Numerical methods and uncertainty quantification for kinetic equations

Lecture 3: Asymptotic Preserving schemes

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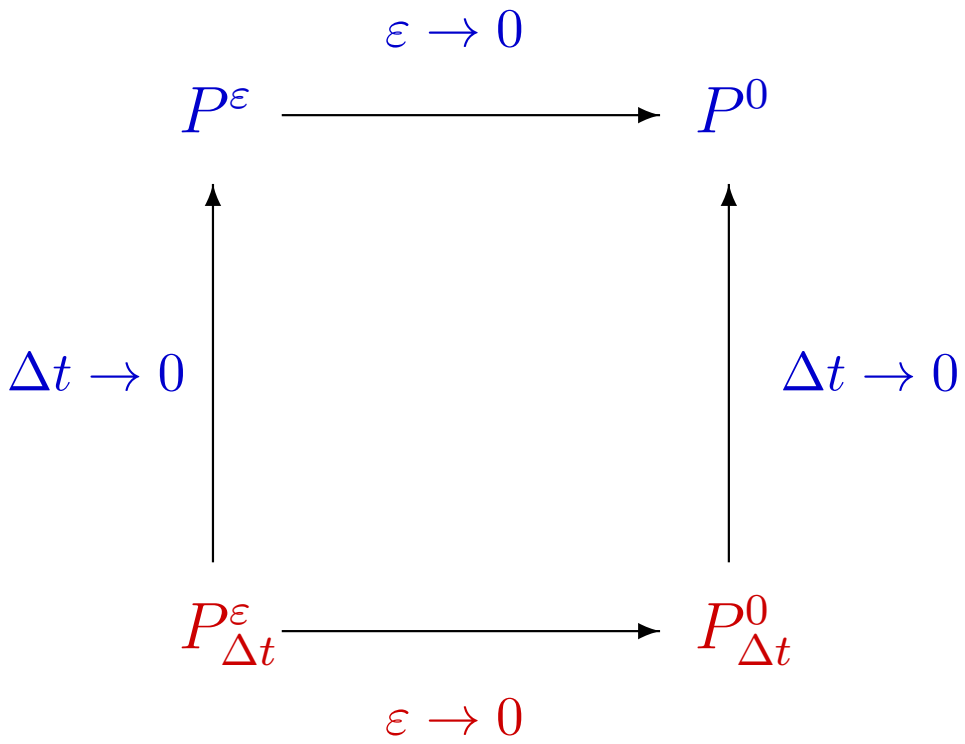
Lecture 3 Outline

Outline

Motivations

- Many problems of interests in applications involve non equilibrium gas flows as hypersonic objects simulations or micro-electro-mechanical devices.
- These kind of problems are characterized by breakdowns of fluid models, either Euler or Navier-Stokes. When the breakdown is localized both in space and time we must deal with connections of continuum and non equilibrium regions.
- To face such problems, the most natural approach is to try to combine numerical schemes for continuum models with microscopic kinetic models which guarantee a more accurate description of the physics when far from the thermodynamical equilibrium.
- Alternatively, we can try to construct numerical methods which address explicitly the multiscale nature of the solutions. Asymptotic Preserving methods represent one class among the possible methodologies.

The AP diagram



In the diagram P^ε is the original singular perturbation problem and $P^\varepsilon_{\Delta t}$ its numerical approximation characterized by a discretization parameter Δt.
The *asymptotic-preserving (AP) property* corresponds to the request that $P^\varepsilon_{\Delta t}$ is a consistent discretization of P^0 as $\varepsilon \to 0$ independently of Δt.

The kinetic model

In the Boltzmann description of RGD [1] in the hydrodynamic scaling, the density $f = f(x, v, t)$ of particles follows the equation

$$\frac{\partial f}{\partial t} + \frac{1}{\varepsilon^\alpha} v \cdot \nabla_x f = \frac{1}{\varepsilon^{1+\alpha}} Q(f, f), \quad x \in \Omega \subset \mathbb{R}^3, v \in \mathbb{R}^3,$$

The parameter $\varepsilon > 0$ is called *Knudsen number* and it is proportional to the mean free path between collisions. The bilinear *collisional operator* $Q(f, f)$ is given by

$$Q(f, f)(v) = \int_{\mathbb{R}^3} \int_{S^2} B(|v - v_*|, \omega)(f(v')f(v'_*) - f(v)f(v_*))dv_* d\omega,$$

where ω is a vector of the unitary sphere $S^2 \subset \mathbb{R}^3$ and for simplicity the dependence of f on x and t has been omitted.
The *collisional velocities* (v', v'_*) are given by the relations

$$v' = \frac{1}{2}(v + v_* + |q|\omega), \quad v'_* = \frac{1}{2}(v + v_* + |q|\omega),$$

where $q = v - v_*$ is the relative velocity.

