Construction of the relaxation matrix (1/2)

Target PDE:

$$\frac{\partial \mathbf{u}}{\partial t} + \boldsymbol{\nabla}_x \cdot \begin{pmatrix} \mathbf{f}(\mathbf{u}) \\ \mathbf{g}(\mathbf{u}) \end{pmatrix} = \boldsymbol{\nabla}_x \left(\mathbf{D} \boldsymbol{\nabla}_x \mathbf{u} \right), \qquad \mathbf{D} = \begin{pmatrix} \mathbf{D}_{xx} & \mathbf{D}_{xy} \\ \mathbf{D}_{yx} & \mathbf{D}_{yy} \end{pmatrix}$$

Kinetic system with relaxation:

$$\frac{\partial \mathbf{F}}{\partial t} + \begin{pmatrix} \Lambda_x \\ \Lambda_y \end{pmatrix} \cdot \boldsymbol{\nabla} \mathbf{F} = \mathbf{Q}^{-1} \begin{pmatrix} \alpha \mathbf{Id}_p & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \beta \mathbf{Id}_p \end{pmatrix} \mathbf{Q} \frac{\mathbb{M} - \mathbf{F}}{\varepsilon}$$

1) Define a Knudsen number ε,
2) Perform an asymptotic expansion for $\varepsilon \ll 1$,
3) Identify the terms $\mathcal{O}(\varepsilon)$ as diffusive terms.

A new explicit local kinetic method for compressible Navier-Stokes equations

Rémi Abgrall

[1] Institute of Mathematics, Universität Zürich, Switzerland

CEA-DAM, 11 décembre 2024

Joint work with Gauthier Wissocq, I-Math, UZH

Acknowledge contributions of Davide Torlo (U. la Sapienza, Roma) and Fatemeh Morrajad (U. Geneva now)

Introduction to kinetic methods

- Work of Jin and Xin around 1995[1].
- Similarities with Lattice Boltzmann methods:
  - in modeling choices: "statistical description",
  - in numerical approximation.
- Advantages :
  - Construction of simple, efficient and low-dissipative numerical methods
  - **Numerical stability** obtained from Entropy considerations.
- Limit : restriction to the purely hyperbolic framework.
  - Problem of introducing diffusive effects
  - Example: Navier-Stokes viscosity and thermal dissipation

[1] S. Jin, Z. Xin, *Communications on Pure and Applied Mathematics* **48**, 235–276, ISSN: 00103640 (1995).

Outline

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Overview

Jin-Xin kinetic method in 1D

We are interested in hyperbolic systems of the form:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \mathbf{0}, \qquad \mathbf{u} \in \mathbb{R}^p. \tag{1}$$

Ex:

- Scalar advection ($p = 1$): $\mathbf{u} = u, \quad \mathbf{f}(\mathbf{u}) = cu, \quad c = cte,$
- Burgers' equation ($p = 1$): $\mathbf{u} = u, \quad \mathbf{f}(\mathbf{u}) = u^2/2,$
- Euler equations ($p = 3$): $\mathbf{u} = [\rho, \rho u, \rho E]^T, \quad \mathbf{f}(\mathbf{u}) = [\rho u, \rho u^2 + p, (\rho E + p)u]^T.$

Principle of Jin-Xin's model[a]: remplace Eq. (1) by

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{v}}{\partial x} = 0, \tag{2}$$

$$\frac{\partial \mathbf{v}}{\partial t} + a^2 \frac{\partial \mathbf{u}}{\partial x} = \frac{1}{\varepsilon}(\mathbf{f}(\mathbf{u}) - \mathbf{v}), \qquad a = cte. \tag{3}$$

When $\varepsilon \to 0$, the solution of (2)-(3) converges formally towards that of (1).

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Jin-Xin kinetic method in 1D

Interest of the Jin-Xin model: transport can be diagonalized:

$$\frac{\partial}{\partial t}\begin{bmatrix}\mathbf{F}_1\\ \mathbf{F}_2\end{bmatrix} + \begin{bmatrix}a & 0\\ 0 & -a\end{bmatrix}\frac{\partial}{\partial x}\begin{bmatrix}\mathbf{F}_1\\ \mathbf{F}_2\end{bmatrix} = \frac{1}{\varepsilon}\left(\begin{bmatrix}\mathbb{M}_1\\ \mathbb{M}_2\end{bmatrix} - \begin{bmatrix}\mathbf{F}_1\\ \mathbf{F}_2\end{bmatrix}\right), \tag{4}$$

where :

- $\mathbf{u} = \mathbf{F}_1 + \mathbf{F}_2$: *moment of order 0*,
- $\mathbf{v} = a(\mathbf{F}_1 - \mathbf{F}_2)$: *moment of order 1*,
- $\begin{bmatrix}\mathbb{M}_1\\ \mathbb{M}_2\end{bmatrix} = \frac{\mathbf{u}}{2}\begin{bmatrix}+\\ -\end{bmatrix}\frac{\mathbf{f}(\mathbf{u})}{2a}$: *Maxwellian or equilibrium function*,
- If $a > |\mathbf{f}'(\mathbf{u})|$, (4) can be shown to have entropy stability properties [Bouchut][2].

Note: Similarity with a Boltzmann equation with two discrete velocities (D1Q2): f_i scalar/vector

$$\frac{\partial f_i}{\partial t} + e_i\frac{\partial f_i}{\partial x} = \frac{1}{\tau}\left(f_i^{eq} - f_i\right) \tag{5}$$

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Generalization of kinetic methods

General writing of a BGK kinetic method[3] in 2D:

$$\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} + \Lambda_y \frac{\partial \mathbf{F}}{\partial y} = \frac{1}{\varepsilon} \left(\mathbb{M}(\mathbf{u}) - \mathbf{F} \right), \qquad \mathbf{F} \in \mathbb{R}^{kp}. \tag{6}$$

- k is the number of waves (Jin-Xin: $k = 2$),
- $\mathbf{u} = \mathbb{P}\mathbf{F}$, with $\mathbb{P} : \mathbb{R}^{kp} \to \mathbb{R}^{p}$ linear mapping nicknamed as "*projector*",
- Λ_x and Λ_y : diagonal matrices with constant coefficients,
- ε constant relaxation time.

We want that the system (6) gets close, when $\varepsilon \to 0$, to the hyperbolic system;

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} + \frac{\partial \mathbf{g}(\mathbf{u})}{\partial y} = \mathbf{0}. \tag{7}$$

Which condition(s) on the Maxwelian $\mathbb{M}$?

[3] P. L. Bhatnagar *et al.*, *Physical Review* **94**, 511–525 (1954), R. Natalini, *Journal of Differential Equations* **148**, 292–317, ISSN: 00220396 (1998), D. Aregba-Driollet, R. Natalini, *SIAM Journal on Numerical Analysis* **37**, 1973–2004, ISSN: 00361429 (2000).

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Conditions on the Maxwellian

Apply $\mathbb{P}$ to (6):

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x}(\mathbb{P}\Lambda_x \mathbf{F}) + \frac{\partial}{\partial y}(\mathbb{P}\Lambda_y \mathbf{F}) = \frac{\mathbb{P}\mathbb{M}(\mathbf{u}) - \mathbf{u}}{\varepsilon} \tag{8}$$

1st condition: conservation

$$\mathbb{P}\mathbb{M}(\mathbf{u}) = \mathbf{u}$$

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x}(\mathbb{P}\Lambda_x \mathbf{F}) + \frac{\partial}{\partial y}(\mathbb{P}\Lambda_y \mathbf{F}) = \frac{\mathbb{P}\mathbb{M}(\mathbf{u}) - \mathbf{u}}{\varepsilon} = \mathbf{0} \tag{9}$$

But $\mathbf{F} \to \mathbb{M}$ when $\varepsilon \to 0$.

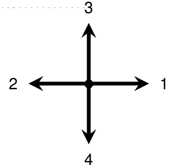
2nd condition: flux

$$\mathbb{P}\Lambda_x\mathbb{M}(\mathbf{u}) = \mathbf{f}(\mathbf{u})$$
$$\mathbb{P}\Lambda_y\mathbb{M}(\mathbf{u}) = \mathbf{g}(\mathbf{u})$$

Example: scalar in 2D with 4 waves

Take $p = 1$ (scalar problem), $k = 4$ (4 waves) in 2D, and

$$\Lambda_x = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & -a & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad \Lambda_y = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & a & 0 \\ 0 & 0 & 0 & -a \end{bmatrix},$$



$$\mathbb{P} = \begin{bmatrix} 1 & 1 & 1 & 1 \end{bmatrix}, \qquad \mathbb{M} = \frac{\mathbf{u}}{4} + \frac{1}{2a} \begin{bmatrix} \mathbf{f}(\mathbf{u}) \\ -\mathbf{f}(\mathbf{u}) \\ \mathbf{g}(\mathbf{u}) \\ -\mathbf{g}(\mathbf{u}) \end{bmatrix}.$$

One can check that: $\mathbb{P}\mathbb{M} = \mathbf{u}$, $\mathbb{P}\Lambda_x\mathbb{M} = \mathbf{f}(\mathbf{u})$, $\mathbb{P}\Lambda_y\mathbb{M} = \mathbf{g}(\mathbf{u})$.

