HDR DEFENSE

Numerical approximation of some hyperbolic problems

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SHORT CV

Academic background

• 1999-2002 :

PHD Thesis at ONERA and Ecole Polytechnique supervised by P.-G LeFloch and F. Coquel

• 2002-2003 (4 months) :

Post-doc position at RWTH Aachen supervised by Prof. Ballmann

2003-present :

Assistant professor at University Paris Diderot-Paris 7 Member of the J.-L. Lions laboratory

2007-2008:

Delegation at CEA Saclay, LETR laboratory

ONERA : French Center for Aerospace Research **CEA :** French Center for Nuclear Research

SHORT CV

Research interests

Theory and Modelling, Numerics and Scientific Computing for

- Hyperbolic systems in conservative and non-conservative form
- Hyperbolic-elliptic systems, nonclassical shocks and phase transitions
- Compressible multi-phase and multi-component flows
- Discretization of sources (asymptotic-preserving schemes)
- Finite Volumes schemes (relaxation schemes, averaging versus sampling)
- Coupling of models
- Traffic flows

OUTLINE OF THE TALK



2 INTERFACIAL COUPLING OF MULTI-PHASE FLOWS





INTERFACIAL COUPLING OF MULTI-PHASE FLOWS

NONCLASSICAL SHOCK:

TRAFFIC FLOWS

OUTLINE OF THE TALK



2 Interfacial coupling of multi-phase flows



TRAFFIC FLOWS

RELAXATION APPROXIMATION

The general idea (numerical viewpoint)

Given a PDE system at equilibrium

$$\partial_t \mathbf{u} + \nabla \mathbf{f}(\mathbf{u}) = 0, \quad \mathbf{u} \in \omega \subset \mathbb{R}^n,$$
 (1)

propose a relaxation system of the form

$$\partial_t \mathbf{U}^{\lambda} + \nabla \mathbf{F}(\mathbf{U}^{\lambda}) = \lambda Q(\mathbf{U}^{\lambda}), \quad \mathbf{U}^{\lambda} \in \Omega \subset \mathbb{R}^N,$$
(2)

such that

- $\lim_{\lambda \to \infty} \mathbf{U}^{\lambda} = \mathbf{u} \ (\lambda > 0 \text{ stands for the relaxation coefficient rate})$
- system (2) with $\lambda = 0$ is easier to handle than (1)

Some remarks

- the litterature is vast on this numerical subject : Jin and Xin '95, Coquel and Perthame '98, Coquel *et al* '01, Bouchut '02... see also Natalini, Serre, Yong, Zumbrun...
- the conservative form of (1) is not a restriction
- *N* may equal *n* + 1, *n* + 2, 2*n*...

RELAXATION APPROXIMATION OF THE EULER EQUATIONS

The governing equations

$$\begin{array}{l} \partial_t \rho + \nabla . \ \rho \mathbf{w} = 0, \quad t > 0, \quad \mathbf{x} \in \mathcal{D} \subset \mathbb{R}^{\mathbf{d}}, \\ \partial_t \rho \mathbf{w} + \nabla . \ (\rho \mathbf{w} \otimes \mathbf{w} + p(\mathbf{u}) \ \mathbf{I}_{\mathbf{d}}) = 0, \\ \partial_t \rho E + \nabla . \ (\rho E + p(\mathbf{u})) \mathbf{w} = 0, \end{array}$$

The relaxation system

$$\begin{array}{l} \partial_t \rho + \nabla . \left(\rho \mathbf{w} \right) = 0, \quad t > 0, \quad \mathbf{x} \in \mathcal{D}, \\ \partial_t (\rho \mathbf{w}) + \nabla . \left(\rho \mathbf{w} \otimes \mathbf{w} + \Pi \mathbf{I_d} \right) = 0, \\ \partial_t (\rho E) + \nabla . \left((\rho E + \Pi) \mathbf{w} \right) = 0, \\ \partial_t (\rho \Pi) + \nabla . \left(\rho \Pi \mathbf{w} \right) + a^2 \nabla . \mathbf{w} = \lambda \rho (p - \Pi), \end{array}$$