[1] C.Cercignani '88

Hydrodynamic equations

If we consider the Boltzmann equation and multiply it for the elementary *collisional invariants* $1, v, |v|^2$ and integrate in v we obtain a system of conservation laws corresponding to conservation of mass, momentum and energy. Clearly the differential system is not closed since it involves higher order moments of the function f.

Formally as $\varepsilon \to 0$ the function f is locally replaced by a Maxwellian. In this case it is possible to compute f from its low order moments thus obtaining to leading order the closed system of *compressible Euler equations*

$$\begin{aligned}
\frac{\partial \rho}{\partial t} &+ \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho u_i) = 0, \\
\frac{\partial}{\partial t}(\rho u_j) &+ \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\rho u_i u_j) + \frac{\partial}{\partial x_j} p = 0, \quad j = 1, 2, 3 \\
\frac{\partial E}{\partial t} &+ \sum_{i=1}^{3} \frac{\partial}{\partial x_i}(E u_i + p u_i) = 0,
\end{aligned}$$

where $p = \rho T$.

Main goal

The goal is to construct simple and efficient time discretizations for the solution of kinetic equations in regions with a large variation of the mean free path.

Requirements

- For large Knudsen numbers, the methods behave as standard explicit methods.
- For intermediate Knudsen numbers, the methods are capable to speed up the computation, allowing larger time steps, without degradation of accuracy.
- In the limit of very small Knudsen numbers, the collision step replaces the distribution function by the local Maxwellian. This property is usually referred to as *asymptotic preserving (AP)* since it implies consistency with the underlying system of *Euler equations* of gas dynamics.
- An high order accuracy should be maintained both in space and time by the numerical scheme for all range of Knudsen numbers. We refer in this case to as *asymptotic accurate (AA)* schemes.

Outline

Numerical approaches

Fully explicit methods

- Non stiff term: $\Delta t \leq \Delta x / \max(v)$ (CFL condition)
- Stiff term: $\Delta t \leq C\varepsilon$.
  Stability will require very small step-sizes for stiff sources, diffusion or relaxation terms (ε small).

Fully implicit methods

- For problems with shocks or steep gradients, implicit methods are not much better than explicit ones (spurious shocks and wrong wave propagation speed when the CFL is violated).
- For convection discretizations with slope limiters, the implicit relations are hard (expensive) to solve even for linear problems.

▶ Thus it is desirable to develop schemes which are Implicit in $\mathcal{G}(U)$ and Explicit in $\mathcal{F}(U)$ (IMEX).

Requirements on IMEX

The combination of the implicit and explicit method should satisfy suitable order conditions. For linear multistep methods (LMM) if both methods are of order p then the IMEX scheme has order p. For Runge-Kutta (RK) schemes we need to satisfy additional mixed compatibility conditions.

Explicit method

- The stability region should be the largest possible.
- Monotonicity requirements

$$\|U^{n+1}\| \leq \|U^n\|, \quad \Delta t \leq \Delta t_*$$

  Strong Stability Preserving (SSP) property[2].