Similar to a D2Q4 lattice for lattice Boltzmann.

Similarities and differences with LBM methods

BGK kinetic methods	Boltzmann methods
$\frac{\partial \mathbf{F}}{\partial t} + \sum_{j,wave\#} \Lambda_j \frac{\partial \mathbf{F}}{\partial x_j} = \frac{1}{\varepsilon}(\mathbb{M} - \mathbf{F})$	$\frac{\partial f_i}{\partial t} + \sum_{j:wave\#} e_{i,j} \frac{\partial f_i}{\partial x_j} = C_i$

- Linear transport with constant speeds
  - **Simples** numerical methods, **low dissipation if**
  - High CFL for all mesh points
  - The **Riemann problems** are very simple.
- Local relaxation: **Very efficient** numerical methods

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- Linear transport with constant speeds
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- Local relaxation: **Very efficient** numerical methods

- $\mathbf{F} \in \mathbb{R}^{kp}$,
- Entropy stability if $\sigma\left(\mathbb{M}'(\mathbf{u})\right) \subset [0, +\infty[$ (Bouchut, 1999[a])
  - Numerical **Stability**
- Only for hyperbolic problems. What about diffusive effects ??

[a] F. Bouchut, *Journal of Statistical Physics* **95**, 113–170, ISSN: 00224715 (1999).

- $(f_i) \in \mathbb{R}^k$
- Numerical stability is complex to analyze
- Viscous effects at 1st order thanks to Chapman-Enskog expansions

We rewrite the Jin-Xin system as:

$$\frac{\partial u}{\partial t} + \frac{\partial v}{\partial x} = 0, \tag{10}$$

$$\frac{\partial v}{\partial t} + \frac{1}{\varepsilon}\frac{\partial p(u)}{\partial x} = \frac{1}{\varepsilon}(f(u) - v), \qquad p'(u) > 0. \tag{11}$$

Eq. (11) gives:

$$v = f(u) - \frac{\partial p(u)}{\partial x} - \varepsilon \frac{\partial v}{\partial t} \xrightarrow[\varepsilon \to 0]{} f(u) - \frac{\partial p(u)}{\partial x},$$

and then in the limit $\varepsilon \to 0$, equation (10) becomes an advection-diffusion equation:

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$$\frac{\partial}{\partial x}\left(K\frac{\partial u}{\partial x}\right)$$

Diffusive limit of the Jin-Xin systems

Diagonalizing the diffusive Jin-Xin model gives:

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Problem of this approach (explicit scheme for transport)

$$\Delta t = \frac{\text{CFL}}{a}\Delta x = \text{CFL}\sqrt{\frac{\varepsilon}{p'(u)}}\Delta x \xrightarrow[\varepsilon\to 0]{} 0$$

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Idea: Chapman-Enskog

Proposed approach: Analogy with how Navier Stokes is obtained from Boltzmann (Chapman-Enskog[4])

Chapman-Enskog

$$\begin{aligned}\text{Boltzmann} &= \text{Euler} + \mathcal{O}(\varepsilon)\\ &= \underbrace{\text{Euler} + \varepsilon\,(\text{“viscous effect/diffusion”})}_{=\text{Navier-Stokes}} + \mathcal{O}(\varepsilon^2),\end{aligned}$$

where ε is the Knudsen number.

Can we apply this approach to kinetic models in order to introduce viscous effects?

1) Define a Knudsen Number ε
2) Write an asymptotic expansion for $\varepsilon \ll 1$ ($\neq$ study the limit when $\varepsilon \to 0$)
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Knudsen number for kinetic methods

1) Definition of the Knudsen number

$$\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} = \frac{1}{\tau}(\mathbb{M} - \mathbf{F})$$

Scaling: let's consider a characteristic problem size ℓ and a characteristic velocity $a = ||\Lambda_x||$.

$$t^* = \frac{at}{\ell}, \qquad x^* = \frac{x}{\ell}, \qquad \Lambda_x^* = \frac{\Lambda}{a}$$

A-Dimensioned kinetic system:

$$\frac{\partial \mathbf{F}}{\partial t^*} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x^*} = \frac{1}{\varepsilon}(\mathbb{M} - \mathbf{F}),$$

Definition of the Knudsen number for BGK

$$\varepsilon = \frac{a\tau}{\ell}$$

Note: In the kinetic theory of BGK gases, $\varepsilon \approx c\tau/\ell$, where c is the speed of sound, characteristic of molecular agitation.

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Chapman-Enskog

2) Asymptotic expansion for $\varepsilon \ll 1$

$$\begin{aligned}\mathbf{F} &= \mathbb{M} - \varepsilon\left(\frac{\partial \mathbf{F}}{\partial t^*} + \Lambda_x^* \frac{\partial \mathbf{F}}{\partial x^*}\right)\\ &= \mathbb{M} - \varepsilon\left(\frac{\partial \mathbb{M}}{\partial t^*} + \Lambda_x^* \frac{\partial \mathbb{M}}{\partial x^*}\right) + \mathcal{O}(\varepsilon^2)\\ &= \mathbb{M} - \tau\left(\frac{\partial \mathbb{M}}{\partial t} + \Lambda_x \frac{\partial \mathbb{M}}{\partial x}\right) + \mathcal{O}(\varepsilon^2)\end{aligned}$$

Hence

$$\mathbb{P}\Lambda_x \mathbf{F} = \mathbf{f}(\mathbf{u}) - \tau\left(\frac{\partial \mathbf{f}(\mathbf{u})}{\partial t} + \frac{\partial(\mathbf{m}_2(\mathbf{u}))}{\partial x}\right) + \mathcal{O}(\varepsilon^2), \qquad \mathbf{m}_2 = \mathbb{P}\Lambda_x^2 \mathbb{M}$$

$\vdots$ (chain rules)

$$\mathbb{P}\Lambda_x \mathbf{F} = \mathbf{f}(\mathbf{u}) + \tau\left[(\mathbf{f}'(\mathbf{u}))^2 - \mathbf{m}_2'(\mathbf{u})\right]\frac{\partial \mathbf{u}}{\partial x} + \mathcal{O}(\varepsilon^2)$$

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3) Identification of the diffusive terms

$$\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} = \frac{1}{\tau}(\mathbb{M} - \mathbf{F})$$

Apply $\mathbb{P}$ and replace $\mathbb{P}\Lambda_x\mathbf{F}$ by its asymptotic expansion:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \frac{\partial}{\partial x}\left(\tau\left[\mathbf{m}_2'(\mathbf{u}) - (\mathbf{f}'(\mathbf{u}))^2\right]\frac{\partial \mathbf{u}}{\partial x}\right) + \mathcal{O}(\varepsilon^2)$$

Target equation:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \frac{\partial}{\partial x}\left(\mathbf{D}\frac{\partial \mathbf{u}}{\partial x}\right), \quad \mathbf{D} : \text{diffusion matrix}$$

Identification for a scalar problem: $\tau = \dfrac{D}{m_2'(u) - (f'(u))^2}$.

But it is not possible to do that in general.

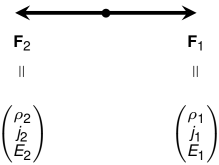
Idea: Relaxation matrix

How can we introduce new parameters to control the $\mathcal{O}(\varepsilon)$ term in the general case?
Idea: Introduction of a relaxation matrix

$$\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} = \boldsymbol{\Omega}(\mathbb{M} - \mathbf{F})$$

- Conservation condition: $\mathbb{P}\boldsymbol{\Omega}(\mathbb{M} - \mathbf{F}) = \mathbf{0}$.
  ➤ Choice of a block matrix: $\boldsymbol{\Omega} = \mathbf{Id}_k \otimes \tilde{\boldsymbol{\Omega}}$.

Example: Navier-Stokes 1D, 2 wave model



$$\frac{\partial}{\partial t}\begin{pmatrix} \rho_1 \\ j_1 \\ E_1 \end{pmatrix} + a\,\frac{\partial}{\partial x}\begin{pmatrix} \rho_1 \\ j_1 \\ E_1 \end{pmatrix} = \tilde{\boldsymbol{\Omega}}\begin{pmatrix} \mathbb{M}_1^{\rho} - \rho_1 \\ \mathbb{M}_1^{j} - j_1 \\ \mathbb{M}_1^{E} - E_1 \end{pmatrix},$$

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho_2 \\ j_2 \\ E_2 \end{pmatrix} - a\,\frac{\partial}{\partial x}\begin{pmatrix} \rho_2 \\ j_2 \\ E_2 \end{pmatrix} = \tilde{\boldsymbol{\Omega}}\begin{pmatrix} \mathbb{M}_2^{\rho} - \rho_2 \\ \mathbb{M}_2^{j} - j_2 \\ \mathbb{M}_2^{E} - E_2 \end{pmatrix}.$$

Relaxation matrix: identification of the diffusive terms

1) Define a Knudsen number ε,
2) Perform an asymptotic expansion for $\varepsilon \ll 1$,
3) Identifiy the $\mathcal{O}(\varepsilon)$ terms as diffusive terms.

