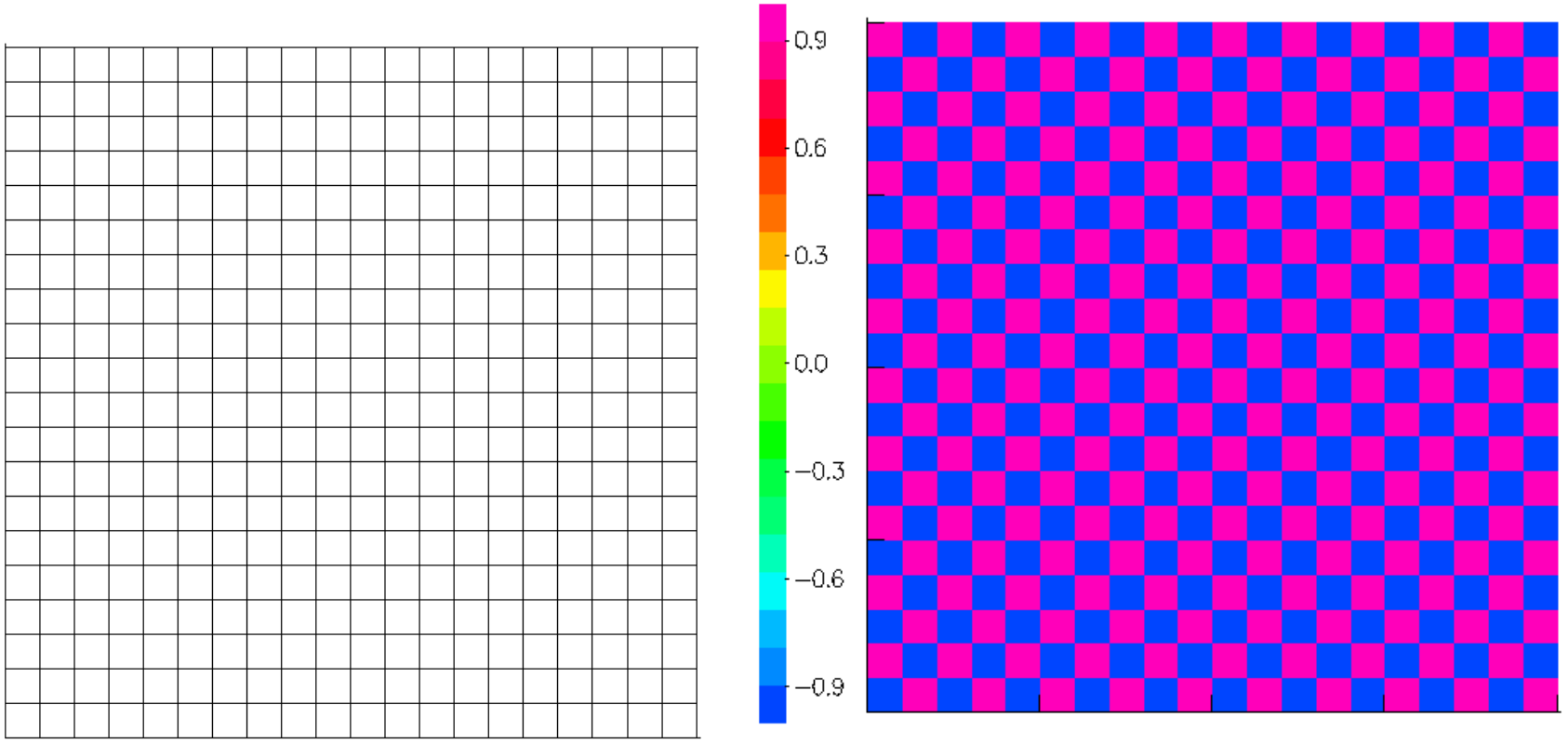
Two behaviour test problems

Now we present two "behavior test problems"... that do not correspond to any physics but show how schemes behave.

- Test 1: "Drifting checkerboard".
- Test 2: "Pulsing checkerboard".



