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AP schemes for intermediate models between a kinetic equation and its diffusive limit

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- Kinetic equation
- First-order closure
- Zeroth-order closure

4 Experiments

- AP properties of the schemes
- Comparisons
- Su-Olson tests

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Kinetic equations

Origin.

Kinetic equations arise in physics and engineering when a huge amount of particles is described statistically by a distribution function f(t, x, v). Some examples:

- semiconductor physics;
- gas dynamics;
- plasma physics;
- collective behaviour models.

Diffusive scaling.

The diffusive scaling is meant to represent a regime in which the mean free path travelled by the particles goes to zero.

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Setting the problem

Kinetic equation.

Take the 1D transport equation

$$arepsilon \partial_t f_arepsilon + v \partial_x f_arepsilon = rac{1}{arepsilon} \mathcal{Q}[f_arepsilon], \qquad \mathcal{Q}[f_arepsilon] = \langle f_arepsilon
angle - f_arepsilon$$

with $(t, x, v) \in [0, T] \times \mathbb{R} \times V$, completed by initial and boundary conditions. Particles are not driven by any force field and interact through a relaxation-type collision operator.

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Setting the	e problem		

The velocity space (V, μ)

V is a space endowed with a measure μ such that it satisfies:

- (i) $\langle 1 \rangle = 1;$
- (ii) $\langle h(v) \rangle = 0$ for any odd function *h*;

(iii)
$$\langle v^2 \rangle = d \in \mathbb{R}_{>0}.$$

In our notations $\langle f \rangle = \int_V f(v) d\mu(v)$.

Examples of (V, μ)

•
$$V = (-1, 1), \qquad d\mu(v) = \frac{1}{2}d\lambda(v);$$

• $V = (-1, 1), \quad \{v_i\}_{i=1}^N \subseteq (-1, 1)^N, \quad d\mu(v) = \frac{1}{N} \sum_{i=1}^N \delta(v = v_i) :$ the points $\{v_i\}_{i=1}^N$ have to be well chosen, otherwise properties (ii) and (iii) do not hold;

•
$$V = \mathbb{R}, \qquad d\mu(v) = \frac{1}{\sqrt{2\pi}}e^{-\frac{v^2}{2}}d\lambda(v)$$

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Heat equation			

Diffusive limit.

As $\varepsilon \to 0$, f_{ε} relaxes to F_0 solution to the **heat equation**:

$$\varepsilon \partial_t f_{\varepsilon} + v \partial_x f_{\varepsilon} = \frac{1}{\varepsilon} \mathcal{Q}[f_{\varepsilon}] \qquad \xrightarrow[\varepsilon \to 0]{} \partial_t F_0 - \left\langle v^2 \right\rangle \partial_{xx}^2 F_0 = 0.$$

Proof.

Formally take the Hilbert expansion in ε

$$f_{\varepsilon} = F_0 + \varepsilon F_1 + \varepsilon^2 F_2 + \dots$$

inject into the kinetic equation and extract the F_i .

Drawbacks.

- The heat equation is not *v*-dependent: no microscopic feature.
- The heat equation transports information at infinite velocity, the transport equation at O (¹/_ε) velocity.

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The P1-approximation

By truncating the Hilbert expansion at first order

$$f_{\varepsilon} \approx F_0 + \varepsilon F_1$$

we obtain the $\mathbb{P}1$ -approximation

$$f_{\varepsilon}(t, x, v) \approx F_0(t, x) - \varepsilon v \partial_x F_0(t, x)$$

which is v-dependent, so that it somehow restores some microscopic features.

Drawbacks

- The P1-approximation might be negative.
- As well as in heat equation, information is transported at infinite velocity.

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Moments

Define the zeroth, first and second order moments by

$$\left(\begin{array}{c}\rho\\J\\\mathbb{P}\end{array}\right) = \left\langle \left(\begin{array}{c}1\\v/\varepsilon\\v^2\end{array}\right)f_{\varepsilon}\right\rangle.$$

Moment equations

Integrating the kinetic equation, we obtain the moment equations

$$\partial_t \rho + \partial_x J = 0$$

$$\varepsilon^2 \partial_t J + \partial_x \mathbb{P} = -J,$$

which need some **closure strategy**, the k^{th} -moment equation being dependent on the $(k + 1)^{th}$ -moment.

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Zeroth-order closure

Two closures are proposed, one at zeroth order and one at first order.

Zeroth order closure

By truncating the modified Hilbert expansion $f_{\varepsilon} = e^{a_0 + \varepsilon a_1 + \varepsilon^2 a_2 + \dots}$ at first order

 $f_{\varepsilon} \approx \exp\left(a_0 + \varepsilon a_1\right)$

and injecting the approximation thus obtained

$$f_{\varepsilon}(t, x, v) \approx \frac{\rho(t, x)}{Z(t, x)} e^{-\varepsilon v \frac{\partial_{x} \rho}{\rho}(t, x)}$$

into the zeroth moment equation, we obtain the following system:

$$\partial_t \rho - \partial_x \left[\frac{\rho}{\varepsilon} \mathbb{G} \left(\varepsilon \frac{\partial_x \rho}{\rho} \right) \right] = 0.$$

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Some notations

We have introduced:

• Z(t,x) is a normalizing factor such that $\langle f_{\varepsilon} \rangle = \rho(t,x)$;

•
$$\mathbb{F}(x) = \langle e^{xv} \rangle;$$

•
$$\mathbb{G}(x) = \frac{\mathbb{F}'}{\mathbb{F}}(x).$$

Examples

If V = (-1, 1) and $d\mu = \frac{1}{2}d\lambda$ (normalized Lebesgue measure), then

$$\mathbb{G}(x) = \coth(x) - \frac{1}{x}.$$

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Entropy Minimization Principle

The first-order closure comes from the following Entropy Minimization Principle:

 $f_{\varepsilon} = \operatorname{argmin}\left\{\left\langle f_{\varepsilon} \log(f_{\varepsilon})\right\rangle\right\}$

under the constraints

$$\left\langle \left(\begin{array}{c} 1\\ \nu/\varepsilon \end{array}\right) f_{\varepsilon} \right\rangle = \left(\begin{array}{c} \rho\\ J \end{array}\right).$$