 \longrightarrow Recall that $\partial_t \rho p(\mathbf{u}) + \nabla \cdot (\rho p(\mathbf{u})\mathbf{w}) + \rho^2 c^2 \nabla \cdot \mathbf{w} = 0$

 $\rightarrow a$ is a given real number subject to a stability condition : $a > \rho c(\mathbf{u})$

 \longrightarrow Question : is it possible to prove that $\lim_{\lambda \to +\infty} \Pi^{\lambda} = p(\mathbf{u})$?

Convergence result

Theorem

- The relaxation system admits smooth solutions that converge towards the *local in time* smooth solutions of the Euler equations as $\lambda \to \infty$
- Arbitrarily large entropic shock of the Euler equations admits a shock profile for the relaxation system

Proof

- Use the structural properties of the relaxation system, and the main convergence result of Yong '99
- Pretty technical, use a detailed analysis of the dynamical system satisfied by the shock profile and the center manifold theorem as well

C. Chalons and J.-F. Coulombel Relaxation approximation of the Euler equations Analysis and Applications (2008)

NUMERICAL PROCEDURE (TIME EXPLICIT SETTING)

Splitting technique

In order to solve $\partial_t \mathbf{U}^{\lambda} + \nabla$. $\mathbf{F}(\mathbf{U}^{\lambda}) = \lambda Q(\mathbf{U}^{\lambda})$

- First, set $\lambda = 0$ and solve $\partial_t \mathbf{U} + \nabla$. $\mathbf{F}(\mathbf{U}) = 0$
- Then, solve $\partial_t \mathbf{U}^{\lambda} = \lambda Q(\mathbf{U}^{\lambda})$ in the asymptotic regime $\lambda \to \infty$

Key point : all the fields of $\partial_t \mathbf{U} + \nabla$. $\mathbf{F}(\mathbf{U}) = 0$ are **linearly degenerate** (the waves behave as linear waves)

Gathering these two steps leads to a standard finite volume scheme

$$\mathbf{u}_{K}^{n+1} = \mathbf{u}_{K}^{n} - \frac{\Delta t}{|K|} \sum_{e \in \partial K} \mathcal{G}_{e,K}^{n} |e|$$

$$\mathcal{G}_{e,K}^n = T_{e,K}^{-1} \mathcal{G}(T_{e,K}\mathbf{u}_K^n, T_{e,K}\mathbf{u}_{K_e}^n; i_1)$$

• $\mathcal{G}(.,.;i_1)$ is built from **the Godunov method** in the first space direction i_1

STABILITY RESULT

Theorem

Under a standard CFL condition and provided that *a* is sufficiently large $(a > \rho c(\mathbf{u}))$, the relaxation scheme

- keeps the invariant domain : $\rho_K^{n+1} > 0$ and $(\rho e)_K^{n+1} = (\rho E)_K^{n+1} \frac{1}{2} \frac{\|(\rho \mathbf{w})_K^{n+1}\|^2}{\rho_K^{n+1}} > 0$
- satisfies an entropy inequality :

$$(\rho S)(\mathbf{u}_{K}^{n+1}) - (\rho S)(\mathbf{u}_{K}^{n}) + \frac{\Delta t}{|K|} \sum_{e \in \partial K} (\rho S \mathbf{w})_{e,K}^{n} \le 0$$

• obeys a maximum principle :

$$S_K^{n+1} \le \max_K S_K^n$$

is exact for stationary contact discontinuities

C. Chalons and F. Coquel Navier-Stokes equations with several independent pressure laws and explicit predictor-corrector schemes Numerisch Math. (2005)

Splitting technique and stationary solutions

Splitting technique

- First, set $\lambda = 0$ and solve $\partial_t \mathbf{U} + \nabla$. $\mathbf{F}(\mathbf{U}) = 0$
- Then, solve $\partial_t \mathbf{U}^{\lambda} = \lambda Q(\mathbf{U}^{\lambda})$ in the asymptotic regime $\lambda \to \infty$

