Asymptotic-Preserving Schemes for Complex Fluids

P. Degond

Department of Mathematics

Imperial College London

United Kingdom

pdegond@imperial.ac.uk (see http://sites.google.com/site/degond/)

Summary

1. Small Mach-number
2. Jamming
3. Multiphase flows
4. Conclusion

1. Small Mach number

joint work with F. Cordier & A. Kumbaro (CEA)

J. Comput. Phys. 231 (2012), 5685-5704

Framework

Problems with coexistence of small & finite Mach numbers

e.g. jets, nozzles, phase changes

When Mach number $\varepsilon \to 0$

compressible $\to$ incompressible

c.f. Klainerman & Majda

Framework: design method for compressible flows

that can handle this limit: all-speed scheme

using Asymptotic-Preserving (AP) methodology

$$\begin{array}{ccc} P^{\varepsilon,h} & \xrightarrow{h\to 0} & P^{\varepsilon} \\ \downarrow{\scriptstyle \varepsilon\to 0} & & \downarrow{\scriptstyle \varepsilon\to 0} \\ P^{0,h} & \xrightarrow{h\to 0} & P^{0} \end{array}$$

Goal

Scheme for compressible Euler

- converges to incompressible Euler as $\varepsilon \to 0$
- full Euler/NS, general EOS
- conservative, 2nd order (MUSCL)
- CFL independent of ε

Previous work on isentropic Euler

- 1st order: D. Tang, CiCP 11 ; 2nd order Tang, KRM 12
- related work: D., Jin, Liu, 07 ; Haack, Jin, Liu, CiCP 12

Other methods

- Analysis: Guillard, Dellacherie, . . .
- Preconditioning: Chorin; Turkel; van Leer; Roe, . . .
- Implicit treatment: Nerrynck; Larrouturou; Klein; . . .
- Hodge decomposition of u: Collela; D., Jin, Liu . . .
- Pressure correction: Patankar; Munz; Fedkiw; Wesseling; Zienkiewicz . . .
- ICE (Implicit Continuous Eulerian): Harlow & Amsden, 76 . . .

Full Euler eq. (scaled form)

$$\partial_t \rho + \nabla \cdot \rho \mathbf{u} = 0$$

$$\partial_t \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \varepsilon^{-2} \nabla p = 0$$

$$\partial_t \rho E + \nabla \cdot (\rho H \mathbf{u}) = 0$$

$$E = e + \varepsilon^2 |u|^2/2, \quad H = h + \varepsilon^2 |u|^2/2, \quad h = e + p/\rho$$

$$\rho = \rho(p, h)$$

Time semi-discrete scheme

$$\Delta t^{-1}(\rho^{n+1} - \rho^n) + \nabla \cdot (\rho \mathbf{u})^n = 0$$

$$\Delta t^{-1}((\rho \mathbf{u})^{n+1} - (\rho \mathbf{u})^n) + \nabla \cdot ((\rho \mathbf{u})^n \otimes \mathbf{u}^n + \alpha p^n \mathrm{Id}) + (\varepsilon^{-2} - \alpha) \nabla p^{n+1} = 0$$

$$\Delta t^{-1}((\rho E)^{n+1} - (\rho E)^n) + \nabla \cdot H^n (\rho \mathbf{u})^{n+1} = 0$$

$$(\rho E)^{n+1} = (\rho e)^{n+1} + \varepsilon^2 \rho^n |u^n|^2/2, \quad (\rho H)^{n+1} = (\rho h)^{n+1} + \varepsilon^2 \rho^n |u^n|^2/2$$

$$h^{n+1} = e^{n+1} + p^{n+1}/\rho^{n+1}, \quad \rho^{n+1} = \rho(p^{n+1}, h^{n+1})$$

Eliminate $(\rho \mathbf{u})^{n+1}$ in energy eq. using momentum eq.

$$(\rho E)^{n+1} - \Delta t^2 (\varepsilon^{-2} - \alpha) \nabla \cdot \big(H^n \nabla p^{n+1} \big) = \phi\big(\rho^n, (\rho \mathbf{u})^n, (\rho E)^n \big)$$

For perfect gas EOS, $e = p/(\gamma - 1)$

$$E^{n+1} = (\gamma - 1)^{-1} p^{n+1} + \varepsilon^2 \rho^n |u^n|^2 / 2$$

$$p^{n+1} - \Delta t^2 (\gamma - 1)(\varepsilon^{-2} - \alpha) \nabla \cdot \big(H^n \nabla p^{n+1} \big) = \tilde{\phi}\big(\rho^n, (\rho \mathbf{u})^n, (\rho E)^n \big)$$

ρ^{n+1} precalculated by mass conservation eq.

For general EOS $\rho = \rho(p, h)$

$$E^{n+1} = (\rho h)^{n+1} - p^{n+1} + \varepsilon^2 \rho^n |u^n|^2 / 2$$

$$\begin{cases} (\rho h)^{n+1} - p^{n+1} - \Delta t^2 (\varepsilon^{-2} - \alpha) \nabla \cdot \big(H^n \nabla p^{n+1} \big) = \hat{\phi}\big(\rho^n, (\rho \mathbf{u})^n, (\rho E)^n \big) \\ \rho(p^{n+1}, h^{n+1}) = \rho^{n+1} \end{cases}$$

System solved for (p^{n+1}, h^{n+1}) by Newton's method

Properties

Spatial discretization

- Implicit terms $\longrightarrow$ centered
- Explicit terms $\longrightarrow$ Rusanov (local Lax-Friedrichs)
- 2nd order by MUSCL + RK2CN in time