The closed system

We can thus express the second moment as

$$\mathbb{P} = \rho \psi \left(\frac{\varepsilon J}{\rho} \right), \qquad \psi(x) = \frac{\mathbb{F}''}{\mathbb{F}} \left(\mathbb{G}^{(-1)}(x) \right),$$

so that the first-order closure reads

$$\partial_t \rho + \partial_x J = 0, \qquad \varepsilon^2 \partial_t J + \partial_x \left[\rho \psi \left(\frac{\varepsilon J}{\rho} \right) \right] = -J.$$

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Reconstruction

The microscopic approximation is reconstructed by

$$\tilde{f}_{\varepsilon}(t,x,v) = \rho(t,x) \frac{\exp\left[\nu \mathbb{G}^{(-1)}\left(\frac{\varepsilon J}{\rho(t,x)}\right)\right]}{\mathbb{F} \circ \mathbb{G}^{(-1)}\left(\frac{\varepsilon J}{\rho(t,x)}\right)}.$$

Notations

We are using the following notations:

$$\mathbb{F}(x) = \langle e^{xv} \rangle, \qquad \mathbb{G}(x) = \frac{\mathbb{F}'}{\mathbb{F}}(x), \qquad \psi(x) = \frac{\mathbb{F}''}{\mathbb{F}}\left(\mathbb{G}^{(-1)}(x)\right).$$

Example

In case V = (-1, 1) and $d\mu = \frac{1}{2}d\lambda$ (normalized Lebesgue measure), we have

$$\mathbb{F}(x) = \frac{\sinh(x)}{x}, \qquad \mathbb{G}(x) = \coth(x) - \frac{1}{x}.$$

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Reconstruction

The microscopic approximation is reconstructed by

$$\tilde{f}_{\varepsilon}(t,x,v) = \rho(t,x) \frac{\exp\left[v\mathbb{G}^{(-1)}\left(\frac{\varepsilon J}{\rho(t,x)}\right)\right]}{\mathbb{F} \circ \mathbb{G}^{(-1)}\left(\frac{\varepsilon J}{\rho(t,x)}\right)}.$$

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Kinetic equation

We propose a splitting scheme for solving the kinetic equation

$$\varepsilon \partial_{t} f_{\varepsilon} + v \partial_{x} f_{\varepsilon} = \frac{1}{\varepsilon} \left(\langle f_{\varepsilon} \rangle - f_{\varepsilon} \right)$$

without need of mesh-resolving parameter ε as it tends to zero.

Decomposition

Split f_{ε} into its mean value plus fluctuations:

$$f_{\varepsilon} = \rho_{\varepsilon} + \varepsilon g_{\varepsilon} = \langle f_{\varepsilon} \rangle + \varepsilon g_{\varepsilon}.$$

Boundedness of the fluctuations

We have from the boundendess in the $L^p(V, \mu)$ -spaces of the collision operator

$$\begin{aligned} \|g_{\varepsilon}\|_{L^{2}_{t,x,v}}^{2} &= \int_{\mathbb{R}\geq 0} \int_{\mathbb{R}} \int_{V} |f_{\varepsilon} - \rho_{\varepsilon}|^{2} dt dx dv \\ &= \int_{\mathbb{R}\geq 0} \int_{\mathbb{R}} \int_{V} |\mathcal{Q}[f_{\varepsilon}]|^{2} dt dx dv \\ &\leq C \int_{\mathbb{R}\geq 0} \int_{\mathbb{R}} \int_{V} |f_{\varepsilon}|^{2} dt dx dv. \end{aligned}$$

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Kinetic equation			

Reformulation

Kinetic equation

Inject the decomposition $f_{\varepsilon} = \rho_{\varepsilon} + \varepsilon g_{\varepsilon}$ into the kinetic equation to obtain

$$\partial_t f_{\varepsilon} + rac{v}{\varepsilon} \partial_x \rho_{\varepsilon} + v \partial_x g_{\varepsilon} = rac{1}{\varepsilon^2} \left(\rho_{\varepsilon} - f_{\varepsilon} \right).$$

First-order splitting strategy

- (i) solve for a Δt -step the equation $\partial_t f_{\varepsilon} = \frac{1}{\varepsilon^2} \left(\rho_{\varepsilon} f_{\varepsilon} \right) \frac{v}{\varepsilon} \partial_x \rho_{\varepsilon}$
- (ii) solve for a Δt -step the equation $\partial_t f_{\varepsilon} + v \partial_x g_{\varepsilon} = 0$.

Evolution of the fluctuations

To complete the scheme, we still need to write the evolution equation for the fluctuations g_{ε} :

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(i)
$$\langle v \rangle = 0 \Longrightarrow \partial_t \rho_{\varepsilon} = 0 \Longrightarrow \partial_t g_{\varepsilon} = -\frac{1}{\varepsilon^2} g_{\varepsilon} - \frac{v}{\varepsilon^2} \partial_x \rho_{\varepsilon};$$

(ii) for **Step** (ii) we use
$$\partial_t g_{\varepsilon} = 0$$
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- (i) solve for a Δt -step the equation $\partial_t f_{\varepsilon} = \frac{1}{\varepsilon^2} \left(\rho_{\varepsilon} f_{\varepsilon} \right) \frac{\nu}{\varepsilon} \partial_x \rho_{\varepsilon}$;
- (ii) solve for a Δt -step the equation $\partial_t f_{\varepsilon} + v \partial_x g_{\varepsilon} = 0$.

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(i)
$$\langle v \rangle = 0 \Longrightarrow \partial_t \rho_{\varepsilon} = 0 \Longrightarrow \partial_t g_{\varepsilon} = -\frac{1}{\varepsilon^2} g_{\varepsilon} - \frac{v}{\varepsilon^2} \partial_x \rho_{\varepsilon};$$

(ii) for Step (ii) we use
$$\partial_t g_{\varepsilon} = 0$$
.