 \longrightarrow At least formally, time convergence to some steady solution U would require

 ∇ . **F**(**U**) = 0 and **Q**(**U**) = 0

Lemma (convergence failure)

Let **U** be such that ∇ . **F**(**U**) = 0 and Q(**U**) = 0 and $a > \rho c$. Then **U** also obeys

 $(a^2 - \rho^2 c^2) \nabla \mathbf{w} = 0$

Remark : ∇ . ρ **w** = 0 but ∇ . **w** \neq 0 in general !

COMPUTATIONS OF STATIONARY SOLUTIONS (TIME-IMPLICIT SETTING)

 \longrightarrow We propose, in order to avoid

 $\nabla \mathbf{F}(\mathbf{U}) = \mathbf{0} = \mathbf{Q}(\mathbf{U})$

and thus to keep the balance

$$\nabla. \mathbf{F}(\mathbf{U}^{\lambda}) = \lambda Q(\mathbf{U}^{\lambda})$$

Prediction-correction technique

- First, solve in a **linearized time-implicit** way $\partial_t \mathbf{U}^{\lambda} + \nabla$. $\mathbf{F}(\mathbf{U}^{\lambda}) = \lambda Q(\mathbf{U}^{\lambda})$ in the limit $\lambda \to \infty$
- Then, solve exactly $\partial_t \mathbf{U}^{\lambda} = \lambda Q(\mathbf{U}^{\lambda})$ in the limit $\lambda \to \infty$

C. Chalons, F. Coquel and C. Marmignon Well-balanced time implicit relaxation schemes for the Euler equations SIAM Journal of Scientific Computing (2008)

NUMERICAL ILLUSTRATIONS



Fig.: ρ (left) and $\| \partial_t \rho \|_{L^2}$ (right)

Some others applications of the relaxation

• Navier-Stokes equations with several independant pressure laws

C. Chalons and F. Coquel Multi-pressure Navier-Stokes equations and predictor-corrector schemes Numerisch Math. (2005)

C. Chalons, F. Coquel and C. Marmignon Time-implicit approximation of the multi-pressure gas dynamics equations to be submitted (2008)

Weakly ionized gases

C. Chalons, C. Marmignon, O. Rouzaud and T. Soubrié Development of a relaxation scheme for weakly ionized gases AIAA paper 05-0603 (2005)

• Two fluid-two pressure diphasic model (non trivial !)

A. Ambroso, C. Chalons, F. Coquel and T. Galié Relaxation and numerical approximation of a two fluid-two pressure model submitted (2008)

OUTLINE OF THE TALK



2 INTERFACIAL COUPLING OF MULTI-PHASE FLOWS





CONTEXT OF THE WORK

 \longrightarrow Collaboration between

Laboratory Jacques-Louis Lions

CC, F. Coquel, E. Godlewski, F. Lagoutière, P.-A. Raviart, N. Seguin

CEA Saclay

A. Ambroso, J. SegréB. Boutin and T. Galié (PhD students)

Also participate

S. Kokh (CEA), J.-M. Hérard (EDF R&D)

 \longrightarrow We want to solve

 $(S_1) : \partial_t \mathbf{u} + \partial_x \mathbf{f}_-(\mathbf{u}) = 0, \quad x < 0$ $(S_2) : \partial_t \mathbf{u} + \partial_x \mathbf{f}_+(\mathbf{u}) = 0, \quad x > 0$

+ a transmission condition (conservation, continuity...) at x = 0

TRAFFIC FLOWS

Some works

 \longrightarrow Both models (S_1) and (S_2) share the same physics (thermohydraulic flow, multiphase flow...) but are associated with different modelling

- different closure laws
- different accuracy of description
- different space dimension...