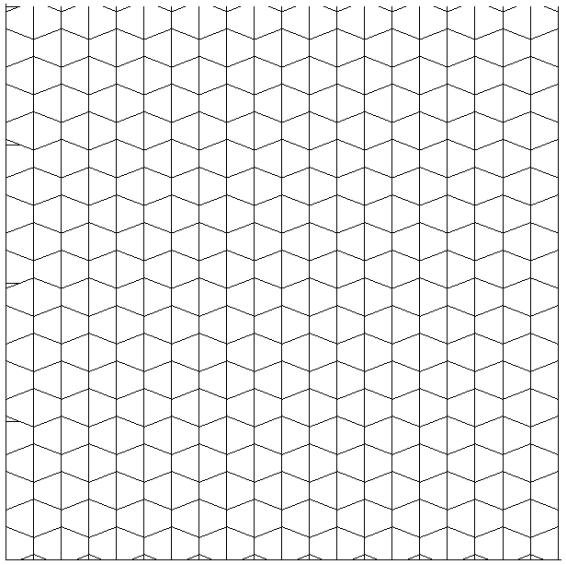
"Drifting checkerboard"

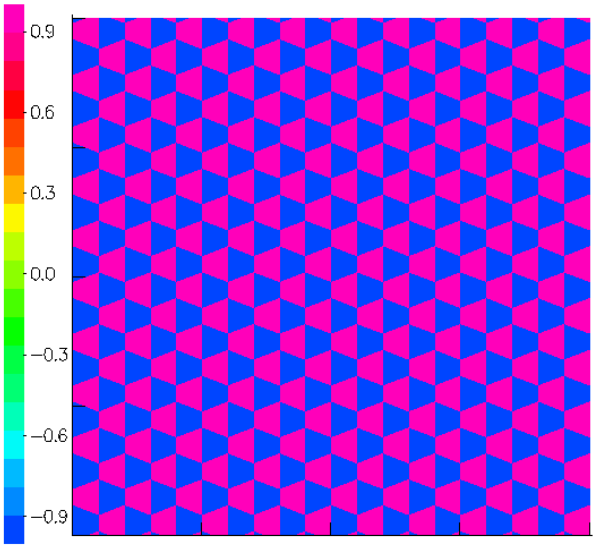


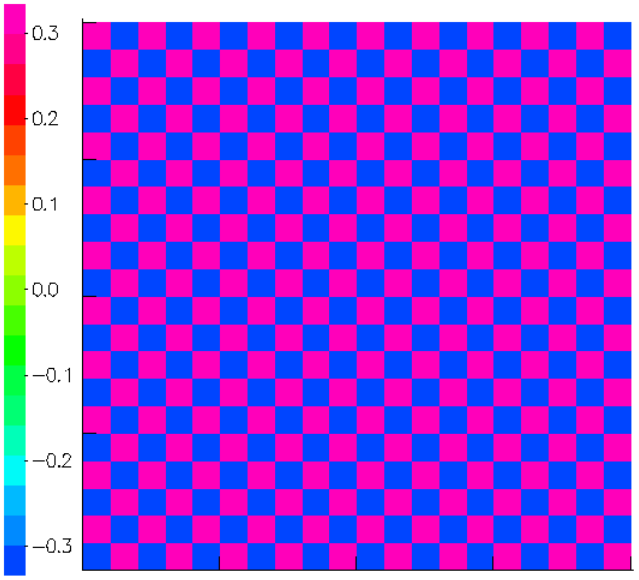
Initialisation : grid ——————————- cells horizontal velocity.

Uniform initialisation except for x-velocity (+1,-1) profile.