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \frac{\partial}{\partial x}\left(\tilde{\boldsymbol{\Omega}}^{-1}\left[\mathbf{m}_2'(\mathbf{u}) - (\mathbf{f}'(\mathbf{u}))^2\right]\frac{\partial \mathbf{u}}{\partial x}\right) + \mathcal{O}(\varepsilon^2)$$

Target problem:

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} = \frac{\partial}{\partial x}\left(\mathbf{D}\frac{\partial \mathbf{u}}{\partial x}\right), \quad \mathbf{D} : \text{diffusion matrix}$$

Condition on the Ω matrix

$$\tilde{\boldsymbol{\Omega}}^{-1} = \mathbf{D}\ \underbrace{\left[\mathbf{m}_2'(\mathbf{u}) - (\mathbf{f}'(\mathbf{u}))^2\right]}_{\text{invertible when } a > |(f)'(\mathbf{u})|}{}^{-1}, \qquad \varepsilon = \frac{\|\mathbf{D}\|}{a\ell}$$

Note: In the kinetic theory of BGK gases, $\varepsilon \approx c\tau/\ell$, where c is the speed of sound, characteristic of molecular agitation.

Discretisation

Crank Nicholson, 1D, and $\Omega = \mathrm{Id}$ to simplify

$$\frac{\mathbf{F}^{n+1} - \mathbf{F}^n}{\Delta t} + \frac{1}{2}\left(\frac{\delta_x \mathbf{F}^{n+1}}{\delta x} + \frac{\delta_x \mathbf{F}^n}{\delta x}\right) - \frac{1}{2\varepsilon}\left(\mathbb{MP}\mathbf{F}^{n+1} - \mathbf{F}^{n+1} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

Difficult to solve, but one can expect second order in time, and space (δ_x), uniformly in ε.

Define

$$L^2(\mathbf{F}) := \mathbf{F} - \mathbf{F}^n + \frac{\Delta t}{2}\left(\frac{\delta_x \mathbf{F}}{\delta x} + \frac{\delta_x \mathbf{F}^n}{\delta x}\right) - \frac{\Delta t}{2\varepsilon}\left(\mathbb{MP}\mathbf{F} - \mathbf{F} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

amounts to solving $L^2(\mathbf{F}) = 0$.

Introduce L^1:

$$L^1(\mathbf{F}) = \mathbf{F} - \mathbf{F}^n + \Delta t \frac{\delta_x \mathbf{F}^n}{\delta x} - \frac{\Delta t}{2\varepsilon}\left(\mathbb{MP}\mathbf{F} - \mathbf{F} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

Discretisation

Crank Nicholson, 1D, and $\Omega = \mathrm{Id}$ to simplify

$$\frac{\mathbf{F}^{n+1} - \mathbf{F}^{n}}{\Delta t} + \frac{1}{2}\left(\frac{\delta_x \mathbf{F}^{n+1}}{\delta x} + \frac{\delta_x \mathbf{F}^{n}}{\delta x}\right) - \frac{1}{2\varepsilon}\left(\mathbb{MP}\mathbf{F}^{n+1} - \mathbf{F}^{n+1} + \mathbb{MP}\mathbf{F}^{n} - \mathbf{F}^{n}\right)$$

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$$\frac{\mathbf{F}^{n+1} - \mathbf{F}^n}{\Delta t} + \frac{1}{2}\left(\frac{\delta_x \mathbf{F}^{n+1}}{\delta x} + \frac{\delta_x \mathbf{F}^n}{\delta x}\right) - \frac{1}{2\varepsilon}\left(\mathbb{MP}\mathbf{F}^{n+1} - \mathbf{F}^{n+1} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

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and note that $L^1(\mathbf{F}) - L^2(\mathbf{F}) = O(\Delta t)$

Discretisation

Crank Nicholson, 1D, and $\Omega = \mathrm{Id}$ to simplify

$$\frac{\mathbf{F}^{n+1} - \mathbf{F}^n}{\Delta t} + \frac{1}{2}\left(\frac{\delta_x \mathbf{F}^{n+1}}{\delta x} + \frac{\delta_x \mathbf{F}^n}{\delta x}\right) - \frac{1}{2\varepsilon}\left(\mathbb{MP}\mathbf{F}^{n+1} - \mathbf{F}^{n+1} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

Difficult to solve, but one can expect second order in time, and space (δ_x), uniformly in ε.
Define

$$L^2(\mathbf{F}) := \mathbf{F} - \mathbf{F}^n + \frac{\Delta t}{2}\left(\frac{\delta_x \mathbf{F}}{\delta x} + \frac{\delta_x \mathbf{F}^n}{\delta x}\right) - \frac{\Delta t}{2\varepsilon}\left(\mathbb{MP}\mathbf{F} - \mathbf{F} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

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Introduce L^1:

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and note that $L^1(\mathbf{F}) - L^2(\mathbf{F}) = O(\Delta t)$ independant of ε

Defered correction technique

Assumptions

If

- for some norm $\|L^1 - L^2\| \leq C\Delta t$, $L^2(\mathbf{F}) = 0$ has a unique solution $\mathbf{F}^\star$ and $\|L^1(\mathbf{F}) - L^1(\mathbf{F}')\| \geq \alpha\Delta t$
- Consider $\mathbf{F}^{(0)} = \mathbf{F}^n$ and define $\mathbf{F}^{(p+1)}$ as

$$L^1\left(\mathbf{F}^{(p+1)}\right) = L^1\left(\mathbf{F}^{(p)}\right) - L^2\left(\mathbf{F}^{(p)}\right)$$

Then, independently of ε

$$\|\mathbf{F}^\star - \mathbf{F}^{(p)}\| \leq C\Delta t^p \|\mathbf{F}^{(0)} - \mathbf{F}^\star\|.$$

Proof.

$$\begin{aligned}\alpha\|\mathbf{F}^{(p+1)} - \mathbf{F}^\star\| &\leq \|L^1(\mathbf{F}^{(p+1)} - L^1(\mathbf{F}^\star)\| = \left\|\left[L^1(\mathbf{F}^{(p)}) - L^2(\mathbf{F}^{(p)})\right] - \left[L^1(\mathbf{F}^\star) - L^2(\mathbf{F}^\star)\right]\right\| \\ &\leq C\Delta t \, \|\mathbf{F}^{(p)} - \mathbf{F}^\star\|\end{aligned}$$

□

Last question: How to solve $L^1 = 0$?

How to solve $L^1 = 0$?

$$\mathbf{F} = \mathbf{F}^n - \Delta t \frac{\delta_x \mathbf{F}}{\Delta t} + \frac{\Delta t}{2\varepsilon}\left(\mathbb{MPF} - \mathbf{F} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

Apply $\mathbb{P}$:

$$\mathbb{P}\mathbf{F} = \mathbb{P}\mathbf{F}^n - \Delta t \frac{\mathbb{P}\delta_x \mathbf{F}}{\Delta t}$$

then

$$\mathbf{F} = \omega^{-1}\left(\mathbf{F}^n + \Delta t \frac{\delta_x \mathbf{F}}{\Delta t}\right) + \frac{\omega^{-1}\Delta t}{2\varepsilon}\left(\mathbb{MPF} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

where $\omega = (1 + \frac{\Delta t}{2\varepsilon})$ so that

$$\frac{\omega^{-1}\Delta t}{2\varepsilon} = \frac{\Delta t}{\Delta t + 2\varepsilon}.$$

Note: $L^1(\mathbf{F}^{(p+1)}) = L^1(\mathbf{F}^{(p)}) - L^2(\mathbf{F}^{(p)})$ writes

$$\mathbf{F}^{(p+1)} = \mathbf{F}^n - \frac{\Delta t}{2}\left(\frac{\delta_x \mathbf{F}^{(p+1)}}{\delta x} + \frac{\delta_x \mathbf{F}^n}{\delta x}\right) - \frac{\Delta t}{2\varepsilon}\left(\mathbb{MP}\mathbf{F}^{(p+1)} - \mathbf{F}^{(p+1)} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

so we can do the same directly on the iteration.

How to solve $L^1 = 0$?

$$\mathbf{F} = \mathbf{F}^n - \Delta t \frac{\delta_x \mathbf{F}}{\Delta t} + \frac{\Delta t}{2\varepsilon}\left(\mathbb{MPF} - \mathbf{F} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

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$$\mathbb{P}\mathbf{F} = \mathbb{P}\mathbf{F}^n - \Delta t \frac{\mathbb{P}\delta_x \mathbf{F}}{\Delta t}$$

then

$$\mathbf{F} = \omega^{-1}\left(\mathbf{F}^n + \Delta t \frac{\delta_x \mathbf{F}}{\Delta t}\right) + \frac{\omega^{-1}\Delta t}{2\varepsilon}\left(\mathbb{MPF} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

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$$\mathbf{F}^{(p+1)} = \mathbf{F}^n - \frac{\Delta t}{2}\left(\frac{\delta_x \mathbf{F}^{(p+1)}}{\delta x} + \frac{\delta_x \mathbf{F}^n}{\delta x}\right) - \frac{\Delta t}{2\varepsilon}\left(\mathbb{MP}\mathbf{F}^{(p+1)} - \mathbf{F}^{(p+1)} + \mathbb{MP}\mathbf{F}^n - \mathbf{F}^n\right)$$

so we can do the same directly on the iteration.