AP property

When $\varepsilon \to 0$, scheme consistent with

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$p = \text{Cst} \quad \text{under suitable boundary conditions}$$

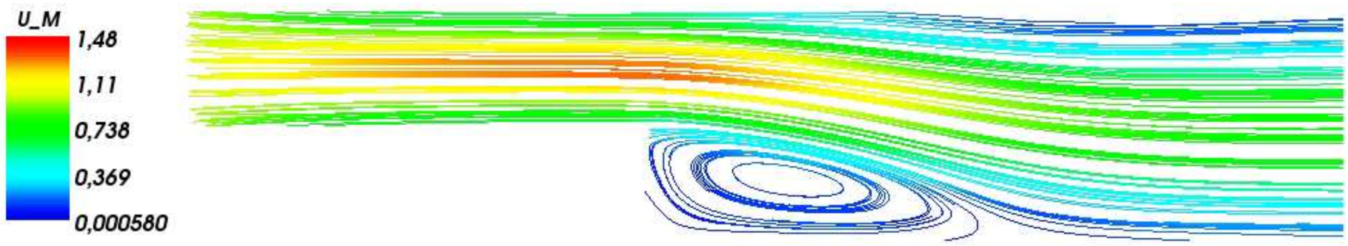
$$\partial_t (\rho e) + \nabla \cdot (\rho h \mathbf{u}) = 0$$

$$h = e - p/\rho, \quad \rho = \rho(p, h)$$

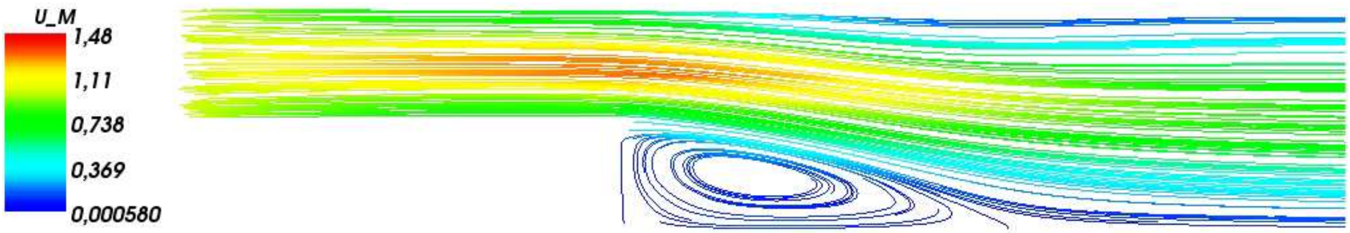
$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla \pi = 0$$