"Drifting checkerboard"





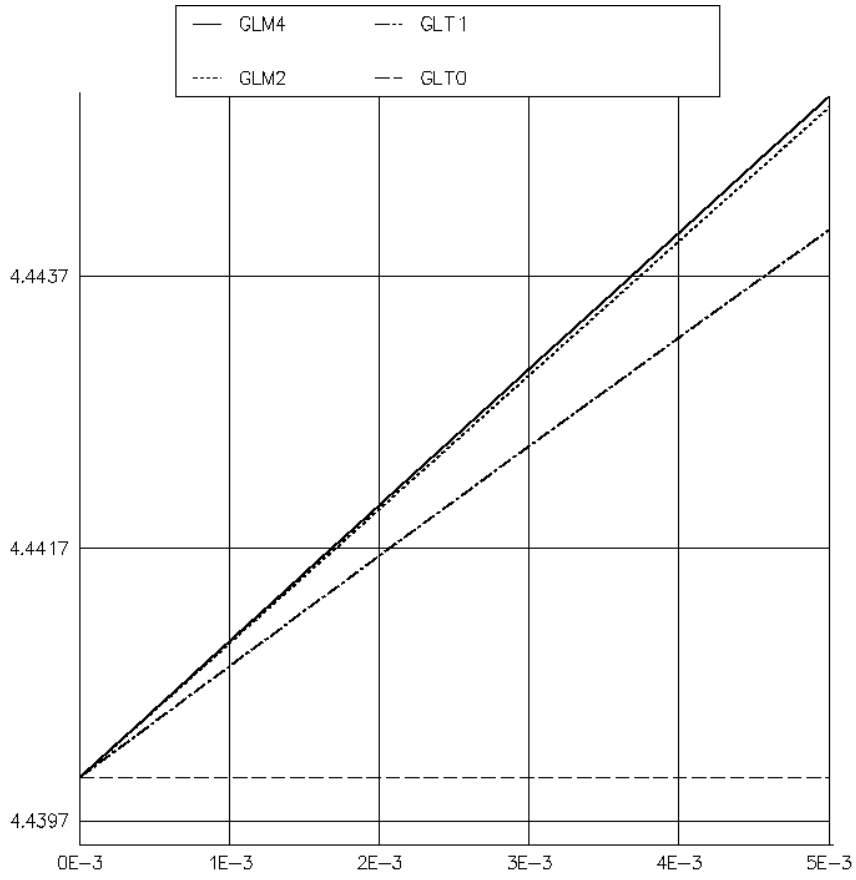


grid-GLACE ———- *velocity-GLACE* ——— *velocity-EUCLHYD.*

Node drift in y-direction with GLACE without smearing of cell velocities (cf. scale). In the contrary for EUCLHYD, no artificial deformation but smearing.

Such behavior that affects real calculations shows how the violation of gas dynamics law when mass matrices are not spherical affects the results.