	Approximations	Asymptotic-preserving schemes	Experiments
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Kinetic equation			
Kinetic eq	uation		

Reformulation

Inject the decomposition $f_{\varepsilon} = \rho_{\varepsilon} + \varepsilon g_{\varepsilon}$ into the kinetic equation to obtain

$$\partial_t f_{\varepsilon} + rac{v}{\varepsilon} \partial_x \rho_{\varepsilon} + v \partial_x g_{\varepsilon} = rac{1}{\varepsilon^2} \left(\rho_{\varepsilon} - f_{\varepsilon} \right).$$

First-order splitting strategy

- (i) solve for a Δt -step the equation $\partial_t f_{\varepsilon} = \frac{1}{\varepsilon^2} \left(\rho_{\varepsilon} f_{\varepsilon} \right) \frac{v}{\varepsilon} \partial_x \rho_{\varepsilon};$
- (ii) solve for a Δt -step the equation $\partial_t f_{\varepsilon} + v \partial_x g_{\varepsilon} = 0$.

Evolution of the fluctuations

To complete the scheme, we still need to write the evolution equation for the fluctuations g_{ε} :

(i)
$$\langle v \rangle = 0 \Longrightarrow \partial_t \rho_{\varepsilon} = 0 \Longrightarrow \partial_t g_{\varepsilon} = -\frac{1}{\varepsilon^2} g_{\varepsilon} - \frac{v}{\varepsilon^2} \partial_x \rho_{\varepsilon};$$

(ii) for Step (ii) we use
$$\partial_t g_{\varepsilon} = 0$$
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Kinetic eq	uation		

Résumé

If we take into account only the leading contribution in ε ,

(i)
$$\partial_t f_{\varepsilon} = -\frac{1}{\varepsilon^2} (f_{\varepsilon} - \rho_{\varepsilon}), \qquad \partial_t g_{\varepsilon} = -\frac{1}{\varepsilon^2} (g_{\varepsilon} + v \partial_x \rho_{\varepsilon}), \qquad \partial_t \rho_{\varepsilon} = 0;$$

(ii) $\partial_t f_{\varepsilon} + v \partial_x g_{\varepsilon} = 0, \qquad \partial_t g_{\varepsilon} = 0.$

Time discretization of the scheme

Dropping ε -subscript for convenience,

Step (i)a relax
$$f$$
: $f^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} f^n + \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) \rho^n$;

Step (i)b relax $g: g^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} g^n - \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) v \partial_x \rho^n;$

Step (i) $\rho^{n+1/2} = \rho^n$; Step (ii) α convect $f: f^{n+1} = f^{n+1/2} - \Delta t \cdot v \partial_x g^{n+1/2}$; Step (iii) α update $\rho: \rho^{n+1} = \langle f^{n+1} \rangle$; Step (ii) α let $g^{n+1} = g^{n+1/2}$; we might use $g^{n+1} = \frac{f^{n+1} - \rho^{n+1}}{\epsilon}$ instead (to be discussed).

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Résumé

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$$\partial_t f_{\varepsilon} = -\frac{1}{\varepsilon^2} (f_{\varepsilon} - \rho_{\varepsilon}), \qquad \partial_t g_{\varepsilon} = -\frac{1}{\varepsilon^2} (g_{\varepsilon} + v \partial_x \rho_{\varepsilon}), \qquad \partial_t \rho_{\varepsilon} = 0;$$

(ii) $\partial_t f_{\varepsilon} + v \partial_x g_{\varepsilon} = 0, \qquad \partial_t g_{\varepsilon} = 0.$

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Dropping ε -subscript for convenience,

Step (i)a relax
$$f: f^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} f^n + \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) \rho^n$$
;
Step (i)b relax $g: g^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} g^n - \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) v \partial_x \rho^n$;
Step (i)c $\rho^{n+1/2} = \rho^n$;
Step (ii)a convect $f: f^{n+1} = f^{n+1/2} - \Delta t \cdot v \partial_x g^{n+1/2}$;
Step (ii)b update $\rho: \rho^{n+1} = \langle f^{n+1} \rangle$;
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Kinetic equation

AP property

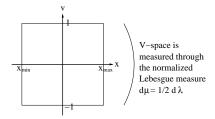
The relaxed scheme $\varepsilon \rightarrow 0$ reads:

- $\partial_t f v^2 \partial_{xx}^2 \rho = 0$, which implies that $\partial_t \rho \langle v^2 \rangle \partial_{xx}^2 \rho = 0$. This is the heat equation with the proper constant;
- $g^{n+1/2} = -v\partial_x \rho^{n+1/2}$, which is coherent with the Hilbert expansion.

The scheme, therefore, relaxes to a solver to the proper heat equation.

The case of normalized Lebesgue measure

Let us use in the following the Lebesgue setting:



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Kinetic equation

AP property

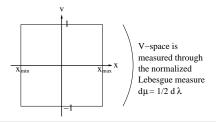
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The case of normalized Lebesgue measure

Let us use in the following the Lebesgue setting:



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Time-space discretized scheme

Step (i)a $f_{i,j}^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} f_{i,j}^n + \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) \rho_i^n;$ Step (i)b $g_{i,j}^{n+1/2} = e^{-\frac{\Delta t}{\varepsilon^2}} g_{i,j}^n + \left(1 - e^{-\frac{\Delta t}{\varepsilon^2}}\right) \overline{\mathbb{D}}_j \rho_i^n;$ Step (i)c $\rho_i^{n+1/2} = \rho_i^n;$ Step (ii)a $f_{i,j}^{n+1} = f_{i,j}^{n+1/2} + \Delta t \overline{\mathbb{D}}_j g_{i,j}^{n+1/2};$ Step (ii)b $g_{i,j}^{n+1} = g_{i,j}^{n+1/2};$ Step (ii)c by a right-rectangluar rule: $\rho_i^{n+1} = \frac{\Delta v}{2} \sum_{i=0}^{j-2} f_{i,i}^{n+1}.$

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The space-derivatives $\mathbb D$ and $\bar{\mathbb D}$