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

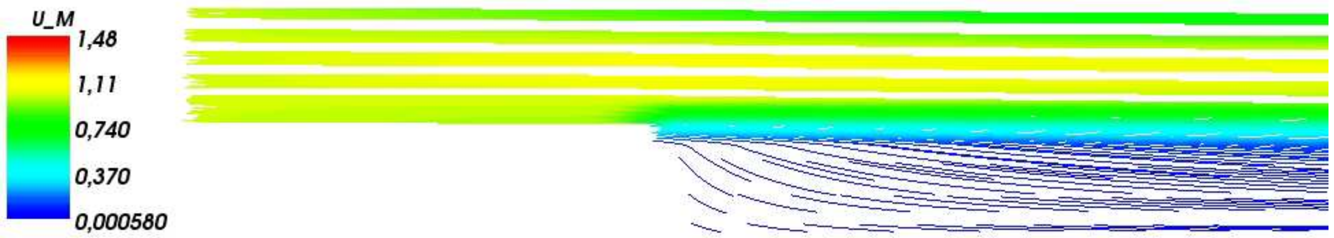
Backwards facing step



(a) Second-order Asymptotic Preserving scheme

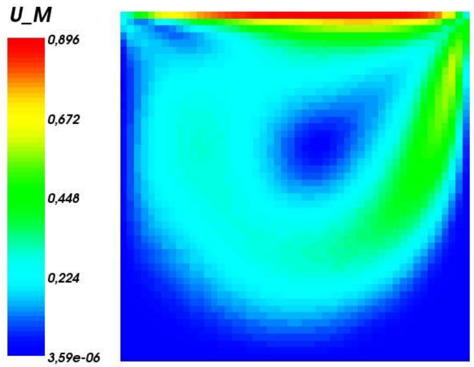


(b) Low Mach Roe scheme

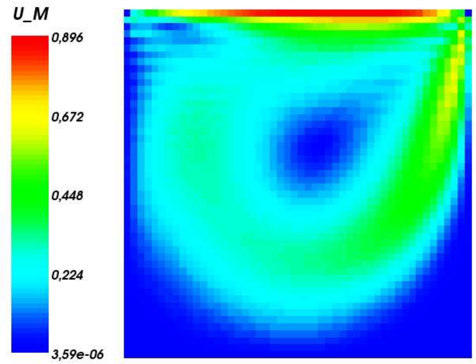


(c) Roe scheme

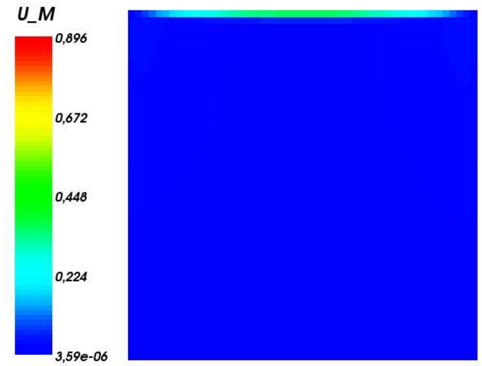
Lid-driven cavity



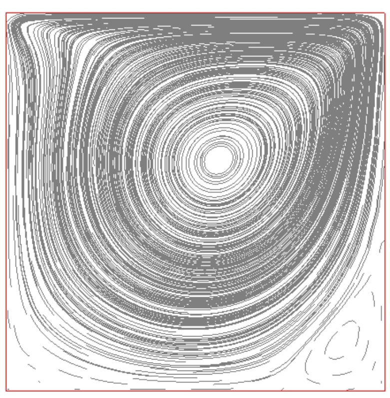
(d) AP scheme



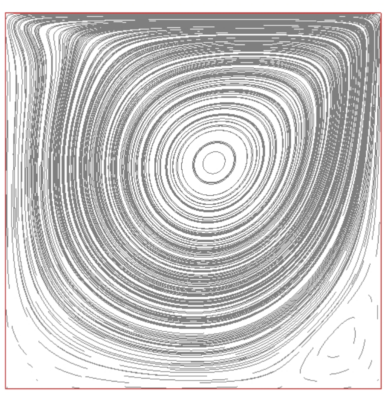
(e) Low Mach



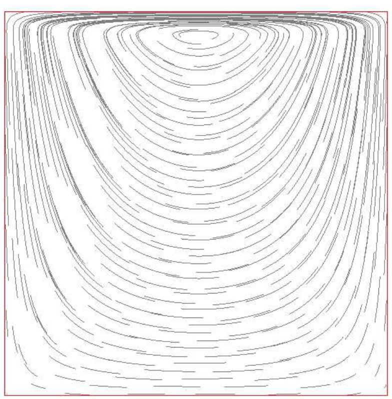
(f) Roe scheme



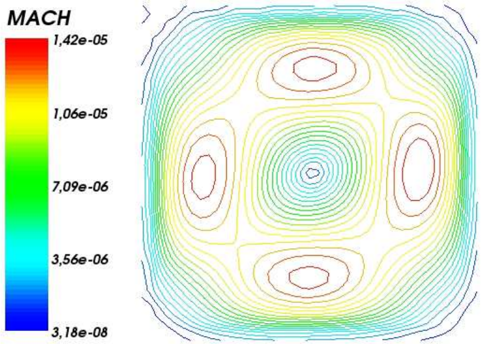
(g) AP scheme



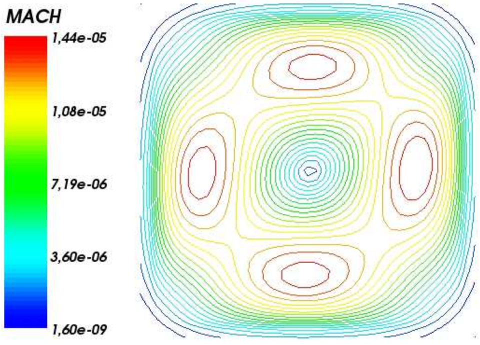
(h) Low Mach



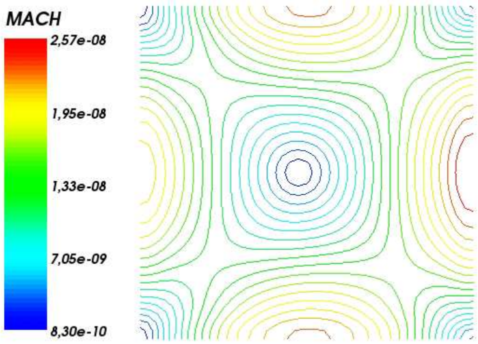
(i) Roe scheme



(j) AP scheme



(k) Low Mach



(l) Roe scheme

2. Jamming

with L. Navoret (Strasbourg) & Jiale Hua (Donghua U. Shanghai)

J. Comput. Phys. 230 (2011) 8057-8088 & 237 (2013) 299-319

Scaled Euler system

$$\partial_t \rho + \nabla(\rho u) = 0$$

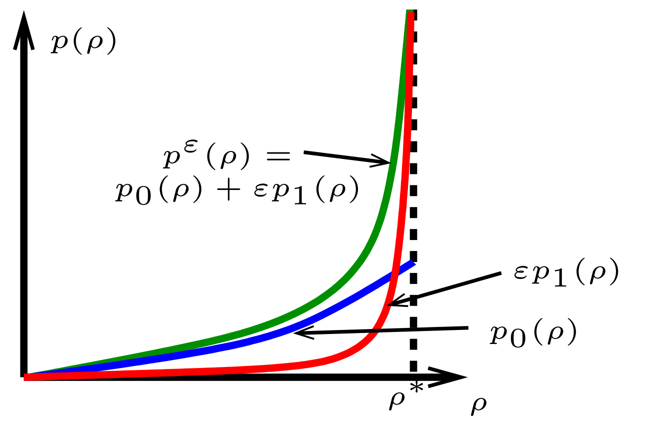
$$\partial_t(\rho u) + \nabla(\rho u \otimes u) + \nabla\big(p_0(\rho) + \varepsilon p_1(\rho)\big) = 0$$