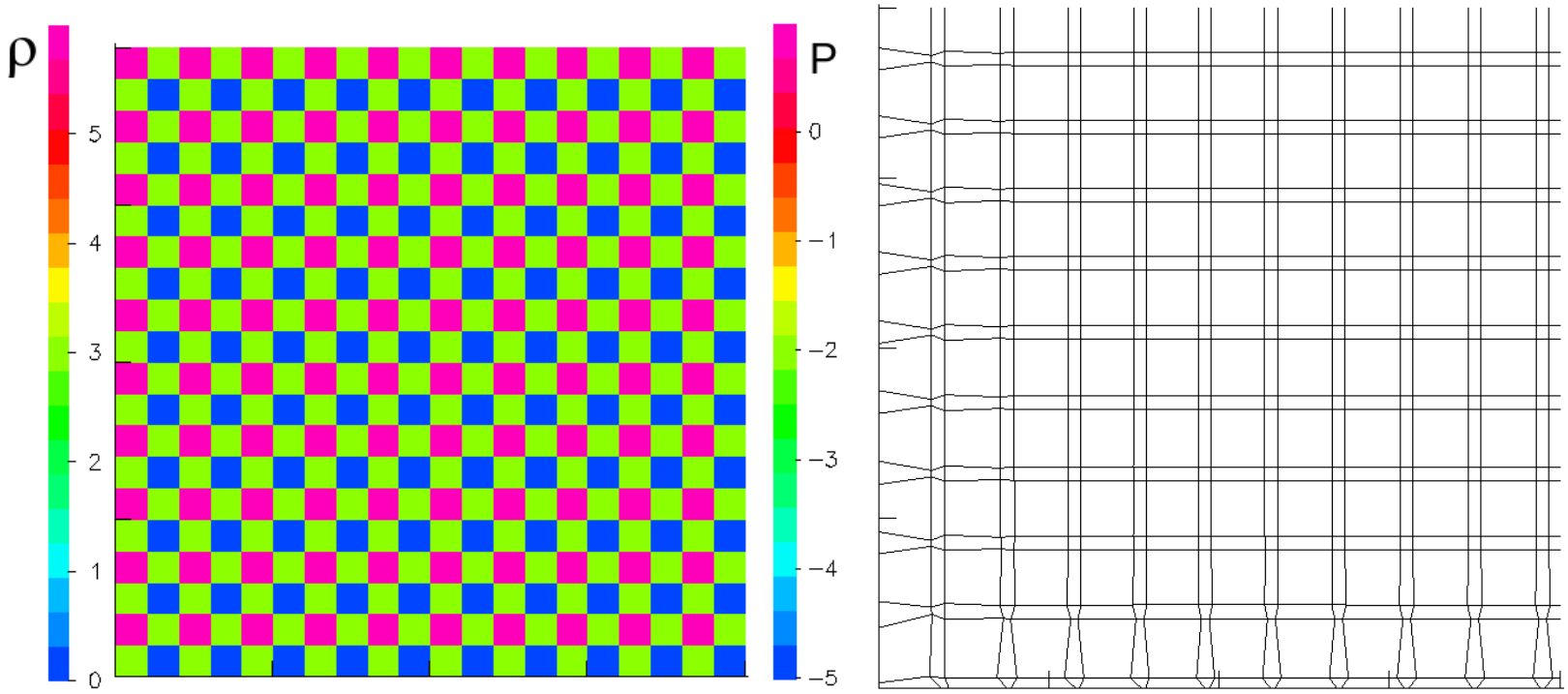
"Drifting checkerboard"



Y-coordinate vs time
of a given vertex
Smearing of extra-diagonal
terms for GLACE
continuous $r = 10^{-4}$,
little broken $r = 10^{-2}$,
chain-dotted $r = 10^{-1}$,
large broken $r = 1$.

Drift decreases as $r \nearrow$ and disappears if extra-diagonal terms are cancelled.