This generalises to other type of temporal discretisation, see Notes.

Spatial discretisation: $(\delta_x w)_j = \hat{\mathbf{f}}_{j+1/2} - \hat{\mathbf{f}}_{j-1/2}$

Ref: Iserle, IMA J. Numer. Anal., vol 2, 1981

First order approximation:

$$\hat{\mathbf{f}}_{j+1/2} = \frac{1}{2}\left(w_j + w_{j+1} + \text{sign }(a)(w_{j+1} - w_j)\right), \quad \text{sign}(a) = \frac{a}{|a|}.$$

Second order:

$$\hat{\mathbf{f}}_{j+1/2} = \frac{1 - \text{ sign }(a)}{12}\left(2w_j + 5w_{j+1} - w_{j+2}\right) + \frac{1 + \text{ sign }(a)}{12}\left(2w_{j+1} + 5w_j - w_{j-1}\right).$$

Fourth order: for δ_4^1 (centered),

$$\hat{\mathbf{f}}_{j+1/2} = a\left(\frac{w_{j+2}}{12} + \frac{3}{4}w_{j+1} + \frac{3}{4}w_j + \frac{w_{j-1}}{12}\right)$$

for δ_4^2 (upwind biased),

$$\begin{aligned}\hat{\mathbf{f}}_{j+1/2} =& \frac{1 - \text{ sign }(a)}{2}\left(\frac{w_{j+3}}{12} - \frac{5}{12}w_{j+2} + \frac{13}{12}w_{j+1} + \frac{w_j}{4}\right)\\ &+ \frac{1 + \text{ sign }(a)}{2}\left(\frac{w_{j+1}}{4} + \frac{13}{12}w_j - \frac{5}{12}w_{j-1} + \frac{w_{j-2}}{12}\right).\end{aligned}$$

Stability analysis, $\Omega = \mathbf{Id}$

Operator	δ_1	δ_2	δ_4^1	δ_4^2
Symbol g	$1 - e^{-i\theta}$	$\frac{1}{3}e^{i\theta} + \frac{1}{2} - e^{-i\theta} + \frac{1}{6}e^{-2i\theta}$	$i\left(\frac{\sin(2\theta)}{6} + \frac{4}{3}\sin\theta\right)$	$\frac{e^{i\theta}}{4} + \frac{5}{6} - \frac{3}{2}e^{-i\theta} + \frac{1}{2}e^{-2i\theta} - \frac{e^{-3i\theta}}{12}$

Table: List of Fourier symbols.

Scheme		# iterations					
Order	δ	1	2	3	4	5	6
2	δ_1	1	1	1	1	1	1
2	δ_2	0	≥ 0.85	≥ 1.22	≥ 1.02	≥ 1.08	≥ 1.23
2	δ_4^1	0	0	≥ 1.45	≥ 1.45	≥ 0.002	≥ 0.01
2	δ_4^2	0	≥ 0.5	≥ 0.69	0.71	0.73	0.73
3	δ_1	6	≥ 1.5	≥ 1.87	≥ 2	≥ 2.23	≥ 2.48
3	δ_2	0	0	1	≥ 2.0447	≥ 2.17120	≥ 2.568
3	δ_4^1	0	0	0	≥ 1.6171	≥ 2.4727	≥ 2.9162
3	δ_4^2	0	0	≥ 0.1	≥ 1.3096	≥ 1.3955	≥ 1.8282

Table: CFL number for stability of the DeC iterations. 0 means that the scheme is unconditionally unstable. If a real number x is given, it means that the scheme is stable up to CFL x, if $\geq x$ is written, this means that the scheme is stable for at least CFL x (and slightly above indeed).

When introducing Ω which is not necessary invertible

Arbitrary order numerical method (Abgrall & Torlo, 2020[5]):

- **First order** in time and space: implicit-explicit upwind
  - ➤ linear stability: $a\frac{\Delta t}{\Delta x} < 1$
- **2nd order** in time/space: Deferred Correction (DeC)
  - ➤ linear stability: $a\frac{\Delta t}{\Delta x} < 0.87$
- **4th order** in time/space: Deferred Correction (DeC)
  - ➤ linear stability: $a\frac{\Delta t}{\Delta x} < 1.04$

These schemes use $\tilde{\mathbf{\Omega}}^{-1}$ and not $\tilde{\mathbf{\Omega}}$.

- Asymptotic preservation (AP): when $\tilde{\mathbf{\Omega}}^{-1} = \mathbf{0}$, consistancy with the hyperbolic system ($\mathbf{D} = \mathbf{0}$).
  - ➤ Example: Euler: $\tilde{\mathbf{\Omega}} = \mathbf{0}$

- $\tilde{\mathbf{\Omega}}^{-1}$ may no be invertible.
  - ➤ Example: Navier-Stokes : $\tilde{\mathbf{\Omega}} = \begin{bmatrix} 0 & 0 & 0 \\ - & - & - \\ - & - & - \end{bmatrix}$

[5] R. Abgrall, D. Torlo, *SIAM Journal on Scientific Computing* **42**, B816–B845, ISSN: 10957197 (2020).

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Overview

Validation: linear acoustic propagation

$$\mathbf{u}(x,0) = \overline{\mathbf{u}} + |\hat{\mathbf{u}}|\cos(2\pi x + \phi(\hat{\mathbf{u}})), \quad |\hat{\mathbf{u}}| \ll \overline{\mathbf{u}},$$

$$\overline{\rho} = 1, \quad \overline{P} = 1, \quad \overline{\mathrm{Ma}} = 2, \quad \gamma = 1.4, \quad \mathrm{Pr} = 0.71,$$

$$\mathbf{u}_{exact}(x,t) = \overline{\mathbf{u}} + |\hat{\mathbf{u}}|\cos(2\pi x - \mathrm{Re}(\omega)t + \phi(\hat{\mathbf{u}}))e^{\mathrm{Im}(\omega)t}$$

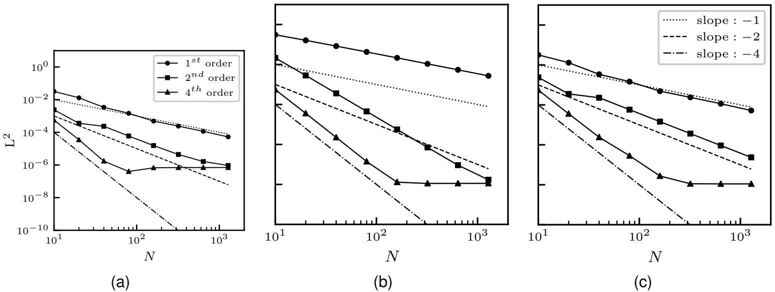


Figure: (a): $\mu = 10^{-3}$, $\varepsilon \approx 1.6\,10^{-3}$, $a = 1.1\ \max(|u| + c)$, (b):$\mu = 10^{-3}$, $\varepsilon \approx 1.8\,10^{-4}$, $a = 10\ \max(|u| + c)$, (c):$\mu = 0$, $\varepsilon = 0$, $a = 1.1\ \max(|u| + c)$

- Expected convergence order
- Observed Plateau =consistency error when ε $\quad (\varepsilon = \mu/(a\ell))$

Validation: linear acoustic propagation

Error convergence study, function of ε
Same test case with

$$N = 1000, \qquad \mu = 0.1, \qquad \text{4th order scheme}$$

(aim: avoid numerical errors)

$a/\max(\lvert u\rvert + c)$	ε	L^2	r
1.1	0.16	$4.6585\ 10^{-4}$	-
2.2	0.08	$2.8028\ 10^{-4}$	0.73
4.4	0.04	$9.7336\ 10^{-5}$	1.53
8.8	0.02	$2.5826\ 10^{-5}$	1.91
17.6	0.01	$6.5393\ 10^{-6}$	1.98
35.2	0.005	$1.6399\ 10^{-6}$	2.00

- We observe a consistency error in $\mathcal{O}(\varepsilon^2)$

Validation: viscous shock

Viscous shock:

$$\mathrm{Ma} = 2, \qquad \mu = 0.001, \qquad \mathrm{Pr} = 3/4, \qquad \gamma = 1.4$$

$N = 10$ points in the characteristic shock width.

Why this test case: analytical solution of NS.