$p_0(\rho) \sim \rho^{\gamma_0}$ background pressure

$p_1(\rho) \sim \left(\frac{\rho\rho^*}{\rho^*-\rho}\right)^{\gamma_1}$ singular pressure

p_1 maintains the bound $\rho \leq \rho^*$

$p^\varepsilon(\rho) = p_0(\rho) + \varepsilon p_1(\rho)$



Literature

1D case: Bouchut et al, J. Nonlinear Sci 00; Berthelin, M3AS 02

Further studies: Labbe Maitre, MAA 13, Perrin Zatorska, CPDE 15

Traffic: Berthelin etal, ARMA 08, M3AS 08, K3M 12; D. Delitala, KRM 08

Hele Shaw: Perthame et al, ARMA 14, Interf. free bdry 14, M3AS 14

Formal limit $\varepsilon \longrightarrow 0$

Free boundary problem:

between compressible and incompressible region

If $\rho < \rho^*$: compressible Euler

$$\partial_t \rho + \nabla(\rho u) = 0$$

$$\partial_t(\rho u) + \nabla(\rho u \otimes u) + \nabla p_0(\rho) = 0$$

Note: if $p_0 = 0$: pressureless gas dynamics

If $\rho = \rho^*$: incompressible Euler

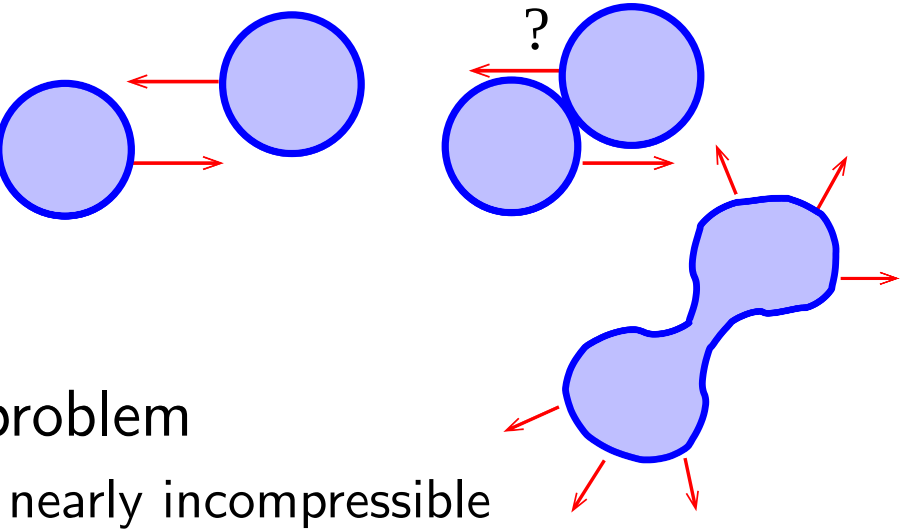
$$\nabla \cdot u = 0$$

$$\rho^* \big(\partial_t u + (u \cdot \nabla) u\big) + \nabla \bar{p} = 0$$

Problem:

What relations at interface between the 2 regions ?
Soved in [D Navoret Hua] if interface smooth
If not (e.g. if topology changes): open problem

Solving the ε-dependent problem



Example of topology change

- droplet collision
- result possibly depends on p_1

Solution: solve the ε-dependent problem

- but for small ε and $\rho \approx \rho^*$: flow is nearly incompressible
- i.e. low Mach: requires use of AP scheme

Strategy: adapt previously developed AP scheme

- note: difficulty if $p_0 = 0$ (infinite Mach limit)

c.f. numerical results for droplet collision

Hydrodynamic model for self-propelled particles:

constant velocity
interact through alignment
subject to noise

$$\partial_t \rho + \nabla(\rho u) = 0$$

$$\rho\big(\partial_t u + c(u \cdot \nabla)u\big) + P_{u^\perp} \nabla p^\varepsilon(\rho) = 0$$

$$|u| = 1$$

$P_{u^\perp}$ = projection on plane $\{u\}^\perp$. Maintains $|u| = 1$
Hyperbolic but non conservative (because term $P_{u^\perp} \nabla p^\varepsilon(\rho)$)
Non galilean-invariant $c \neq 1$

Literature

Based on particle model proposed by Vicsek et al, PRL95

Derivation of SOH by D Motsch, M3AS 08

Related to (but $\neq$ from) Toner & Tu, PRL 95

Study of SOH model: J.G. Liu, Frouvelle, T. Yang, H. Yu, . . .

If $\rho < \rho^*$: standard (i.e. compressible) SOH

$$\partial_t \rho + \nabla(\rho u) = 0$$

$$\rho\big(\partial_t \rho + (u \cdot \nabla) u\big) + P_{u^\perp} \nabla p_0(\rho) = 0$$

$$|u| = 1$$

if $p_0 = 0$: pressureless gas dynamics with $c \neq 1$

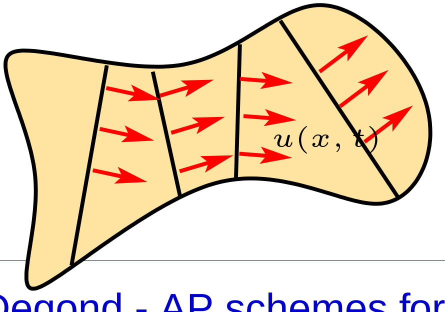
If $\rho = \rho^*$: incompressible SOH

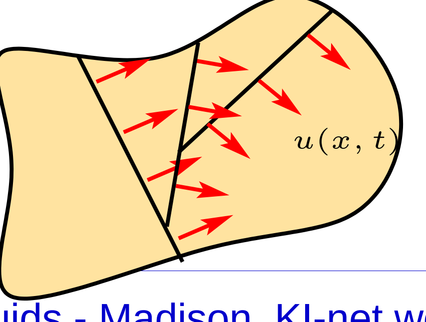
$$\nabla \cdot u = 0$$

$$\rho^* \big(\partial_t u + c(u \cdot \nabla) u\big) + P_{u^\perp} \nabla \bar{p} = 0$$

$$|u| = 1$$

fields s.t. $|u| = 1$ and $\nabla \cdot u = 0$ are singular





The ε-dependent SOH problem

Difficulty with interface dynamics

- even if interface is smooth, motion of interface unknown
- SOH non-conservative system $\Rightarrow$ shock speed unknown
- Interface treatment $\approx$ shock [D Navoret et al, JSP 10]
- Resolution of ε-dependent problem even more necessary