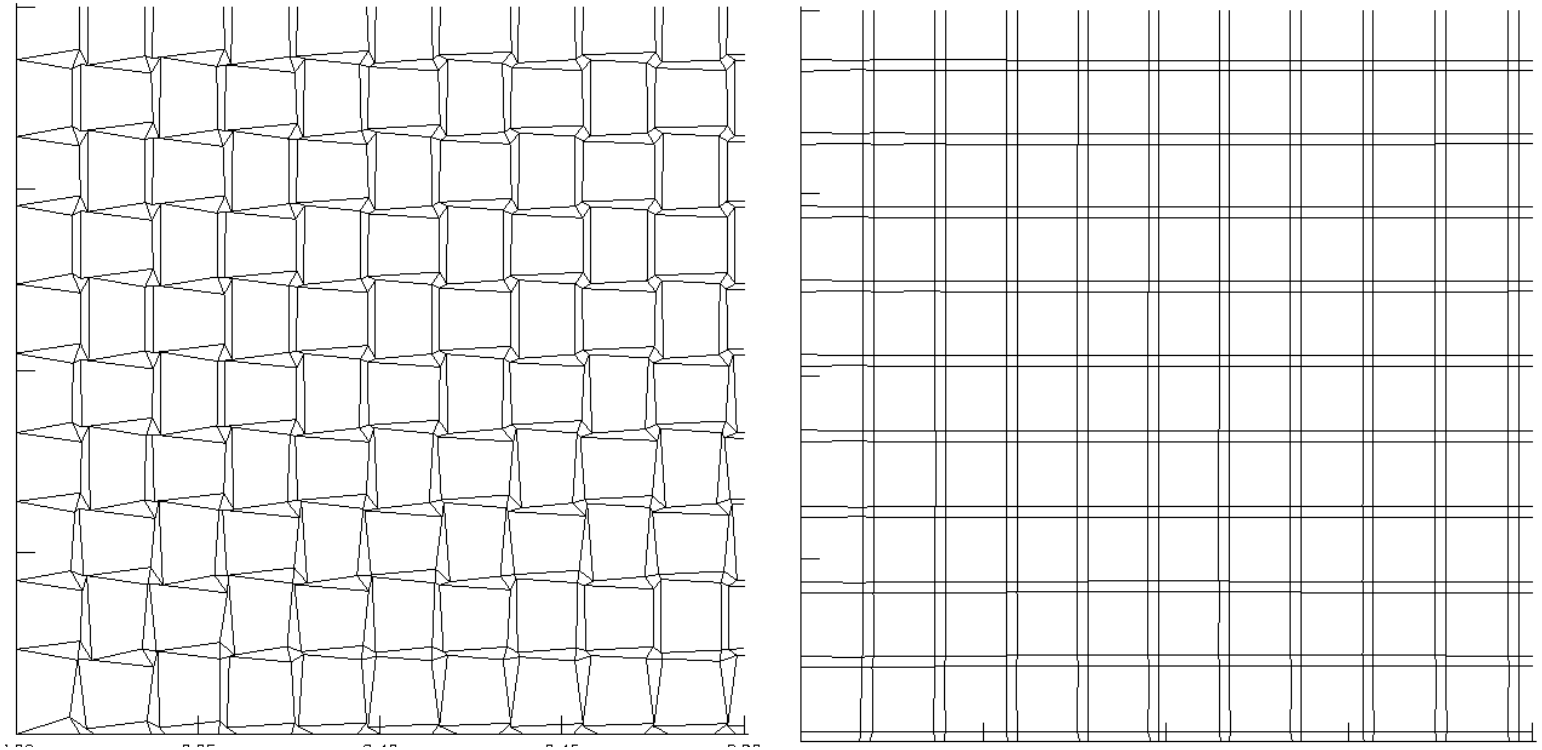
"Pulsing checkerboard" - Staggered scheme



Uniform initialisation except for density and pressure (log scale) and mesh for Schulz artificial viscosity (staggered scheme)

Non-uniform thermodynamics states induce cells pulsations. Instabilities appear at domain boundary (sliding line), are damped and propagate inside the computational domain depending on the scheme.

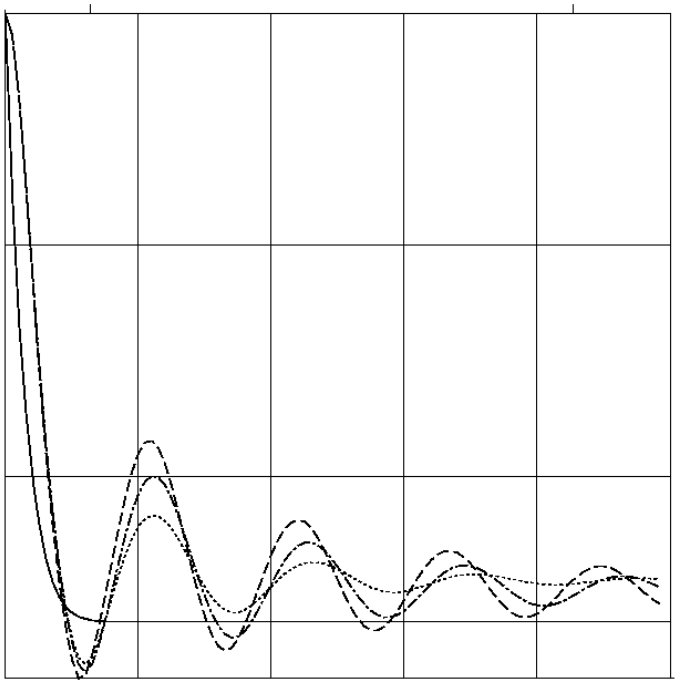
"Pulsing checkerboard" - Collocated scheme



GLACE ——————————— EUCLHYD

Collocated schemes: instabilities on the whole domain for GLACE. They remain *quite* tiny and stay near the boundary for EUCLHYD.