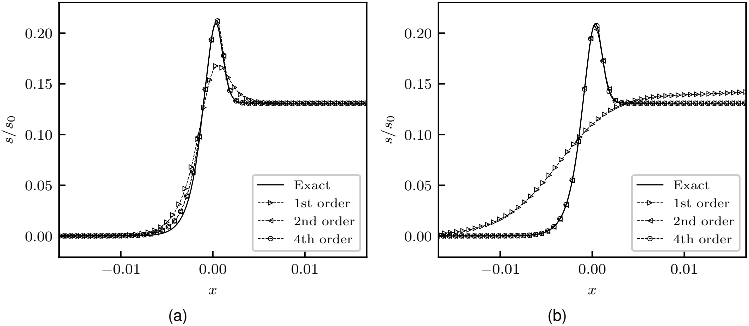


Figure: (a): $a = 1.1 \max(|u| + c)$ ($\varepsilon \approx 0.16$), (b): $a = 10 \max(|u| + c)$ ($\varepsilon \approx 0.017$)

q

Overview

Example: relaxation matrix in 2D

Writing a 2D matrix-relaxation kinetic model:

$$\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} + \Lambda_y \frac{\partial \mathbf{F}}{\partial y} = \mathbf{\Omega} \frac{\mathbb{M} - \mathbf{F}}{\varepsilon}$$

Target model: advection diffusion.

$$\begin{aligned}\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{f}(\mathbf{u})}{\partial x} + \frac{\partial \mathbf{g}(\mathbf{u})}{\partial y} &= \frac{\partial}{\partial x}\left(\mathbf{D}_{xx}\frac{\partial \mathbf{u}}{\partial x} + \mathbf{D}_{xy}\frac{\partial \mathbf{u}}{\partial y}\right) \\ &+ \frac{\partial}{\partial y}\left(\mathbf{D}_{yx}\frac{\partial \mathbf{u}}{\partial x} + \mathbf{D}_{yy}\frac{\partial \mathbf{u}}{\partial y}\right)\end{aligned}$$

With respect to 1D, 2 difficulties:

- How to take into account the terms ($\mathbf{D}_{xy}$ and $\mathbf{D}_{yx}$)?
- How to construct a relaxation matrix $\mathbf{\Omega}$ that satisfies the conservation condition: $\mathbb{P}\mathbf{\Omega}(\mathbb{M} - \mathbf{F}) = \mathbf{0}$?

Description in the moment space

Idea : Rewrite the problem in the moment space

Definition: Moment matrix

$$\mathbf{Q} = \begin{pmatrix} \mathbb{P} \\ \mathbb{P}\Lambda_x \\ \mathbb{P}\Lambda_y \\ \mathbb{H} \end{pmatrix} \quad \begin{matrix} \leftarrow \textit{moment of order 0} \\ \leftarrow \textit{moment of order 1} \\ \leftarrow \textit{moment of order 1} \\ \leftarrow \textit{high order moments} \end{matrix}$$

Q: square invertible matrix ($kp \times kp$)

$\mathbb{H}$: this matrix is constructed **arbitrarily** in order to make **Q** a square and invertible matrix.

Proposition

If $\mathbb{M}$ is a linear function of the $(\mathbf{u}, \mathbf{f}(\mathbf{u}), \mathbf{g}(\mathbf{u}))$, then one can choose $\mathbb{H}$ so that $\mathbb{H}\mathbb{M} = \mathbf{0}$.

In the following, we assume that $\mathbb{H}\mathbb{M} = \mathbf{0}$.

Example: 4 waves model

$$\Lambda_x = \mathrm{diag}(a, -a, 0, 0), \quad \Lambda_y = \mathrm{diag}(0, 0, a, -a), \quad \mathbb{M} = \frac{\mathbf{u}}{4} + \frac{1}{2a}\begin{bmatrix} \mathbf{f}(\mathbf{u}) \\ -\mathbf{f}(\mathbf{u}) \\ \mathbf{g}(\mathbf{u}) \\ -\mathbf{g}(\mathbf{u}) \end{bmatrix}.$$

One can choose the following moment matrix:

$$\mathbf{Q} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ a & -a & 0 & 0 \\ 0 & 0 & a & -a \\ a^2 & a^2 & -a^2 & -a^2 \end{pmatrix}.$$

One can check that:

$$\mathbf{Q}\mathbb{M} = [\mathbf{u}, \mathbf{f}(\mathbf{u}), \mathbf{g}(\mathbf{u}), \mathbf{0}]^T.$$

Note: $\mathbb{H} = \begin{pmatrix} a^2 & a^2 & -a^2 & -a^2 \end{pmatrix} = \mathbb{P}(\Lambda_x^2 - \Lambda_y^2)$: this justifies the denomination "*high order moment*".

Relaxation matrix in the basis of moments

We choose to describe the relaxation matrix $\mathbf{\Omega}$ in the basis of moments as

$$\mathbf{\Omega} = \mathbf{Q}^{-1} \begin{pmatrix} \alpha \mathbf{Id}_p & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \beta \mathbf{Id}_p \end{pmatrix} \mathbf{Q}$$

where

- $\alpha, \beta \in \mathbb{R}$ are two parameters to be defined,
- $\mathbf{C}$ is a $(2p \times 2p)$ square matrix to determine.

With this choice, we have

$$\mathbb{P}\mathbf{\Omega} = \alpha \mathbb{P} \quad \Rightarrow \quad \mathbb{P}\mathbf{\Omega}(\mathbb{M} - \mathbf{F}) = \alpha \mathbb{P}(\mathbb{M} - \mathbf{F}) = \mathbf{0}.$$

- How to take into account the terms $\mathbf{D}_{xy}$ and $\mathbf{D}_{yx}$?
- How to construct a relaxation matrix $\mathbf{\Omega}$ such that: $\mathbb{P}\mathbf{\Omega}(\mathbb{M} - \mathbf{F}) = \mathbf{0}$? ✓

Construction of the relaxation matrix (2/2)

- As in 1D, the Knudsen can be defined as:

$$\varepsilon = \frac{||\mathbf{D}||}{a\ell}.$$

- The 1st order terms in ε can be identified as diffusion terms when

$$\mathbf{C}^{-1} = \mathbf{D}\left(\mathbf{J}_\Lambda - \mathbf{J}_f\right)^{-1}, \qquad \mathbf{J}_\Lambda = \begin{pmatrix} \mathbb{P}\Lambda_x^2\mathbb{M}'(\mathbf{u}) & \mathbb{P}\Lambda_x\Lambda_y\mathbb{M}'(\mathbf{u}) \\ \mathbb{P}\Lambda_x\Lambda_y\mathbb{M}'(\mathbf{u}) & \mathbb{P}\Lambda_y^2\mathbb{M}'(\mathbf{u}) \end{pmatrix},$$

$$\mathbf{J}_f = \begin{pmatrix} \mathbf{f}'(\mathbf{u})^2 & \mathbf{f}'(\mathbf{u})\mathbf{g}'(\mathbf{u}) \\ \mathbf{f}'(\mathbf{u})\mathbf{g}'(\mathbf{u}) & \mathbf{g}'(\mathbf{u})^2 \end{pmatrix}$$

  - As in 1D, $\mathbf{J}_\Lambda - \mathbf{J}_f$ is invertible if $a > \max\Big(\rho(\mathbf{f}'(\mathbf{u})), \rho(\mathbf{g}'(\mathbf{u}))\Big)$.

- The parameters α and β play NO role in the expansion at 1st order:
  - α never play a role
  - β would play a role for higher order expansions

Regularisation

As in 1D, the matrix Ω appears only via its inverse:

$$\boldsymbol{\Omega}^{-1} = \mathbf{Q}^{-1} \begin{pmatrix} 1/\alpha \mathbf{Id}_p & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 1/\beta \mathbf{Id}_p \end{pmatrix} \mathbf{Q}$$

Regularisation inspired by regularised LBM (Latt 2006 (*8*))

"$1/\alpha = 0$", "$1/\beta = 0$", and then:

$$\boldsymbol{\Omega}^{-1} = \boldsymbol{\Omega}^{-1} = \mathbf{Q}^{-1} \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{C}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \mathbf{Q}$$

Effect of regularization on high-order moments

The kinetic system is written as

$$\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} + \Lambda_y \frac{\partial \mathbf{F}}{\partial y} = \mathbf{\Omega}(\mathbb{M} - \mathbf{F}),$$

or, equivalently :

$$\mathbf{F} - \mathbb{M} - \mathbf{\Omega}^{-1}\left(\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} + \Lambda_y \frac{\partial \mathbf{F}}{\partial y}\right).$$

Multiply on the left by $\mathbb{H}$ (high-order moment matrix):

$$\mathbb{H}\mathbf{F} = \underbrace{\mathbb{H}\mathbb{M}}_{=0} - \underbrace{\mathbb{H}\mathbf{\Omega}^{-1}}_{=0}\left(\frac{\partial \mathbf{F}}{\partial t} + \Lambda_x \frac{\partial \mathbf{F}}{\partial x} + \Lambda_y \frac{\partial \mathbf{F}}{\partial y}\right) = \mathbf{0}$$

Principle of regularization: filter out high-order moments

Numerical schemes for Navier-Stokes

- Numerical methods similar to those presented in 1D: orders 1, 2 and 4
- Method used in the following: 4-wave system ($\sim$ D2Q4), with regularized relaxation matrix
- $a = 2.1\,\mathrm{max}(u + c, v + c)$ (existence of an entropy)
- Kinetic system equivalent to a Jin-Xin system with relaxation matrix:

$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{u}\\ \mathbf{v}_x\\ \mathbf{v}_y\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\ a^2/2 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}\frac{\partial}{\partial x}\begin{pmatrix}\mathbf{u}\\ \mathbf{v}_x\\ \mathbf{v}_y\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ a^2/2 & 0 & 0\end{pmatrix}\frac{\partial}{\partial y}\begin{pmatrix}\mathbf{u}\\ \mathbf{v}_x\\ \mathbf{v}_y\end{pmatrix}$$
$$= \begin{bmatrix}\mathbf{0}\\ \mathbf{C}\begin{pmatrix}\mathbf{f}(\mathbf{u}) - \mathbf{v}_x\\ \mathbf{g}(\mathbf{u}) - \mathbf{v}_y\end{pmatrix}\end{bmatrix}$$

➤ Memory cost reduction

q

Overview

Scalar case, no viscosity

Consider the two-dimensional advection equation:

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} = 0, \ (x, y, t) \in [-2, 2] \times [-2, 2] \times \mathbb{R}^+,$$

and periodic boundary conditions. We consider the following initial condition:

$$u_0(x, y) = \sin(\pi x + \pi y), \ (x, y) \in (-2, 2) \times (-2, 2).$$

The CFL number is set to 1. The convergence for the density is shown in Tables 3 and 4 for final time $T = 10$ for orders 2 and 4, which result in the predicted convergence rates of second and fourth order, respectively.