Difficulty with resolution of ε-dependent problem

- non-conservativity of the model due to $|u| = 1$ constraint
- Strategy: use relaxation model [Motsch Navoret, MMS 11] i.e. solve

$$\partial_t(\rho v) + c\nabla \cdot (\rho v \otimes v) + \nabla p^\varepsilon(\rho) = \beta^{-1}(1 - |v|^2)\rho v, \qquad \beta \ll 1$$

without constraint on v

Time splitting: over each timestep Δt:

- First solve conservative model for (ρ, v) without rhs: $\beta^{-1} = 0$
- Then normalize the velocity: $u = v/|v|$
- During conservative step, use AP-method to handle $\varepsilon \ll 1$

Two-fluid model

Two groups of pedestrians (denoted $+$ or $-$)

moving against each-other

Each pedestrian has preferred velocity $w_\pm$

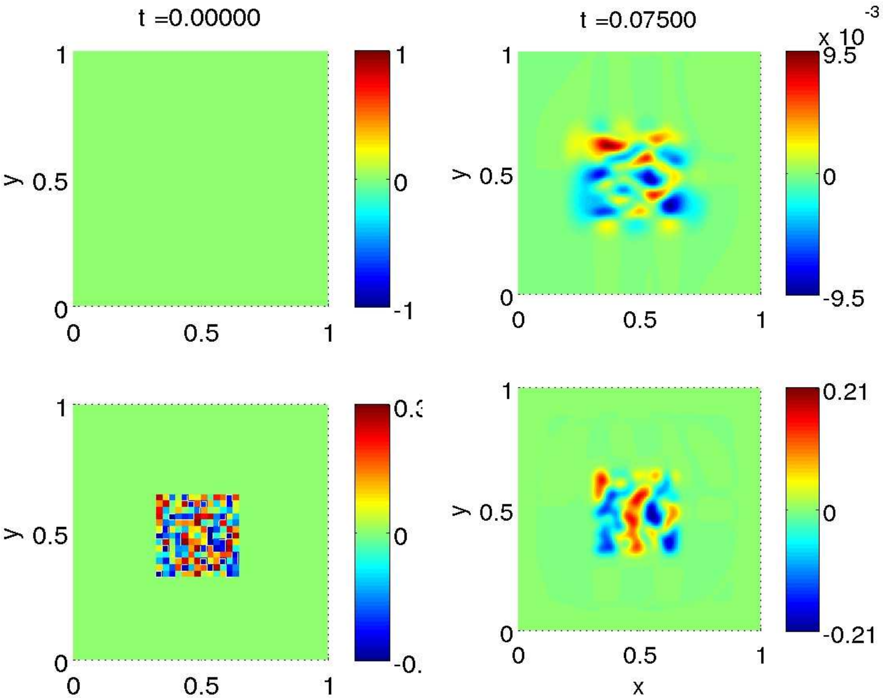
Actual velocity $u_\pm$ relaxes to $w_\pm$ with rate β

Congestion treated by singular pressure $p^\varepsilon(\rho)$ with $\rho = \rho_+ + \rho_-$

$$\partial_t \rho_\pm + \nabla \cdot (\rho_\pm u_\pm) = 0$$

$$\partial_t(\rho_\pm u_\pm) + \nabla \cdot (\rho_\pm u_\pm \otimes u_\pm) + \nabla p^\varepsilon(\rho) = \beta^{-1} \rho_\pm (w_\pm - u_\pm)$$

$$\partial_t(\rho_\pm w_\pm) + \nabla \cdot (\rho_\pm w_\pm \otimes u_\pm) = 0$$



Evolution of a random patch of pedestrians
top: excess flow. bottom: excess density
left: $t = 0$. right: $t > 0$

3. Multiphase flows

joint work with F. Cordier & A. Kumbaro (CEA)

J. Sci. Comput. 58 (2014) 115-148

Problem when a phase appears / disappears

- passage between 1-fluid to 2-fluid and vice-versa
- applications for safety in nuclear power plants: water / vapor
- important in many other applications, e.g. meteorology (clouds)

Model: isentropic 2-phase model with pressure equilibrium

- $\neq$ Baer-Nunziato model (pressures are not in equilibrium)
- case of vapor disappearance. $\alpha_v = \varepsilon \bar\alpha_v$, $\bar\alpha_v = \mathcal{O}(1)$

$$\partial_t(\bar\alpha_v \rho_v) + \partial_x(\bar\alpha_v \rho_v u_v) = 0$$

$$\partial_t(\alpha_\ell \rho_\ell) + \partial_x(\alpha_\ell \rho_\ell u_\ell) = 0$$

$$\partial_t(\bar\alpha_v \rho_v u_v) + \partial_x(\bar\alpha_v \rho_v u_v^2) + \bar\alpha_v \partial_x p + \varepsilon\, \bar\alpha_v \alpha_\ell \tilde\rho\, u_r^2\, \delta\, \partial_x \bar\alpha_v = 0$$

$$\partial_t(\alpha_\ell \rho_\ell u_\ell) + \partial_x(\alpha_\ell \rho_\ell u_\ell^2) + \alpha_\ell \partial_x p + \varepsilon\, \bar\alpha_v \alpha_\ell \tilde\rho\, u_r^2\, \delta\, \partial_x \alpha_\ell = 0$$

$$\rho_v = \rho_v(p), \quad \rho_\ell = \rho_\ell(p), \quad \varepsilon \bar\alpha_v + \alpha_\ell = 1$$

When the vapor disappears . . .