"Pulsing checkerboard"



Density vs time for a cell having an initial high density.

Respectively: continuous collocated scheme GLACE and EUCLHYD; little broken staggered scheme Shulz-like, chain-dotted staggered scheme vertex Tensor, dotted staggered scheme Schulz. Pulsations if staggered scheme but none for collocated schemes because of locking and the fact that for such schemes the cells vertex have no inertia history (momentum, kinetic energy) due to the lack of *unsteadiness* of the algebraic jump relations and the O(Δt).

Conclusion

- GLACE and EUCLHYD are good candidates for industrial applications (*see literature*).
- Extra-diagonal terms deserve to be... *not to be*. Several tracks, only shown here.
- Because of the full MultiD context of Lagrange framework some extra fix-like treatments are necessary. *But that's Lagrange!*.
- Time and space accuracy is a key point.

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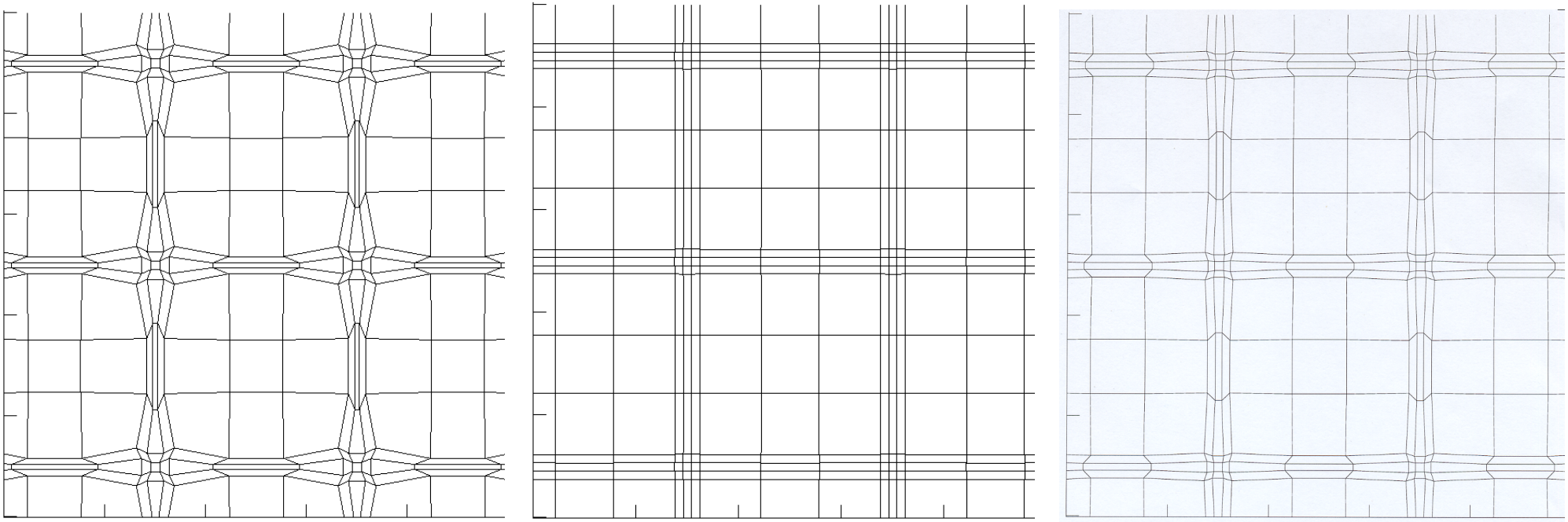
"Pulsing checkerboard"

Constants states are now discretize by a 3x3 cell block.