Scalar case, no viscosity

Table: Convergence study for the advection equation for order 2 at $T = 10$.

h	L^1-error	slope	L^2-error	slope	L^∞-error	slope
0.05	$1.0698.10^{+1}$	-	$2.8479.10^{0}$	-	$9.3878.10^{-1}$	-
0.025	$3.5595.10^{0}$	1.59	$9.6212.10^{-1}$	1.57	$3.3039.10^{-1}$	1.51
0.0125	$6.8578.10^{-1}$	2.38	$1.8812.10^{-1}$	2.35	$6.5662.10^{-2}$	2.33
0.00625	$1.4701.10^{-1}$	2.22	$4.0558.10^{-2}$	2.21	$1.4243.10^{-2}$	2.20
0.003125	$3.4890.10^{-2}$	2.08	$9.6578.10^{-3}$	2.07	$3.4037.10^{-3}$	2.07

Table: Convergence study for the advection equation for order 4 at $T = 10$.

h	L^1-error	slope	L^2-error	slope	L^∞-error	slope
0.05	$4.7601.10^{0}$	-	$1.2919.10^{0}$	-	$4.1702.10^{-1}$	-
0.025	$3.1678.10^{-1}$	3.91	$8.5482.10^{-2}$	3.92	$2.9212.10^{-2}$	3.84
0.0125	$1.8698.10^{-2}$	4.08	$5.1232.10^{-3}$	4.06	$1.7850.10^{-3}$	4.03
0.00625	$1.1427.10^{-3}$	4.03	$3.1527.10^{-4}$	4.02	$1.1072.10^{-4}$	4.01
0.003125	$7.0804.10^{-5}$	4.01	$1.9599.10^{-5}$	4.01	$6.9070.10^{-6}$	4.00

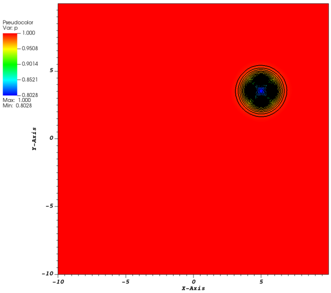
The initial conditions are given by

$$\rho = \left[1 - \frac{(\gamma - 1)\beta^2}{32\gamma\pi^2} \exp\left(1 - r^2\right)\right]^{\frac{1}{\gamma-1}}, p = \rho^\gamma,$$

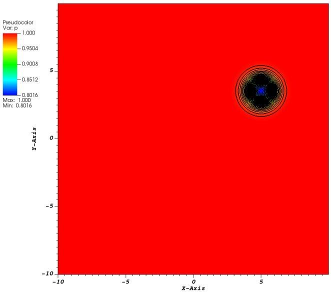
$$v_x = 1 - \frac{\beta}{4\pi} \exp\left(\frac{1 - r^2}{2}\right)(y - y_c), v_y = \frac{\sqrt{2}}{2} + \frac{\beta}{4\pi} \exp\left(\frac{1 - r^2}{2}\right)(x - x_c),$$

where $\gamma = 1.4$, $\beta = 5$ and $r = \sqrt{(x - x_c)^2 + (y - y_c)^2}$. The computational domain is a square $[-10, 10] \times [-10, 10]$. Also, the free stream conditions are given by:

$$\rho_\infty = 1, \quad v_{x,\infty} = 1, \quad v_{y,\infty} = \frac{\sqrt{3}}{2}, \quad p_\infty = 1.$$



(a) 4-th order scheme in space and time



(b) Exact

Figure: Plot of the pressure for the vortex problem at $T = 5$.

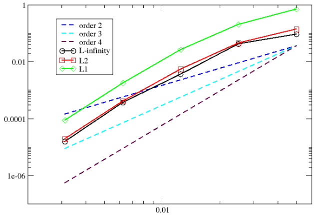
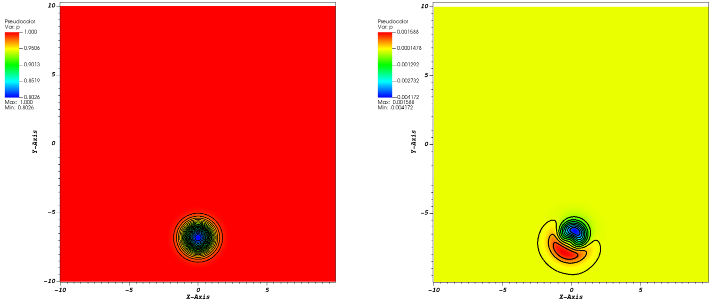


Figure: Convergence plot of density for the fourth order scheme in space and time at $T = 5$.

More

In order to illustrate the long time behavior of the scheme, we show the pressure for $T = 200$ and the error between the computed pressure and the exact one on Fig. 5 and a 200×200 grid. Note that the typical time for a vortex to travel across the domain is about 10.



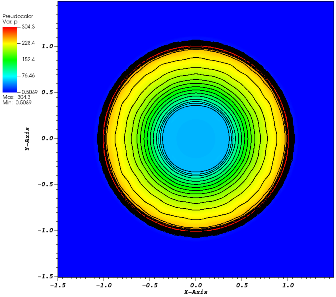
(a) p (b) error

Figure: Pressure and error between the computed solution and the exact one at $T = 200$ on a 200×200 grid. We have $p_{i,j} - p^{ex}_{i,j} \in [-4.2\ 10^{-3}, 1.6\ 10^{-3}]$.

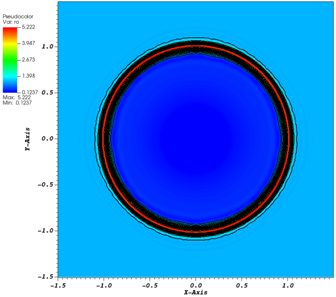
Strong shock

The problem is defined on $[-1.5, 1.5] \times [-1.5, 1.5]$ for $T = 0.025$. We had to use the MOOD technique to get the results, the shocks are too strong.

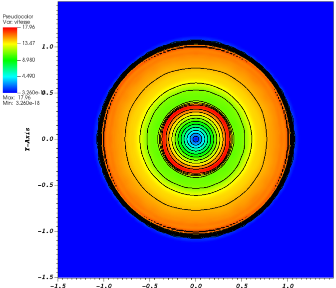
$$(\rho_0, v_{x,0}, v_{y,0}, p_0) = \begin{cases} (1, 0, 0, 1000) & \text{if } r \leq 0.5 \\ (1, 0, 0, 1) & \text{else.} \end{cases} \tag{13}$$

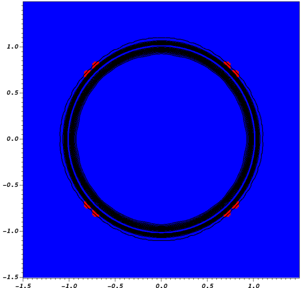

Pseudocolor
Var: p
304.3
228.4
152.4
76.46
0.5089
Max: 304.3
Min: 0.5089
Y-Axis
X-Axis

(a) p


Pseudocolor
Var: ro
5.222
3.947
2.673
1.398
0.1237
Max: 5.222
Min: 0.1237
Y-Axis
X-Axis

(b) ρ


Pseudocolor
Var: vitesse
17.96
13.47
8.980
4.490
Max: 17.96
Min: 3.260e-18
Y-Axis


Y-Axis

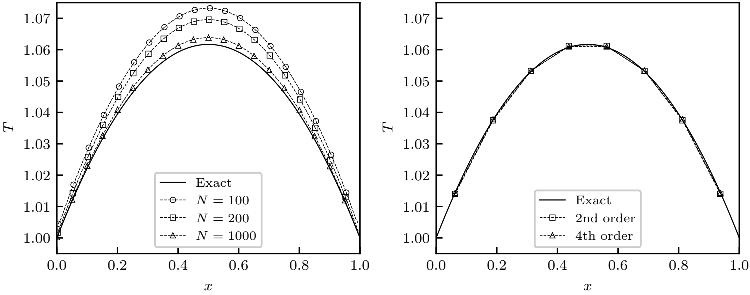
Validation: isothermal Couette flow

Initial conditions:

$$\rho_0 = 1, \qquad (u, v)_0 = (0, 0), \qquad P_0 = 1,$$
$$\gamma = 1.4, \qquad \mathrm{Pr} = 0.73, \qquad \mu = 0.01.$$