In the fully-relaxed scheme, we obtain $\rho_i^{n+1} = \rho_i^n + \Delta t \mathbb{D}_j \overline{\mathbb{D}}_j \rho_i^n$. In order to recover the classical three-point centered scheme for the heat equation, needed for the scheme to be stable, \mathbb{D} and $\overline{\mathbb{D}}$ must be taken in aternate direction. We define, therefore:

$$\begin{split} \left[\mathbb{D}_{j}\varphi\right]_{i} &= \frac{1}{\Delta x} \begin{cases} -\nu_{j}\left(\varphi_{i}-\varphi_{i-1}\right) & \text{if } \nu_{j} \in V_{+} \\ -\nu_{j}\left(\varphi_{i+1}-\varphi_{i}\right) & \text{if } \nu_{j} \in V_{-} \end{cases} \\ \left[\bar{\mathbb{D}}_{j}\varphi\right]_{i} &= \frac{1}{\Delta x} \begin{cases} -\nu_{j}\left(\varphi_{i+1}-\varphi_{i}\right) & \text{if } \in V_{+} \\ -\nu_{j}\left(\varphi_{i}-\varphi_{i-1}\right) & \text{if } \nu_{j} \in V_{-} \end{cases} \end{split}$$

where we have also introduced $V_{\pm} = \{j \in \{0, \dots, N_{\nu} - 1\}$ such that $\nu_j \in \mathbb{R}_{\pm}\}$.

Boundary conditions

Boundary conditions should enforce mass conservation during the advection step:

$$\sum_{i=1}^{N_{x}-2} \sum_{j} \mathbb{D}_{j} g_{i,j}^{n+1/2} = 0 \iff \begin{cases} g_{0,k}^{n+1/2} = \frac{-1}{v_{k} \#[V_{+}]} \sum_{v_{j} \in V_{-}} v_{j} g_{1,j}^{n+1/2} & \text{for } k \in V_{+} \\ g_{N_{x}-1,k}^{n+1/2} = \frac{-1}{v_{k} \#[V_{-}]} \sum_{v_{j} \in V_{+}} v_{j} g_{N_{x}-2,j}^{n+1/2} & \text{for } k \in V_{-}. \end{cases}$$

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Outline

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- Motivation
- Setting

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- Heat equation and \mathbb{P}^1 -approximation
- Intermediate models

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Zeroth-order closure

4 Experiments

- AP properties of the schemes
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- Su-Olson tests

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Numerics for the first-order closure

We recall the first-order closure (dropping ε -dependency):

$$\partial_t \rho + \partial_x J = 0$$

 $\varepsilon^2 \partial_t J + \partial_x \left[\rho \psi \left(\frac{\varepsilon J}{\rho} \right) \right] = -J$

Strategy

We introduce a new unknown z(t, x) and two new parameters λ and α ; the non-linear equation for the first moment is now an advection equation and the non-linearities only appear at a right hand side:

$$\begin{pmatrix} \partial_t t & \partial_x & 0\\ 0 & \varepsilon^2 \partial_t & \partial_x\\ 0 & \varepsilon^2 \lambda^2 \partial_x & \partial_t \end{pmatrix} \begin{pmatrix} \rho\\ J\\ z \end{pmatrix} = \begin{pmatrix} 0\\ -J\\ \frac{1}{\alpha} \left(\rho \psi(u) - z\right) \end{pmatrix},$$

with $u = \frac{\varepsilon J}{\rho}$. As $\alpha \to 0$, this system relaxes towards the original system.

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First-order closure

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First-order closure

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Numerics for the first-order closure

Diagonalization

We diagonalize it by means of a linear transformation of its unknowns ($\mu = \varepsilon \lambda$)

$$\begin{pmatrix} \rho \\ J \\ z \end{pmatrix} = \begin{pmatrix} \frac{1}{\mu^2} & \frac{1}{\mu^2} & \frac{1}{\mu^2} \\ 0 & \frac{1}{\varepsilon\mu} & -\frac{1}{\varepsilon\mu} \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} f_0 \\ f_+ \\ f_- \end{pmatrix},$$

Splitting

then apply splitting technique between the α -relaxations and the ε -relaxations:

$$\begin{pmatrix} \partial_t & 0 & 0\\ 0 & \partial_t + \frac{\mu}{\varepsilon} \partial_x & 0\\ 0 & 0 & \partial_t - \frac{\mu}{\varepsilon} \partial_x \end{pmatrix} \begin{pmatrix} f_0\\ f_+\\ f_- \end{pmatrix} = \begin{pmatrix} -\frac{1}{\alpha} \left(\rho\psi(u) - z\right)\\ -\frac{f_+}{\varepsilon^2} + \frac{z}{2\varepsilon^2} + \frac{1}{2\alpha} \left(\rho\psi(u) - z\right)\\ -\frac{f_-}{\varepsilon^2} + \frac{z}{2\varepsilon^2} + \frac{1}{2\alpha} \left(\rho\psi(u) - z\right) \end{pmatrix}$$

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Numerics for the first-order closure

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Numerics for the first-order closure

Stiffness in Step 1.

Step 1 is again stiff as $\varepsilon \to 0$:

$$\partial_t f_{\pm} \pm \frac{\mu}{\varepsilon} \partial_x f_{\pm} = -\frac{1}{\varepsilon^2} \left[f_{\pm} - \frac{z}{2} \right],$$

which means that f_{\pm} is relaxed towards $\frac{z}{2}$, so we apply the same strategy as before and split f_{\pm} into the following sum:

$$f_{\pm} = \frac{z}{2} + \varepsilon g_{\pm}$$

and follow the same calculations as before.

Asymptotic-preserving schemes

Numerics for the first-order closure

Solving Step 1.