Limit $\varepsilon \to 0$

$$\partial_t(\bar\alpha_v \rho_v) + \partial_x(\bar\alpha_v \rho_v u_v) = 0$$
$$\partial_t \rho_\ell + \partial_x(\rho_\ell u_\ell) = 0$$
$$\partial_t(\bar\alpha_v \rho_v u_v) + \partial_x(\bar\alpha_v \rho_v u_v^2) + \bar\alpha_v \partial_x p = 0$$
$$\partial_t(\rho_\ell u_\ell) + \partial_x(\rho_\ell u_\ell^2) + \partial_x p = 0$$
$$\rho_v = \rho_v(p), \quad \rho_\ell = \rho_\ell(p)$$

Vapor and liquid decouple

- standard isentropic Euler for (ρ_ℓ, u_ℓ) with p s.t. $\rho_\ell = \rho_\ell(p)$
- pressureless gas dynamics for $(\bar\alpha_v \rho_v, \bar\alpha_v \rho_v u_v)$ with r.h.s.

Pressureless gas dynamics not hyperbolic

- double eigenvalue u_v with non-diagonalizable jacobian
- as $\varepsilon \to 0$, model loses hyperbolicity (2 eigenvalues collapse)
- the matrix of eigenvectors becomes singular
- any method (eg Roe) based on eigenvector matrix collapses

General non-conservative system

$$\partial_t V + A(V)\partial_x V = 0$$

Generalized Roe Scheme [Toumi & Kumbaro, JCP 96]

$$\Delta t^{-1}(V_i^{n+1} - V_i^n) + \Delta x^{-1}\big(\phi^-(V_i^n, V_{i+1}^n) + \phi^+(V_{i-1}^n, V_i^n)\big) = 0$$

$$\phi^{\pm}(V_i, V_{i+1}) = A^{\pm}(V_{i+1/2})\,(V_{i+1} - V_i), \quad V_{i+1/2} = (V_i + V_{i+1})/2$$

$$A^{\pm} = (A + |A|)/2$$

Formula for $|A|$:

If $A = R\,\text{diag}(\lambda_1, \ldots, \lambda_N)\,R^{-1}$ then $|A| = R\,\text{diag}(|\lambda_1|, \ldots, |\lambda_N|)\,R^{-1}$

But R becomes singular as $\varepsilon \longrightarrow 0$!

Functional calculus

Let Φ: $I \to \mathbb{R}$ continuous. $I \supseteq \text{Sp}(A) = \{\lambda_1, \ldots, \lambda_N\}$

Then $\Phi(A) = R\,\text{diag}\big(\Phi(\lambda_1), \ldots, \Phi(\lambda_N)\big)\, R^{-1}$

$\Phi(A)$ only depends on the values $(\Phi(\lambda_k))_{k=1}^N$ of Φ on $\text{Sp}(A)$

Other expression of $\Phi(A)$ involving a polynomial

$P(\lambda) = \sum_{p=0}^N a_p \lambda^p$ polynomial interpolating $(\lambda_k, \Phi(\lambda_k))_{k=1}^N$

Then $\Phi(A) = P(A) = \sum_{p=0}^N a_p A^p$

$P(A)$ can be evaluated without calling for R

$P(A)$ is well-defined even when A is non-diagonalizable

If $A^\varepsilon \to A$ as $\varepsilon \to 0$, then $\Phi(A^\varepsilon) = P(A^\varepsilon) \to P(A)$

Approximate polynomial

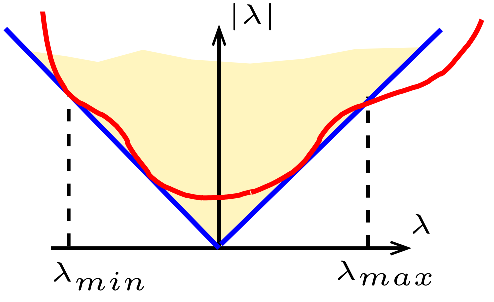
If $P^\delta \to \Phi$ as $\delta \to 0$, pointwise on $\text{Sp}(A)$ then $P^\delta(A) \to \Phi(A)$