Isotherm wall condition (lateral walls):

$$[u, v, T]_L = [0, 1.3\sqrt{\gamma}, 1], \qquad [u, v, T]_R = [0, 0, 1].$$



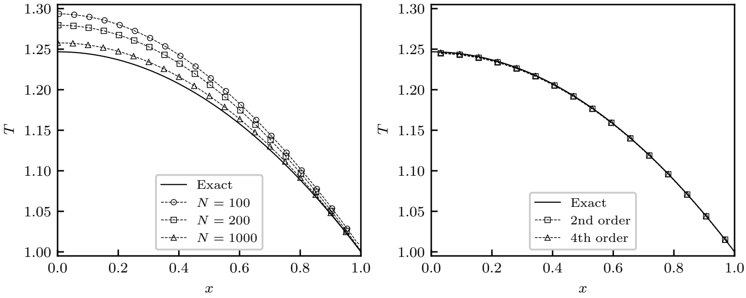
(a) 1st order (b) 2nd, 4th order with $N = 8$ points

Validation: Couette flow, adiabatic walls

Initial conditions:

$$\rho_0 = 1, \qquad (u, v)_0 = (0, 0), \qquad P_0 = 1,$$
$$\gamma = 1.4, \qquad \mathrm{Pr} = 0.73, \qquad \mu = 0.01.$$

Left wall, adiabatic

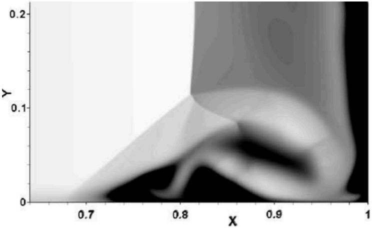


(c) 1st order

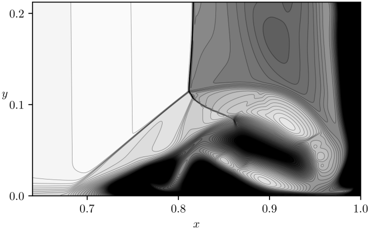
(d) 2nd and 4th order with $N = 16$ points

Shock-boundary layer interaction

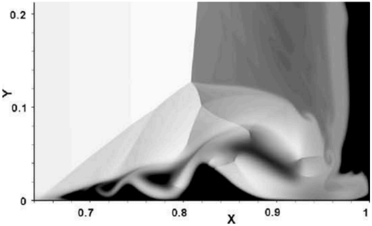
Left: reference solution (Daru & Tenaud, 2009[6], OSMP7), right: kinetic method 4th order, (4000 $\times$ 2000) points.



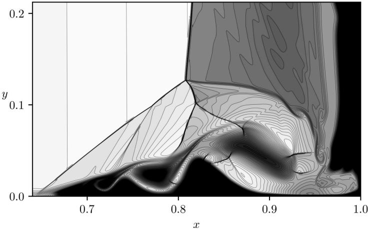
(e) Ref: Temperature, $\mathrm{Re} = 200$, t=0.6



(f) Temperature isolines, $\mathrm{Re} = 200$, t=0.6



(g) Ref: Temperature, $\mathrm{Re} = 1000$, t=0.6

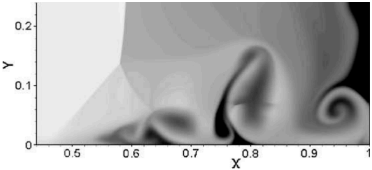


(h) Ref: Temperature, $\mathrm{Re} = 1000$, t=0.6

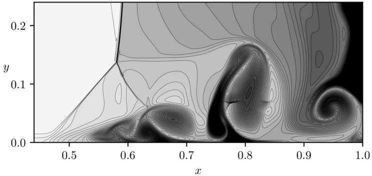
[6] V. Daru, C. Tenaud, *Computers and Fluids* **38**, 664–676, ISSN: 00457930 (2009).

Shock-boundary layer interaction

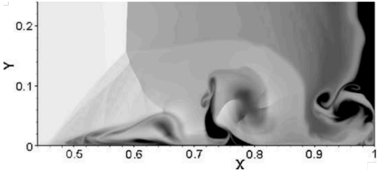
Left: reference solution (Daru & Tenaud, 2009[7], OSMP7), right: kinetic method 4th order, (4000×2000) points.



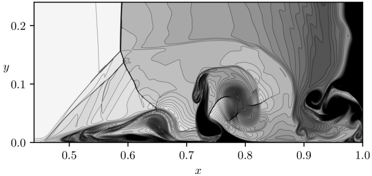
(i) Ref, Temperature, t=1,$\mathrm{Re} = 200$



(j) Temperature isolines, t=1, $\mathrm{Re} = 200$



(k) Ref: Temp, t=1, $\mathrm{Re} = 200$

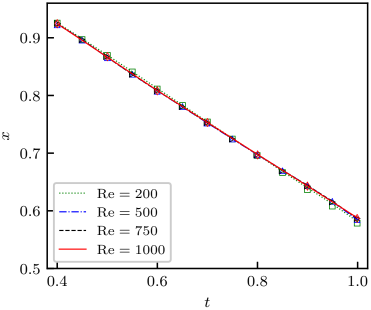


(l) Temperature isolines, t=1, $\mathrm{Re} = 1000$

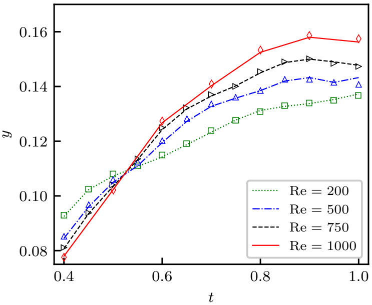
[7] V. Daru, C. Tenaud, *Computers and Fluids* **38**, 664–676, ISSN: 00457930 (2009).

Shock-boundary layer interaction

Localisation of the lambda shock:



(m)



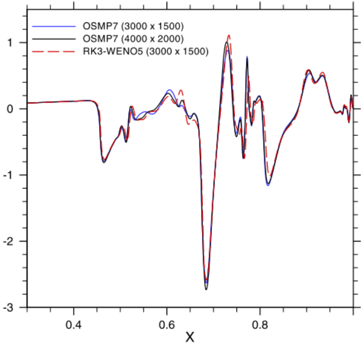
(n)

(Symbols : Reference solution Daru & Tenaud[8]).

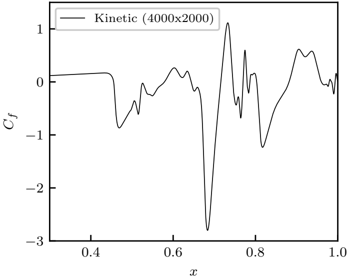
Very good qualitative agreement

[8] V. Daru, C. Tenaud, *Computers and Fluids* **38**, 664–676, ISSN: 00457930 (2009).

Skin friction, $Re = 1000$



(o) Tenaud-Daru

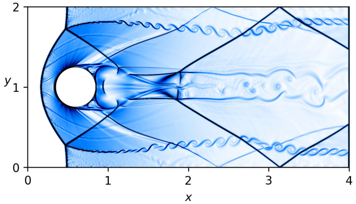


(p) Present

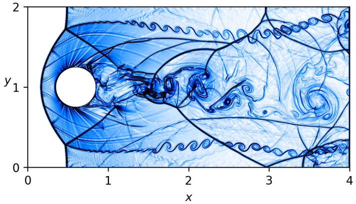
$$c_f = \frac{\mathbf{n}^T \boldsymbol{\tau} \mathbf{n}}{\frac{1}{2}\rho_\infty u_\infty^2}.$$

Flow around a cylinder

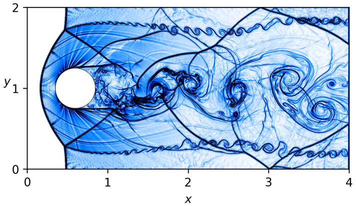
Flow at Mach=3



(q) $\mathrm{Re} = 10^4$



(r) $\mathrm{Re} = 10^5$

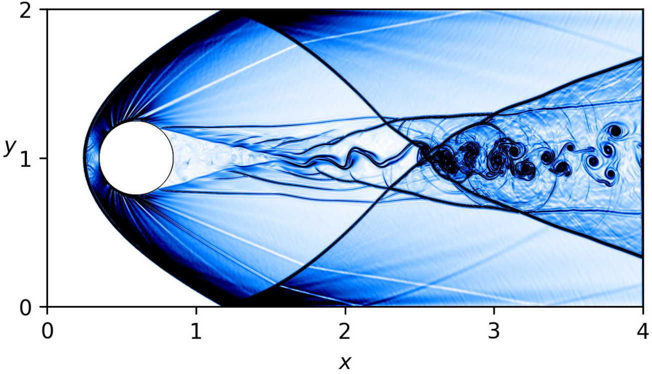


(s) $\mathrm{Re} = 10^7$

Note : "Staircase" boundary conditions on the cylinder. To be improved . . .