Developping all the computations and rewriting the system in the original variables we get:

$$\begin{split} \boldsymbol{z}^{n+1/2} &= \boldsymbol{z}^n + \frac{\varepsilon(1-e^{-\Delta t/\varepsilon^2})}{2} \left(\bar{\mathbb{D}}_+(\boldsymbol{z}^n) + \bar{\mathbb{D}}_-(\boldsymbol{z}^n) \right) + \Delta t \left[\mathbb{D}_+ \left(e^{-\Delta t/\varepsilon^2} \frac{\mu J^n}{2} \right. \\ &+ (1-e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_+(\boldsymbol{z}^n)}{2} \right) + \mathbb{D}_- \left(e^{-\Delta t/\varepsilon^2} \frac{(-\mu J^n)}{2} + (1-e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_-(\boldsymbol{z}^n)}{2} \right) \right] \\ \boldsymbol{J}^{n+1/2} &= e^{-\Delta t/\varepsilon^2} \boldsymbol{J}^n + \frac{1-e^{-\Delta t/\varepsilon^2}}{2\mu} \left(\bar{\mathbb{D}}_+(\boldsymbol{z}^n) - \bar{\mathbb{D}}_-(\boldsymbol{z}^n) \right) + \frac{\Delta t}{\varepsilon\mu} \left[\mathbb{D}_+ \left(e^{-\Delta t/\varepsilon^2} \frac{\mu J^n}{2} \right) \right] \\ &+ (1-e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_+(\boldsymbol{z}^n)}{2} \right) - \mathbb{D}_- \left(e^{-\Delta t/\varepsilon^2} \frac{(-\mu J^n)}{2} + (1-e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_-(\boldsymbol{z}^n)}{2} \right) \right] \\ &\rho^{n+1/2} &= \rho^n + \frac{\Delta t}{\mu^2} \left(\mathbb{D}_+ \left(e^{-\Delta t/\varepsilon^2} \frac{\mu J^n}{2} + (1-e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_+(\boldsymbol{z}^n)}{2} \right) \\ &+ \mathbb{D}_- \left(e^{-\Delta t/\varepsilon^2} \frac{(-\mu J^n)}{2} + (1-e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_-(\boldsymbol{z}^n)}{2} \right) \right). \end{split}$$

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Numerics for the first-order closure

Solving Step 2.

Step 2 just involves relaxations, and no more details are given; after reconstructing the original variables we obtain

$$\begin{aligned} z^{n+1} &= e^{-\Delta t/\alpha} z^{n+1/2} + (1 - e^{-\Delta t/\alpha}) \rho^{n+1/2} \psi^{n+1/2} \\ J^{n+1} &= J^{n+1/2} \\ \rho^{n+1} &= \rho^{n+1/2}. \end{aligned}$$

Asymptotic-preserving schemes

Numerics for the first-order closure

Derivatives

Discretized derivatives are subjected to upwinding and are taken in alternate directions, in order to rescue the classical three-points centered scheme for the Laplacian of the heat equation in the ($\alpha \rightarrow 0, \varepsilon \rightarrow 0$)-scheme:

$$\begin{split} \left(\bar{\mathbb{D}}_{+}(\varphi) \right)_{i} &= -\frac{\mu}{\Delta x} \left(\varphi_{i+1} - \varphi_{i} \right) \\ \left(\mathbb{D}_{+}(\varphi) \right)_{i} &= -\frac{\mu}{\Delta x} \left(\varphi_{i} - \varphi_{i-1} \right) \\ \left(\bar{\mathbb{D}}_{-}(\varphi) \right)_{i} &= \frac{\mu}{\Delta x} \left(\varphi_{i} - \varphi_{i-1} \right) \\ \left(\mathbb{D}_{-}(\varphi) \right)_{i} &= -\frac{\mu}{\Delta x} \left(\varphi_{i+1} - \varphi_{i} \right). \end{split}$$

Boundary conditions

Homogeneous Neumann conditions are used to enforce mass conservation:

$$\rho_0^n = \rho_1^n, \ \rho_{N_x-1}^n = \rho_{N_x-2}^n, \ z_0^n = z_1^n, \ z_{N_x-1}^n = z_{N_x-2}^n, \ J_0^n = -J_1^n, \ J_{N_x-1}^n = -J_{N_x-2}^n.$$

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Asymptotic-preserving schemes

Numerics for the first-order closure

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Approximations

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First-order closure

Numerics for the first-order closure

AP properties: the limit $\alpha \rightarrow 0$

$$\begin{split} J^{n+1} &= e^{-\Delta t/\varepsilon^2} J^n + \frac{1 - e^{-\Delta t/\varepsilon^2}}{2\mu} \left(\bar{\mathbb{D}}_+(\rho^n \psi^n) - \bar{\mathbb{D}}_-(\rho^n \psi^n) \right) \\ &+ \frac{\Delta t}{\varepsilon\mu} \left[\mathbb{D}_+ \left(e^{-\Delta t/\varepsilon^2} \frac{\mu J^n}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_+(\rho^n \psi^n)}{2} \right) \right. \\ &- \mathbb{D}_- \left(e^{-\Delta t/\varepsilon^2} \frac{(-\mu J^n)}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_-(\rho^n \psi^n)}{2} \right) \right], \\ \rho^{n+1} &= \rho^n + \frac{\Delta t}{\mu^2} \left(\mathbb{D}_+ \left(e^{-\Delta t/\varepsilon^2} \frac{\mu J^n}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_+(\rho^n \psi^n)}{2} \right) \right. \\ &+ \mathbb{D}_- \left(e^{-\Delta t/\varepsilon^2} \frac{(-\mu J^n)}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_-(\rho^n \psi^n)}{2} \right) \right). \end{split}$$

AP properties: the limit $\varepsilon \to 0$

$$\rho^{n+1} = \rho^n + \psi(0) \frac{\Delta t}{(\Delta x)^2} (\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n).$$

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Approximations

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First-order closure

Numerics for the first-order closure

AP properties: the limit $\alpha \rightarrow 0$

$$\begin{split} J^{n+1} &= e^{-\Delta t/\varepsilon^2} J^n + \frac{1 - e^{-\Delta t/\varepsilon^2}}{2\mu} \left(\bar{\mathbb{D}}_+(\rho^n \psi^n) - \bar{\mathbb{D}}_-(\rho^n \psi^n) \right) \\ &+ \frac{\Delta t}{\varepsilon\mu} \left[\mathbb{D}_+ \left(e^{-\Delta t/\varepsilon^2} \frac{\mu J^n}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_+(\rho^n \psi^n)}{2} \right) \right. \\ &- \mathbb{D}_- \left(e^{-\Delta t/\varepsilon^2} \frac{(-\mu J^n)}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_-(\rho^n \psi^n)}{2} \right) \right], \\ \rho^{n+1} &= \rho^n + \frac{\Delta t}{\mu^2} \left(\mathbb{D}_+ \left(e^{-\Delta t/\varepsilon^2} \frac{\mu J^n}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_+(\rho^n \psi^n)}{2} \right) \right. \\ &+ \mathbb{D}_- \left(e^{-\Delta t/\varepsilon^2} \frac{(-\mu J^n)}{2} + (1 - e^{-\Delta t/\varepsilon^2}) \frac{\bar{\mathbb{D}}_-(\rho^n \psi^n)}{2} \right) \right). \end{split}$$