CC, P.-A. Raviart and N. Seguin *The interface coupling of the gas dynamics equations Quarterly of Applied Mathematics (2008)*

A. Ambroso, CC, F. Coquel, E. Godlewski, F. Lagoutière, P.-A. Raviart and N. Seguin Coupling of general Lagrangian systems Mathematics of Computation (2008)

A. Ambroso, CC, F. Coquel, E. Godlewski, F. Lagoutière, P.-A. Raviart and N. Seguin The coupling of homogeneous models for two-phase flows International Journal of Finite Volumes (2007)

OUTLINE OF THE TALK



2 Interfacial coupling of multi-phase flows





GOVERNING EQUATIONS

The model under consideration

$$\begin{cases} \partial_t u + \partial_x f(u) = 0, & u(x, t) \in \mathbb{R}, \ (x, t) \in \mathbb{R} \times \mathbb{R}^+, \\ u(x, 0) = u_0(x), \end{cases}$$

+ $\partial_t S(u) + \partial_x Q(u) \le 0$ (single entropy inequality)



FIG .: Concave-convex flux function

These works are motivated by the computation of phase transitions in van der Waals fluids and nonlinear elastic two-phase material (see for instance my PhD)

MATHEMATICAL DIFFICULTIES

→ The Riemann problem admits (up to) *a one-parameter family of solutions* => non-uniqueness

 \longrightarrow Some of them are both **nonclassical** (they violate the standard Lax shock inequalities) and **physically relevant**

The kinetic relation

 \longrightarrow Non-uniqueness can be fixed with an **additional algebraic condition** on each nonclassical shock (σ, u_-, u_+)

 \longrightarrow The kinetic relation takes the form

 $u_{+} = \varphi(u_{-})$ for all nonclassical shocks, (3)

where φ is the kinetic function, and σ is given by the Rankine-Hugoniot relation

See LeFloch '02 monograph

NUMERICAL DIFFICULTIES

\longrightarrow Nonclassical solutions are very sensitive w.r.t. small scales and numerical diffusion

$$u = \lim_{\epsilon \to 0} u^{\epsilon} \quad \text{with} \quad \partial_t u^{\epsilon} + \partial_x f(u^{\epsilon}) = \mathcal{R}(\epsilon \partial_{xx} u^{\epsilon}, \epsilon^2 \partial_{xxx} u^{\epsilon})$$



FIG .: Numerical solutions obtained with the Godunov scheme

NUMERICAL DIFFICULTIES

In the literature, we can distinguish between :

→ **the diffuse interface methods :** these methods are *conservative* but work pretty *bad for shocks with large amplitude* Hayes and LeFLoch '98, LeFloch and Rohde '00...

 \rightarrow the sharp interface methods : these methods work *very well*, are *not strictly conservative* (but *convergent*) and *pretty expensive* in general Hou, Rozakis and LeFloch '99, Merkle and Rohde '06...

Our objective could be ...

To get a numerical scheme which :

- is not expensive
- works even for shocks with large amplitude
- provides sharp interfaces
- is conservative

THE TRANSPORT-EQUILIBRIUM STRATEGY

The main idea (2 steps)

 \longrightarrow First, at each interface treat the nonclassical shock as a stationary discontinuity

- \longrightarrow Then, propagate this discontinuity using a Glimm strategy
 - The method is not expensive, works very well, provides sharp interfaces and seems to be convergent
 - It is not strictly conservative as the Glimm scheme !

C. Chalons Transport-Equilibrium Schemes for Computing Nonclassical Shocks Numerical Methods for Partial Differential Equations (2008)

C. Chalons Numerical approximation of a macroscopic model of pedestrian flows SIAM Journal of Scientific Computing (2007)

The reconstruction strategy (see Lagoutière '07, '08)

The main idea

Understand u_j^n as **the projection of a nonclassical discontinuity** related to the Riemann solution associated with initial states $u_l = u_{j-1}^n$ and $u_r = u_{j+1}^n$



FIG.: A general discontinuous reconstruction with conservation property (the general case).