GLACE ——————— EUCLHYD ——————— $[p^* \equiv]$

Meshes obtained with GLACE, EUCLHYD and $[p^* \equiv] \, constant$ (see below): stiffness with EUCLHYD, distorsion with GLACE. Notice if extra-diagonal terms are cancelled in GLACE scheme, one obtains EUCLHYD results. Intermediate results with $[p^* \equiv] \, constant$.

$p^* \equiv$ constant on dual mesh

p_v^* is taken uniformly constant around node v and instead of the previous 2x2 system for $\mathbf{u}^*$ one writes two scalar relations:

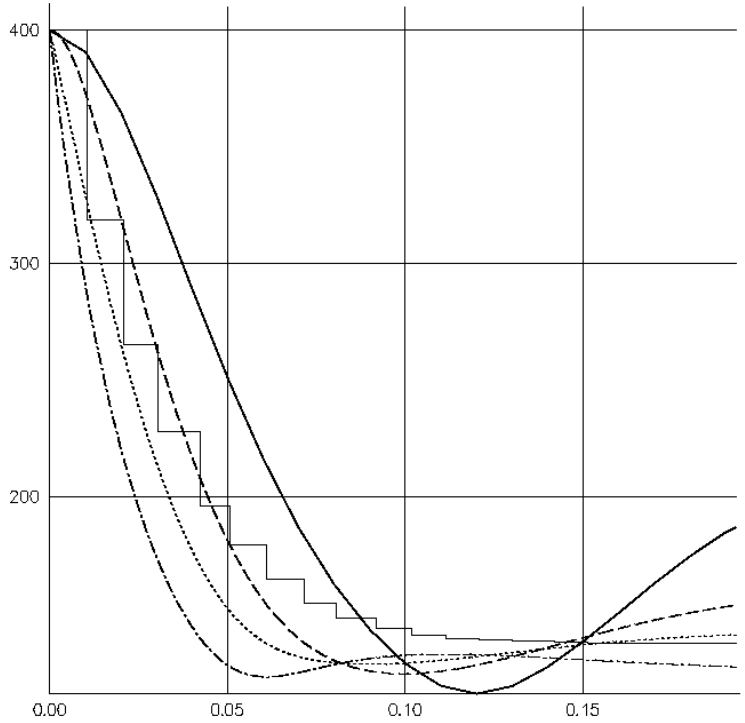
$$\mathbf{u}_v^* = \frac{\sum_{c \ni v} \rho_c s_c L_{vc}^d \mathbf{u}_c - \sum_{c \ni v} [p_c L_{vc} \mathbf{n}_{vc}]}{\sum_{c \ni v} \rho_c s_c L_{vc}^d} \qquad p_v^* = \frac{\sum_{c \ni v} \frac{L_{vc}^d}{\rho_c s_c} p_c - \sum_{c \ni v} [L_{vc} \mathbf{u}_{vc}.\mathbf{n}_{vc}]}{\sum_{c \ni v} \frac{L_{vc}^d}{\rho_c s_c}}$$

In 1D it reduces to:

$$u_v^* = \rho_l s_l u_l + \rho_r s_r u_r - \frac{(p_l - p_r)}{\rho_l s_l + \rho_r s_r}, \qquad p_v^* = \rho_r s_r p_l + \rho_l s_l p_r - \frac{(u_{pl} - u_{pr})}{\rho_l s_l + \rho_r s_r}$$

- No more relation $\left\{ p^* = \mathcal{R}\left(\mathbf{u}^*\right) \text{ and } \mathbf{u}^* = \mathcal{R}^{-1}\left(p^*\right) \right\}$!!!
- Even less good entropy !!!!!!
- But $\overline{\overline{M}}^v = \sum_{c \ni v} \rho_c s_c L_{vc}^d \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$!

"Pulsing checkerboard"



Density(t)

Density vs time for cells having initially a high density value. Continuous line = vertex tensor (1x1 block); piecewise constant = EUCLHYD (1x1) other lines = density of 3 cells obtained with EUCLHYD (3x3). In this last case, pulsations are present with low amplitudes. EUCLHYD is O(Δt,Δx) here.