AP properties: the limit $\varepsilon \to 0$

$$\rho^{n+1} = \rho^n + \psi(0) \frac{\Delta t}{(\Delta x)^2} (\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n).$$

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Zeroth-order closure Outline

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- Intermediate models

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Zeroth-order closure

Numerics for the zeroth-order closure

We recall the the zeroth-order closure reads

$$\partial_t \rho - \partial_x \left[\frac{\rho}{\varepsilon} \mathbb{G} \left(\varepsilon \frac{\partial_x \rho}{\rho} \right) \right] = 0.$$

Strategy

The zeroth-order closure is seen as the limit $\alpha \rightarrow 0$ of the following system:

$$\begin{pmatrix} \partial_t & \partial_x \\ \frac{\mu^2}{\varepsilon^2} \partial_x & \partial_t \end{pmatrix} \begin{pmatrix} \rho \\ J \end{pmatrix} = \begin{pmatrix} 0 \\ -\frac{1}{\alpha} \left[J + \frac{\rho}{\varepsilon} \mathbb{G} \left(\varepsilon \frac{\partial_x \rho}{\rho} \right) \right] \end{pmatrix}$$

Diagonalization

We diagonalize the system by changing variables $f_{\pm} = \frac{\rho}{2} \pm \frac{\varepsilon J}{2\mu}$ thus obtaining the system

$$\partial_t f_{\pm} \pm \frac{\mu}{\varepsilon} \partial_x f_{\pm} = \frac{1}{\alpha} \left[\frac{\rho}{2} - f_{\pm} \mp \frac{\rho}{2\mu} \mathbb{G} \left(\varepsilon \frac{\partial_x \rho}{\rho} \right) \right].$$

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Zeroth-order closure

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The zeroth-order closure is seen as the limit $\alpha \rightarrow 0$ of the following system:

$$\left(\begin{array}{cc}\partial_t & \partial_x\\ \frac{\mu^2}{\varepsilon^2}\partial_x & \partial_t\end{array}\right)\left(\begin{array}{c}\rho\\ J\end{array}\right) = \left(\begin{array}{c}0\\ -\frac{1}{\alpha}\left[J + \frac{\rho}{\varepsilon}\mathbb{G}\left(\varepsilon\frac{\partial_x\rho}{\rho}\right)\right]\end{array}\right).$$

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We diagonalize the system by changing variables $f_{\pm} = \frac{\rho}{2} \pm \frac{\varepsilon J}{2\mu}$ thus obtaining the system

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Zeroth-order closure

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We diagonalize the system by changing variables $f_{\pm} = \frac{\rho}{2} \pm \frac{\varepsilon J}{2\mu}$ thus obtaining the system

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Decomposition

We follow the same decomposition strategy of splitting into average and fluctuations:

$$g_{\pm} = \frac{1}{\varepsilon} f_{\pm} - \frac{1}{2\varepsilon} \rho.$$

First-order splitting strategy

We solve the resulting system

$$\partial f_{\pm} \pm \mu \partial_x g_{\pm} = \frac{1}{\alpha} \left[\frac{\rho}{2} - f_{\pm} \mp \frac{\rho}{2\mu} \mathbb{G} \left(\varepsilon \frac{\partial_x \rho}{\rho} \right) \right] \mp \frac{\mu}{2\varepsilon} \partial_x \rho$$
 by splitting it into:

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Step (i) solve for a Δt -time step

$$\partial f_{\pm} = rac{1}{lpha} \left[rac{
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ho}{2\mu} \mathbb{G} \left(arepsilon rac{\partial_x
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ight)
ight] \mp rac{\mu}{2arepsilon} \partial_x
ho;$$

Step (ii) solve for a Δt -time step

$$\partial_t f_{\pm} \pm \frac{\mu}{\varepsilon} \partial_x f_{\pm} = 0, \qquad \partial_t g_{\pm} = 0.$$

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Numerics for the zeroth-order closure

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$$\partial_t f_{\pm} \pm \frac{\mu}{\varepsilon} \partial_x f_{\pm} = 0, \qquad \partial_t g_{\pm} = 0.$$

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Numerics for the zeroth-order closure

Discretized system

Step (i)a

$$f_{\pm}^{n+1/2} = e^{-\Delta t/\alpha} f_{\pm}^{n} + \frac{\rho^{n}}{2} (1 - e^{-\Delta t/\alpha}) \left[1 \mp \frac{1}{\mu} \mathbb{G} \left(\mp \frac{\varepsilon}{\mu} \frac{\bar{\mathbb{D}}_{\pm} \rho^{n}}{\rho^{n}} \right) \right] \\ + \alpha (1 - e^{-\Delta t/\alpha}) \frac{1}{2\varepsilon} \bar{\mathbb{D}}_{\pm} \rho^{n};$$

Step (i)b

$$g_{\pm}^{n+1/2} = \frac{1}{\varepsilon} f_{\pm}^{n+1/2} - \frac{1}{2\varepsilon} \rho^{n+1/2};$$

Step (ii)a

$$f_{\pm}^{n+1} = f_{\pm}^{n+1/2} + \Delta t \mathbb{D}_{\pm} g_{\pm}^{n+1/2};$$

Step (ii)b

$$g_{\pm}^{n+1} = g_{\pm}^{n+1/2}.$$

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Numerics for the zeroth-order closure

AP properties: the relaxed scheme $\alpha \rightarrow 0$

Step (i)a results into

$$f_{\pm}^{n+1/2} = \frac{\rho^n}{2} \left[1 + \frac{1}{\mu} \mathbb{G} \left(\frac{\varepsilon}{\mu} \frac{\bar{\mathbb{D}}_{\pm} \rho^n}{\rho^n} \right) \right],$$

while Step (i)a into

$$g_{\pm}^{n+1/2} = \frac{\rho^n}{2\mu\varepsilon} \mathbb{G}\left(\frac{\varepsilon}{\mu}\frac{\bar{\mathbb{D}}_{\pm}\rho^n}{\rho^n}\right)$$