THE RECONSTRUCTION STRATEGY

Two requirements

- \longrightarrow The reconstruction should be **conservative** in the usual sense
- ----- The reconstruction should be exact for any isolated nonclassical discontinuity



FIG.: A general discontinuous reconstruction with conservation property (the general case).

Stability properties in the case $f' \ge 0$

Theorem

Under a usual CFL restriction and some physical assumptions on f and φ , the scheme

- is conservative and consistent in the usual sense of finite volume schemes
- is **exact** on each cell C_i if u_i and u_r are two initial states such that $u_r = \varphi(u_i)$:

$$u_j^n = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u(x, t^n) dx, \qquad j \in \mathbb{Z}, \ n \in \mathbb{N},$$

In particular, the numerical discontinuity is diffused on one cell at most

• The method is not expensive, works very well, provides sharp interfaces and is conservative in the usual sense

B. Boutin, C. Chalons, F. Lagoutière and P.-G. LeFloch A conservative scheme for nonclassical solutions based on kinetic relations Interfaces and Free Boundaries (2008)

NUMERICAL ILLUSTRATION



OUTLINE OF THE TALK



2 Interfacial coupling of multi-phase flows





SEVERAL MACROSCOPIC MODELS

We denote

- ρ : car density
- R: maximal density
- v : car velocity
- (LWR '56)

$$\partial_t \rho + \partial_x \rho v = 0, \quad v = v(\rho)$$

• (Aw-Rascle '00)

$$\begin{cases} \partial_t \rho + \partial_x (\rho v) = 0\\ \partial_t \rho w + \partial_x \rho v w = 0 \end{cases}$$

 $w = v(\rho, w) + p(\rho), \ p(\rho) = V_{ref} \ln(\rho/R), \ V_{ref}$ is a reference velocity

• (Colombo '02)

$$\begin{cases} \partial_t \rho + \partial_x (\rho v) = 0\\ \partial_t q + \partial_x (q v - Q v) = 0 \end{cases}$$

 $v = v(\rho, q), q$ is a weighted momentum and Q a road parameter

A TRAFFIC FLOW MODEL WITH PHASE TRANSITIONS

Experimental data : Kerner '00 (Daimler Benz AG)



Free flow : $(\rho, q) \in \Omega_f$

Congested flow : $(\rho, q) \in \Omega_c$

 $\begin{cases} \partial_t \rho + \partial_x \rho v = 0 \\ q = \rho V \end{cases} \qquad \qquad \begin{cases} \partial_t \rho + \partial_x \rho v = 0 \\ \partial_t q + \partial_x (q - Q) v = 0 \end{cases}$

 $v_f(\rho) = (1 - \frac{\rho}{R})V \qquad \qquad v_c(\rho, q) = (1 - \frac{\rho}{R})\frac{q}{\rho}$

(Colombo '02)

A TRAFFIC FLOW MODEL WITH PHASE TRANSITIONS

Experimental data



$$\Omega_{f} = \left\{ (\rho, q) \in [0, R] \times \mathbb{R}^{+} \colon v_{f}(\rho) \geq V_{f}, \ q = \rho \cdot V \right\}$$
$$\Omega_{c} = \left\{ (\rho, q) \in [0, R] \times \mathbb{R}^{+} \colon v_{c}(\rho, q) \leq V_{c}, \ \frac{q - Q}{\rho} \in \left[\frac{Q^{-} - Q}{R}, \frac{Q^{+} - Q}{R} \right] \right\}$$
(Colombo '02)

Model

A TRAFFIC FLOW MODEL WITH PHASE TRANSITIONS

The Riemann problem (Colombo '02) has been solved uniquely under some consistency conditions and using phase transitions (u₋, u₊, σ) such that

$$\rho v_c(\mathbf{u}_+) - \rho v_f(\mathbf{u}_-) = \sigma \left(\rho(\mathbf{u}_+) - \rho(\mathbf{u}_-) \right)$$

(see Colombo, Goatin and Priuli '06 for the Cauchy problem)