Polynomial schemes

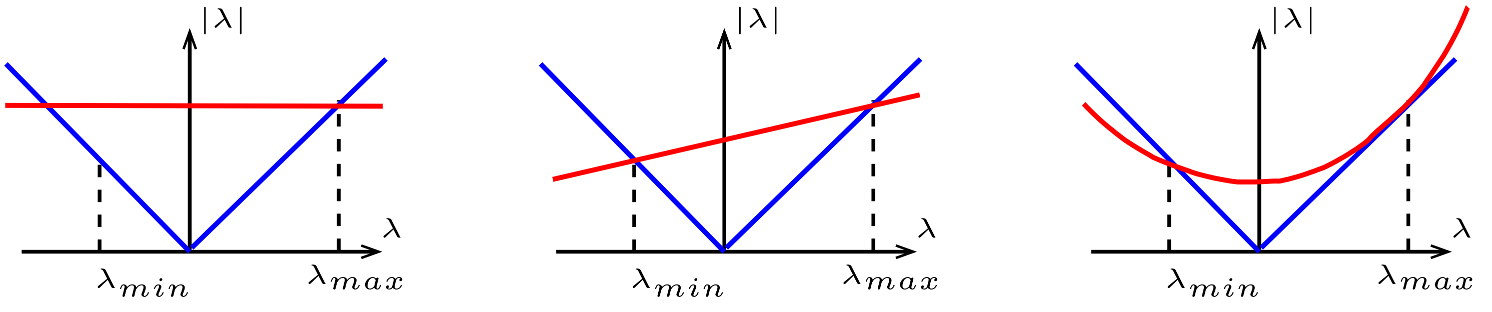
Application to the computation of the Roe matrix $|A|$

[D, Peyrard, Russo, Villedieu, CRAS 99]

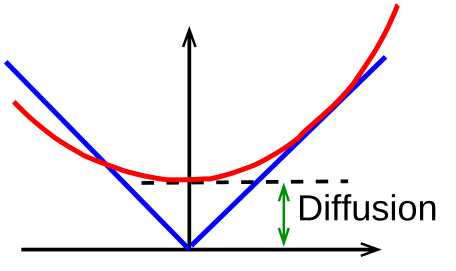
Stability request (under CFL)



Polynomial schemes $P0$, $P1$ and $P2$



Too much diffusion



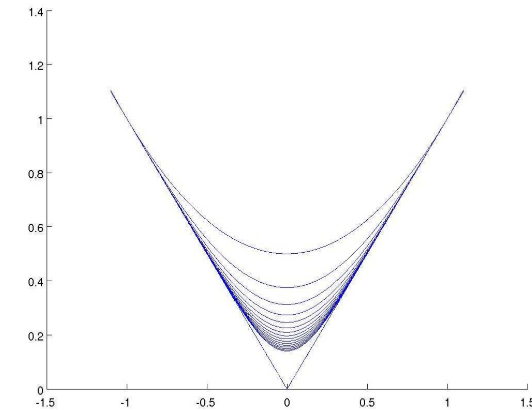
Approximation by a high degree polynomial

Polynomial independent of A

Even polynomial, high degree

approximation of $\lambda \to |\lambda|$

but construction ill-conditionned



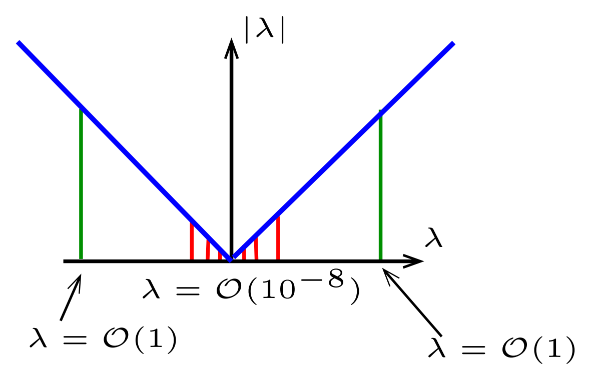
Polynomial dependent on A

Use specificity of A in 2-phase model

Eigenvalues organized in 2 groups

One group is $\mathcal{O}$(sound speed)

One group is $\mathcal{O}(10^{-8})$ smaller



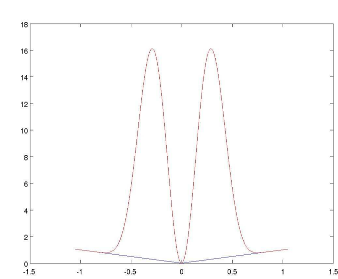
Construction:

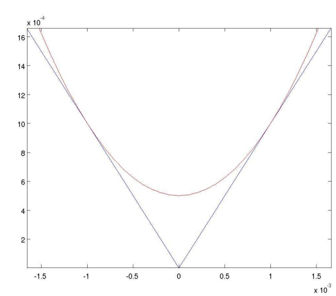
High order approx. of large λ

2nd order approx of one of the small λ

Allow large oscillations in between

Possibility to tune the diffusion





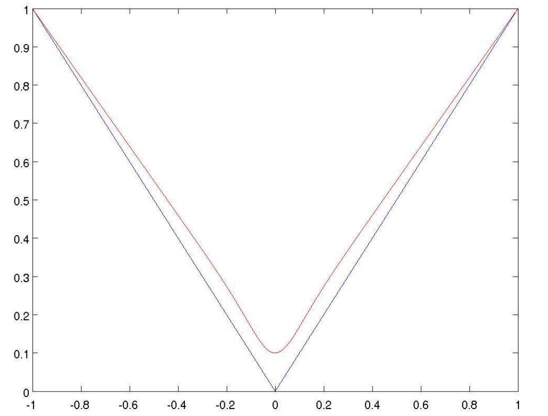
Hyperbolic tangent approximation

Use following approximation of $\lambda \to |\lambda|$

$$\Phi(\lambda) = \tau + (1-\tau)\,\lambda\,\mathrm{tanh}(\lambda/\tau)\,\mathrm{cotanh}(1/\tau)$$

To compute $\mathrm{tanh}(s)$, use differential eq.