Therefore, in terms of the mean value ρ , we have

$$\rho^{n+1} = \rho^n + \Delta t \left\{ \mathbb{D}_+ \left[\frac{\rho^n}{2\varepsilon\mu} \mathbb{G}\left(\frac{\varepsilon}{\mu} \frac{\bar{\mathbb{D}}_+ \rho^n}{\rho^n} \right) \right] + \mathbb{D}_- \left[\frac{\rho^n}{2\varepsilon\mu} \mathbb{G}\left(\frac{\varepsilon}{\mu} \frac{\bar{\mathbb{D}}_- \rho^n}{\rho^n} \right) \right] \right\}.$$

AP properties: $\varepsilon \rightarrow 0$

As $\varepsilon \to 0$, the system relaxes to a scheme for the heat equation, as long as the derivatives \mathbb{D}_{\pm} and $\overline{\mathbb{D}}_{\pm}$ are taken in alternate directions to recover the classical centered three-point scheme.

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AP properties: the relaxed scheme $\alpha \rightarrow 0$

Step (i)a results into

$$f_{\pm}^{n+1/2} = \frac{\rho^n}{2} \left[1 + \frac{1}{\mu} \mathbb{G} \left(\frac{\varepsilon}{\mu} \frac{\bar{\mathbb{D}}_{\pm} \rho^n}{\rho^n} \right) \right],$$

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AP properties of the schemes

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Relaxation to the heat equation $\varepsilon \to 0$

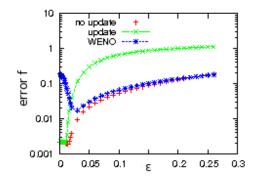


Figure: $L_{t,x,v}^2$ -error of the distribution function f with respect to the solution of the heat equation with a symmetric initial datum, for a mesh of 100x100, with respect to ε .

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Relaxation $\alpha \rightarrow 0$ for a fixed ε

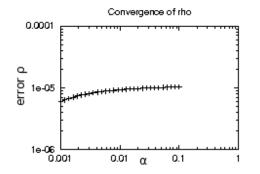


Figure: $L_{t,x}^2$ -error of the densities ρ for the $\alpha > 0$ method with respect to the completely relaxed scheme $\alpha = 0$ for $\varepsilon = 0.01$.

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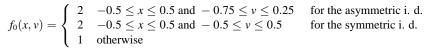
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Comparison between closures

We plot here the $L^2_{t,x,v}$ -difference between the $f_{\varepsilon}(t, x, v)$ given by the kinetic scheme and the $\tilde{f}_{\varepsilon}(t, x, v)$ reconstructed from heat equation or closure schemes. As initial datum we choose a symmetric f_0 and an asymmetric f_0 :



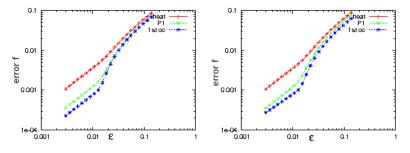


Figure: Left: symmetric initial datum. Right: asymmetric initial datum.

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The system

$$\begin{cases} \partial_t f_{\varepsilon} + \frac{v}{\varepsilon} \partial_x f_{\varepsilon} = \frac{1}{\varepsilon^2} \left(\langle f_{\varepsilon} \rangle - f_{\varepsilon} \right) + \sigma_a (\Theta - \rho) + S \\ \partial_t \Theta = \sigma_a (\rho - \Theta) \\ S = S(t, x) = \text{a given source.} \end{cases}$$

Strategy

We shall write numerical schemes for three levels, exactly as for the case of the benchmark kinetic equation:

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- kinetic level;
- first-order closure;
- zeroth-order closure.

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The system

$$\begin{cases} \partial_t f_{\varepsilon} + \frac{v}{\varepsilon} \partial_x f_{\varepsilon} = \frac{1}{\varepsilon^2} \left(\langle f_{\varepsilon} \rangle - f_{\varepsilon} \right) + \sigma_a(\Theta - \rho) + S \\ \partial_t \Theta = \sigma_a(\rho - \Theta) \\ S = S(t, x) = \text{a given source.} \end{cases}$$

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- kinetic level;
- first-order closure;
- zeroth-order closure.

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Kinetic level

The distribution function is split into average and fluctuations $f_{\varepsilon} = \rho_{\varepsilon} + \varepsilon g_{\varepsilon}$, then a first-order splitting procedure is adopted:

Step (i) Solve for Δt

$$\begin{cases} g^{n+1/2} = e^{-\Delta t/\varepsilon^2} g^n - (1 - e^{-\Delta t/\varepsilon^2}) v \partial_x \rho^n, \\ f^{n+1/2} = e^{-\Delta t/\varepsilon^2} f^n + (1 - e^{-\Delta t/\varepsilon^2}) \rho^n, \\ \Theta^{n+1/2} = e^{-\sigma_a \Delta t} \Theta^n + \sigma_a (1 - e^{-\sigma_a \Delta t}) \rho^n, \\ \rho^{n+1/2} = \rho^n; \end{cases}$$

Step 2.- Solve for Δt the convection equation

$$\partial_t f + v \partial_x g = \sigma_a (\Theta - \rho) + S,$$

then update ρ^{n+1} .