Flow around a cylinder

Euler ($\mu = 0$), Mach=100



q

Overview

Conclusion and outlook

- It is possible to develop robust and accurate numerical schemes for compressible Euler. Can be arbitrary accurate. Run at CFL$\geq$ 1.
- Show how to develop kinetic schemes for advection diffusion/Navier Stokes that can be arbitrary accurate.
- Show the properties, in particular consistency. Ru at CFL $\approx$ 1.
- Show preliminary results for high Mach number flow problems
- Must improve boundary conditions (in progress). Heat flux ??
- Can be used for unstructured/polygonal meshes, starting from a scalar convection solver.

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First order Kinetic scheme

First order scheme *(Abgrall & Torlo, 2020*[9]*)*:

- Spatial approximation on Cartesian meshes: $\partial/\partial x \to \delta_x^{(1)}/\Delta x$ (upwinding)

$$\frac{\mathrm{d}\mathbf{F}}{\mathrm{d}t} = -\Lambda_x \frac{\delta_x^{(1)}\mathbf{F}}{\Delta x} + \Omega(\mathbb{P}\mathbf{F})\left[\mathbb{M}(\mathbb{P}\mathbf{F}) - \mathbf{F}\right]$$

- In time: implicit/explicit
  - ➤ Transport: Explicit Euler, first order
  - ➤ Relaxation: Implicit Euler, first order

$$\mathbf{F}^{n+1} = \mathbf{F}^n - \frac{\Delta t}{\Delta x}\Lambda_x \delta_x^{(1)}\mathbf{F}^n + \Delta t\, \Omega_{n+1}\left[\mathbb{M}_{n+1} - \mathbf{F}^{n+1}\right]$$

The implicit scheme can be made explicit in 2 steps:

$$(1)\quad \mathbf{u}^{n+1} := \mathbb{P}\mathbf{F}^{n+1} = \mathbf{u}^n - \frac{\Delta t}{\Delta x}\mathbb{P}\Lambda_x \delta_{x(1)}\mathbf{F}^n$$

$$(2)\quad \mathbf{F}^{n+1} = \left(\Omega_{n+1}^{-1} + \Delta t \mathbf{Id}\right)^{-1}\left\{\Omega_{n+1}^{-1}\left[\mathbf{F}^n - \frac{\Delta t}{\Delta x}\Lambda_x \delta_{x(1)}\mathbf{F}^n\right] + \Delta t\, \mathbb{M}_{n+1}\right\}$$

[9] R. Abgrall, D. Torlo, *SIAM Journal on Scientific Computing* **42**, B816–B845, ISSN: 10957197 (2020).

Arbitrary order kinetic scheme (1/3)

Arbitrary order scheme *(Abgrall & Torlo, 2020[10])*:

- Spatial approximation on Cartesian meshes: $\partial/\partial x \to \delta_x^{(q)}/\Delta x$ (spatial approximation of order q)

$$\frac{\mathrm{d}\mathbf{F}}{\mathrm{d}t} = -\Lambda_x \frac{\delta_x^{(q)}\mathbf{F}}{\Delta x} + \Omega(\mathbb{P}\mathbf{F})\left[\mathbb{M}(\mathbb{P}\mathbf{F}) - \mathbf{F}\right] := \mathcal{F}(\mathbf{F})$$

- In time: Try to use implicit Runge-Kutta of order q, with s sub-iterations: Butcher tableau $A \in \mathcal{M}_s(\mathbb{R})$:

$$\hat{\mathbf{F}} = \mathbf{F}^n + \Delta t\, \mathbf{A}\mathcal{F}(\hat{\mathbf{F}}), \qquad \hat{\mathbf{F}} = \begin{bmatrix} \mathbf{F}_1 \\ \vdots \\ \mathbf{F}_s \end{bmatrix} \qquad \text{et} \quad \mathbf{F}^{n+1} = \mathbf{F}_s.$$

Example : Order 2, Lobato IIIC: $\mathbf{A} = \begin{pmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{pmatrix}$

Problem: implicit scheme difficult to solve. . .

[10] R. Abgrall, D. Torlo, *SIAM Journal on Scientific Computing* **42**, B816–B845, ISSN: 10957197 (2020).

Arbitrary order kinetic scheme (2/3)

Idea: Deferred correction (DeC, CITE)

- We define a "high order" operator $\mathcal{L}^2$:

$$\mathcal{L}^2(\hat{\mathbf{F}}) = \hat{\mathbf{F}} - \mathbf{F}^n + \frac{\Delta t}{\Delta x} \mathbf{A} \, \Lambda_x \delta_x^{(q)} \hat{\mathbf{F}} - \Delta t \, \mathbf{A} \Omega(\mathbb{P}\hat{\mathbf{F}}) \left[\mathbb{M}(\mathbb{P}\hat{\mathbf{F}}) - \hat{\mathbf{F}} \right].$$

The scheme writes: $\mathcal{L}^2(\hat{\mathbf{F}}) = 0$.
Difficult problem

- We define a first order scheme 1, $\mathcal{L}^1$, easier to solve:

$$\mathcal{L}^1(\hat{\mathbf{F}}) = \hat{\mathbf{F}} - \mathbf{F}^n + \frac{\Delta t}{\Delta x} \mathbf{C} \, \Lambda_x \delta_x^{(q)} \hat{\mathbf{F}} - \Delta t \, \mathbf{A} \Omega(\mathbb{P}\hat{\mathbf{F}}) \left[\mathbb{M}(\mathbb{P}\hat{\mathbf{F}}) - \hat{\mathbf{F}} \right],$$

where **C** is a matrix associated to an explicit RK scheme. This can be solved explicitly as for the first order case above.

Arbitrary order kinetic scheme (3/3)

Principle of DeC:

1) Define : $\hat{\mathbf{F}}^{(0)} = \mathbf{F}_n$.
2) Iterative solution

$$\mathcal{L}^1(\hat{\mathbf{F}}^{(p+1)}) = \mathcal{L}^1(\hat{\mathbf{F}}^p) - \mathcal{L}^2(\hat{\mathbf{F}}^p).$$

3) After q iterations, $\hat{\mathbf{F}}^{(q)}$ approximates $\mathbf{F}(t_{n+1})$ with order q.

We get

$$(1) \quad \hat{\mathbf{u}}^{(p+1)} = \hat{\mathbf{u}}^n - \frac{\Delta t}{\Delta x}\mathbf{A}\mathbb{P}\Lambda_x\delta_x^{(q)}\hat{\mathbf{F}}^{(p)}, \qquad (\hat{\mathbf{u}}^{(p)} = \mathbb{P}\hat{\mathbf{F}}^p),$$

$$(2) \quad \hat{\mathbf{F}}^{(p+1)} = \Omega^{-1}\left[\Omega^{-1} + \mathbf{A}\Delta t\right]^{-1}\left(\mathbf{F}^n - \frac{\Delta t}{\Delta x}\mathbf{A}\Lambda_x\delta_x^{(q)}\hat{\mathbf{F}}^{(p)}\right) + \Delta t\,\mathbf{A}\left[\Omega^{-1} + \mathbf{A}\Delta t\right]^{-1}\mathbb{M}(\hat{\mathbf{u}}^{(p+1)})$$

1st, 2nd and 4th order scheme

1st order: upwind

$$\delta_x^{(1)}\mathbf{F} = \begin{cases} \mathbf{F}_k - \mathbf{F}_{k-1} & \text{si } a \geq 0, \\ \mathbf{F}_{k+1} - \mathbf{F}_k & \text{sinon,} \end{cases}$$

Linear stability: $a\dfrac{\Delta t}{\Delta x} < 1.$

2nd order

$$\delta_x^{(2)}\mathbf{F} = \begin{cases} \mathbf{F}_{k+1}/3 + \mathbf{F}_k/2 - \mathbf{F}_{k-1} + \mathbf{F}_{k-2}/6 & \text{if } a \geq 0, \\ -\mathbf{F}_{k-1}/3 - \mathbf{F}_k/2 + \mathbf{F}_{k+1} - \mathbf{F}_{k+2}/6 & \text{else.} \end{cases}$$

$$\mathbf{A} = \begin{pmatrix} 1/2 & -1/2 \\ 1/2 & 1/2 \end{pmatrix},$$

linear stability: $a\dfrac{\Delta t}{\Delta x} < 0.87.$

4th Order:

$$\delta_x^{(4)} = \begin{cases} \mathbf{F}_{k+1}/4 + 5\mathbf{F}_k/6 - 3\mathbf{F}_{k-1}/2 + \mathbf{F}_{k-2}/2 - \mathbf{F}_{k-3}/12 & \text{if } a \geq 0, \\ -\mathbf{F}_{k-1}/4 - 5\mathbf{F}_k/6 + 3\mathbf{F}_{k+1}/2 - \mathbf{F}_{k+2}/2 + \mathbf{F}_{k+3}/12 & \text{else,} \end{cases}$$

$$\mathbf{A} = \begin{pmatrix} 1/6 & -1/3 & 1/6 \\ 1/6 & 5/12 & -1/12 \\ 1/6 & 2/3 & 1/6 \end{pmatrix},$$

linear stability: $a\dfrac{\Delta t}{\Delta x} < 1.04.$