• $\Omega_f \cup \Omega_c$ is not convex \Longrightarrow the Godunov method fails in general



NUMERICAL APPROXIMATION : A NEW VERSION OF THE GODUNOV SCHEME



Instead of setting

$$\mathbf{u}_{j}^{n+1} = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} \mathbf{v}(x, \Delta t) dt$$

we propose

$$\overline{\mathbf{u}}_{j}^{n+1} = \frac{1}{\overline{\Delta x_{j}}} \int_{\overline{x_{j-1/2}}}^{\overline{x}_{j+1/2}} \mathbf{v}(x, \Delta t) dt$$

followed by **sampling procedure** to recover the initial mesh and define \mathbf{u}_i^{n+1}

UPDATE FORMULAS



Let be given $(a_n)_n$ a well-distributed random sequence within $]0, \Delta x[$ (*e.g.* van der Corput sequence)

Random choice procedure gives

$$\mathbf{u}_{j}^{n+1} = \begin{cases} \overline{\mathbf{u}}_{j-1}^{n+1} & \text{if} & a_{n+1} \in (0, \frac{\Delta t}{\Delta x} \sigma_{j-1/2}^{+}) \\ \overline{\mathbf{u}}_{j}^{n+1} & \text{if} & a_{n+1} \in [\frac{\Delta t}{\Delta x} \sigma_{j+1/2}^{+}, 1 + \frac{\Delta t}{\Delta x} \sigma_{j+1/2}^{-}) \\ \overline{\mathbf{u}}_{j+1}^{n+1} & \text{if} & a_{n+1} \in [1 + \frac{\Delta t}{\Delta x} \sigma_{j+1/2}^{-}, 1) \end{cases}$$

 $\sigma_{j+1/2}$ is the speed of the possible phase transition coming from $x_{j+1/2}$ $\sigma_{j+1/2}^+ = \max(\sigma_{j+1/2}, 0), \sigma_{j+1/2}^- = \min(\sigma_{j+1/2}, 0)$

REMARKS AND ILLUSTRATIONS

- The algorithm coincides with Godunov's scheme in absence of phase transitions
- The algorithm coincides with Glimm's scheme for an isolated phase transition
- Extension to *L*¹-stable second-order scheme (MUSCL and RK approaches)



C. Chalons and P. Goatin Godunov scheme and sampling technique for phase transitions in traffic flows Interfaces and Free Boundaries (2008)

NUMERICAL APPROXIMATION OF THE AW-RASCLE MODEL

The model

$$\begin{aligned} \partial_t \rho + \partial_x (\rho v) &= 0 \\ \partial_t \rho (v + p) + \partial_x \rho v (v + p) &= 0 \end{aligned}$$

Maximum principle

Under an usual CFL condition, the proposed Transport-Equilibrium scheme satisfies the following maximum principles

$$\begin{cases} \inf_{j \in \mathbb{Z}} v_j^0 \le v_j^n \le \sup_{j \in \mathbb{Z}} v_j^0, \\ \inf_{j \in \mathbb{Z}} (v_j^0 + p(\rho_j^0)) \le v_j^n + p(\rho_j^n) \le \sup_{j \in \mathbb{Z}} (v_j^0 + p(\rho_j^0)). \end{cases}$$

Remark : these maximum principles are satisfied by a Riemann solution

NUMERICAL APPROXIMATION OF THE AW-RASCLE MODEL



C. Chalons and P. Goatin Transport-Equilibrium schemes for contact discontinuities in traffic flows Communications in Mathematical Sciences (2007)

CONCLUSION

- Numerical problems for hyperbolic systems
- Motivated by real applications in fluid mechanics for instance (ONERA, CEA, IFP)
- Construction of new numerical schemes that are handy and able to treat non standard situations
- Which raises sometimes theoretical and scientific computing questions...

ONERA : French Center for Aerospace Research **CEA :** French Center for Nuclear Research **IFP :** French Center for Oil Research