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First-order closure

The system

$$\begin{cases} \partial_t \rho + \partial_x J = \sigma_a(\Theta - \rho) + S, \\ \varepsilon^2 \partial_t J + \partial_x \left[\rho \psi \left(\frac{\varepsilon J}{\rho} \right) \right] = -J \\ \partial_t \Theta = \sigma_a(\rho - \Theta). \end{cases}$$

is seen as the relaxation, as $\alpha \rightarrow 0$, of the following:

$$\begin{cases} \partial_t \rho + \partial_x J = \sigma_a(\Theta - \rho) + S, \\ \varepsilon^2 \partial_t J + \partial_x z = -J, \\ \partial_t z + \varepsilon^2 \lambda^2 \partial_x J = \frac{1}{\alpha} \left(\rho \psi(\varepsilon J/\rho) - z \right) \\ \partial_t \Theta = \sigma_a(\rho - \Theta). \end{cases}$$

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First-order closure: strategy

Diagonalize the system using f_0 and f_{\pm} , then split:

Step (i) Solve

$$\begin{aligned} \partial_t f_0 &= \mu^2 \left(\sigma_a (\Theta - \rho) + S \right), \\ \partial_t f_\pm &= -\frac{f_\pm}{\varepsilon^2} + \frac{z}{2\varepsilon^2} \mp \mu \partial_x g_\pm \mp \frac{\mu}{2\varepsilon} \partial_x z, \\ \partial_t \Theta &= \sigma_a (\rho - \Theta), \end{aligned}$$

Step (ii) Solve the ODE

$$\partial_t f_0 = -\frac{1}{\alpha} (\rho \psi(u) - z),$$

$$\partial_t f_{\pm} = \frac{1}{2\alpha} (\rho \psi(u) - z),$$

$$\partial_t \Theta = 0.$$

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Zeroth-order closure

$$\begin{cases} \partial_t \varrho - \partial_x \Big(\frac{\varrho}{\varepsilon} \mathbb{G} \Big(\varepsilon \frac{\partial_x \varrho}{\varrho} \Big) \Big) = \sigma_a (\Theta - \rho) + S, \\ \partial_t \Theta = \sigma_a (\rho - \Theta), \end{cases}$$

is seen as the relaxation, when α tends to 0, of

$$\begin{cases} \partial_t \rho + \partial_x J = \sigma_a(\Theta - \rho) + S, \\ \partial_t J + \frac{\mu^2}{\varepsilon^2} \partial_x \rho = -\frac{1}{\alpha} \left[J + \frac{\rho}{\varepsilon} \mathbb{G} \left(\varepsilon \frac{\partial_x \rho}{\rho} \right) \right], \\ \partial_t \Theta = \sigma_a(\rho - \Theta). \end{cases}$$

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Su-Olson tests

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Solver

Following the same strategy as for the zeroth-order closure of the benchmark system, and relaxing the numerical scheme to $\alpha = 0$, we obtain the following

$$\begin{split} \Theta^{n+1} &= e^{-\sigma_a \Delta t} \Theta^n + \sigma_a (1 - e^{-\sigma_a \Delta t}) \rho^n. \\ \rho^{n+1} &= \rho^n + \Delta t \left\{ \mathbb{D}_+ \left[\frac{\rho^n}{2\varepsilon\mu} \mathbb{G} \left(\frac{\varepsilon}{\mu} \frac{\bar{\mathbb{D}}_+ \rho^n}{\rho^n} \right) \right] + \mathbb{D}_- \left[\frac{\rho^n}{2\varepsilon\mu} \mathbb{G} \left(\frac{\varepsilon}{\mu} \frac{\bar{\mathbb{D}}_- \rho^n}{\rho^n} \right) \right] \right\} \\ &+ \Delta t \left(\sigma_a (\Theta^{n+1} - \rho^n) + S^n \right). \end{split}$$

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Numerical results

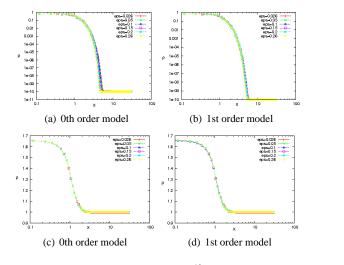


Figure: t = 1; (a) and (b): $f_0 = \rho_0 = \Theta_0 = 10^{-10}$; (c) and (d): $f_0 = \rho_0 = \Theta_0 = 1$.

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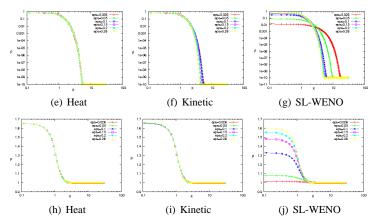


Figure: Su-Olson test: Comparison of the density ρ computed by the different models as ε varies at time t = 1 (continued).

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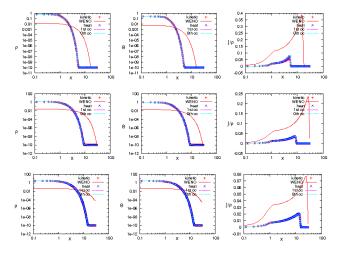


Figure: $\varepsilon = 0.026$, the initial datum is $f_0 = \rho_0 = \Theta_0 = 10^{-10}$.

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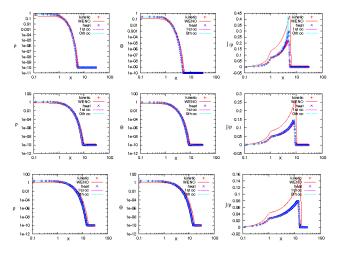


Figure: $\varepsilon = 0.1$, the initial datum is $f_0 = \rho_0 = \Theta_0 = 10^{-10}$.

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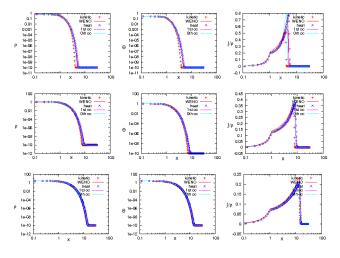


Figure: $\varepsilon = 0.26$, the initial datum is $f_0 = \rho_0 = \Theta_0 = 10^{-10}$.

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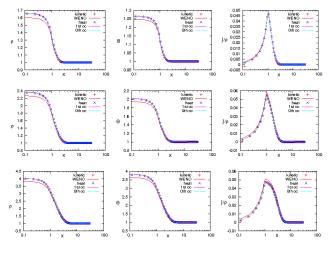


Figure: $\varepsilon = 0.26$, the initial datum is $f_0 = \rho_0 = \Theta_0 = 1$.

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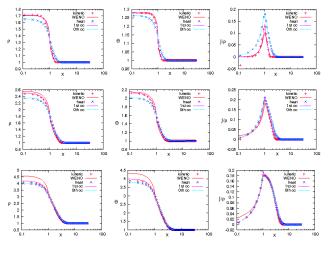


Figure: $\varepsilon = 1$, the initial data is $f_0 = \rho_0 = \Theta_0 = 1$.