$$\frac{d}{ds}(\mathrm{tanh}(\alpha s)) = \alpha(1-\mathrm{tanh}^2(\alpha s))$$



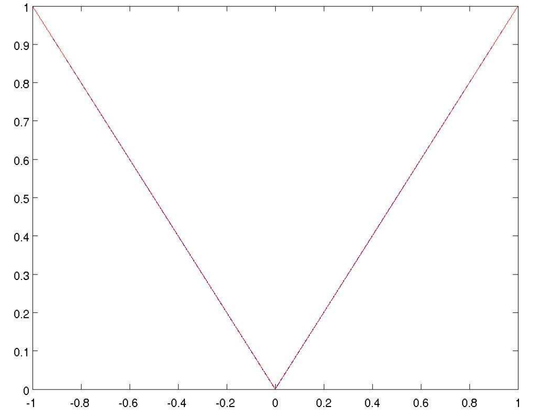
Matrix formula for $B(s) = \mathrm{tanh}(sA)$

$$\frac{dB}{ds} = A\,(\mathrm{Id} - B(s)^2),\ B(0) = 0$$

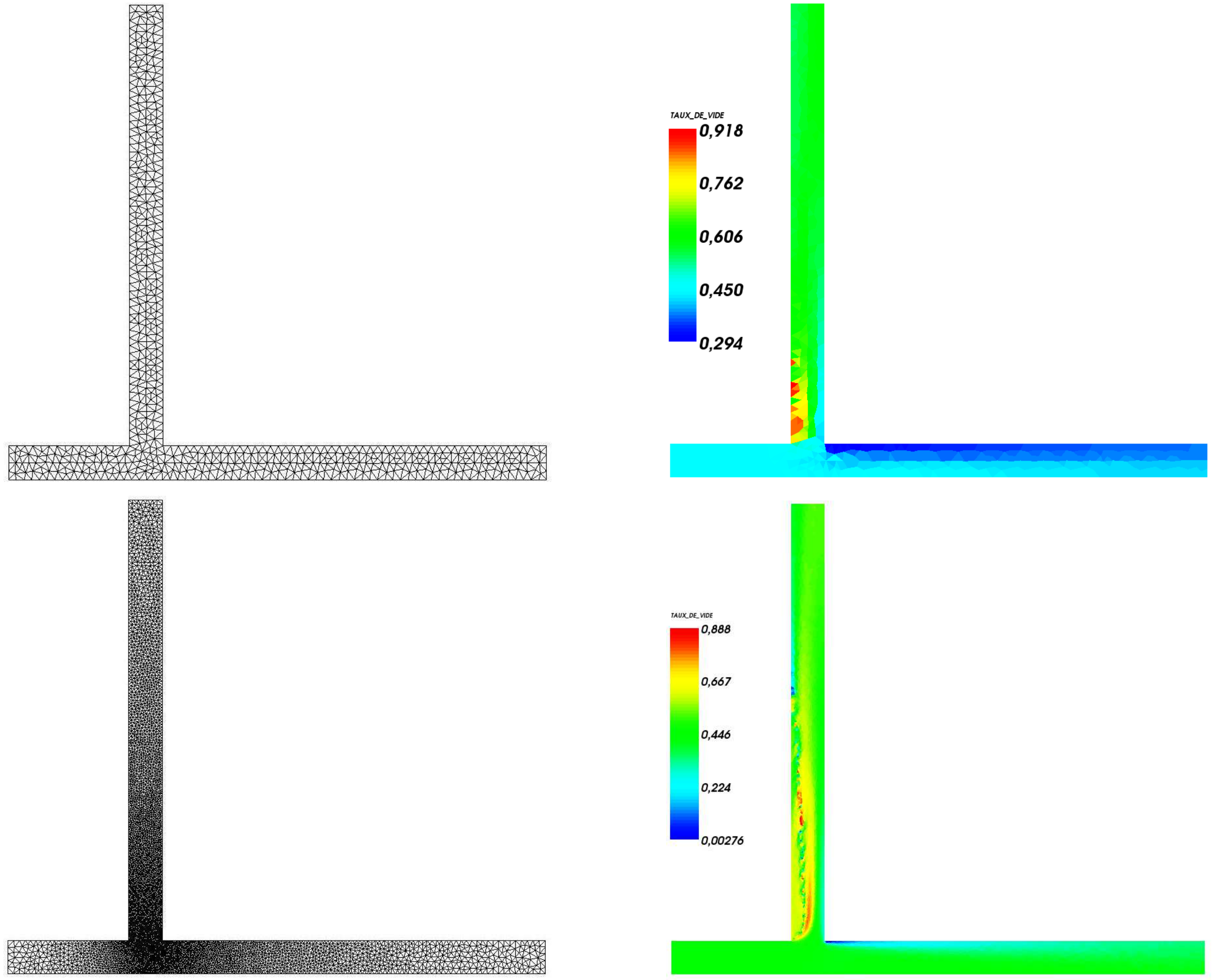
Solve this differential eq. by implicit Euler

$$B^{k+1} = B^k + h\,A\,(\mathrm{Id} - (B^{k+1})^2)$$

Method works but too costly



Numerical results: Tee junction



4. Conclusion

Conclusion

Construction of AP schemes

- for full Euler or NS in the small Mach number regime
- Semi-implicit treatment
- Reduces to solving an elliptic equation for the pressure
- Proved AP Property

Applications to jamming phase transition

- Compressible to incompressible
- For standard isentropic fluids
- For Self-Organized Hydrodynamics (adding $|u| = 1$ constraint)

For multi-phase flows

- Method that sustains phase appearance / disappearance
- Based on polynomial schemes
- Does not require the eigenvector matrix
- Proved robust in very stiff cases