Implicit method

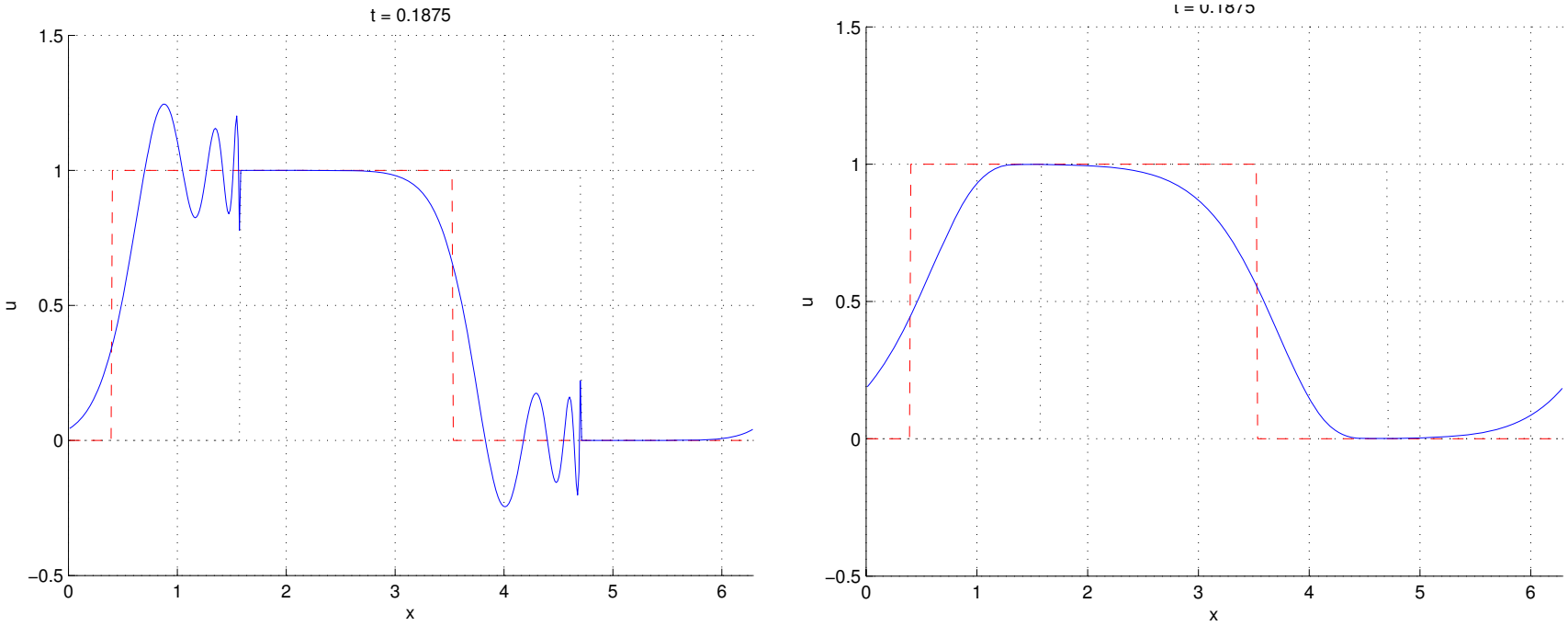
- Stable for stiff systems, and good damping properties.
- The method should be Asymptotic Preserving (AP) namely it should be consistent with the model reduction that may occur in very stiff regimes [3].

[2] S.Gottlieb, C-W.Shu, E.Tadmor '01, R.Spiteri, S.Ruth, '02

[3] S.Jin '99

Why SSP?

Linear advection $F(U) = aU$ with first order upwind. Solution for $a = -1$ at $t = 0.1875$ for Crank-Nicolson (left) and Backward Euler (right).



Here the example is for implicit methods since the concept is the same, but the numerical results are more evident. All Runge-Kutta and multi-step methods of order greater than one have a step-size restriction to be SSP.

Implicit-explicit methods

We consider the system of stiff ODE's

System of stiff ODEs

$$U' = \mathcal{F}(U) + \mathcal{G}(U)$$

where $\mathcal{F}$ is non stiff and $\mathcal{G}$ is a stiff term.

Splitting methods

- Solve separately the advection problem and the stiff source problem

$$U' = \mathcal{F}(U), \quad t \in [0, T] \qquad U' = \mathcal{G}(U), \quad t \in [0, T].$$

- Although it is only first order accurate (even if the two steps are exact, unless the operators commute), it is very popular due to its simple concept and the freedom in choosing different solvers for advection and sources.
- Higher order splitting (ex. Strang splitting) can be constructed but may present a loss of accuracy when the source term is highly stiff.

IMEX Runge-Kutta methods[4]

IMEX Runge-Kutta

$$
\begin{aligned}
U_i &= U^n + \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} \mathcal{F}(t_0 + \tilde{c}_j \Delta t, U_j) + \Delta t \sum_{j=1}^{\nu} a_{ij} \mathcal{G}(t_0 + c_j \Delta t, U_j), \\
U^{n+1} &= U^n + \Delta t \sum_{i=1}^{\nu} \tilde{w}_i \mathcal{F}(t_0 + \tilde{c}_i \Delta t, U_i) + \Delta t \sum_{i=1}^{\nu} w_i \mathcal{G}(t_0 + c_i \Delta t, U_i).
\end{aligned}
$$

$\tilde{A} = (\tilde{a}_{ij})$, $\tilde{a}_{ij} = 0$, $j \geq i$ and $A = (a_{ij})$: $\nu \times \nu$ matrices.
The coefficient vectors are $\tilde{c} = (\tilde{c}_1, \ldots, \tilde{c}_\nu)^T$, $\tilde{w} = (\tilde{w}_1, \ldots, \tilde{w}_\nu)^T$, $c = (c_1, \ldots, c_\nu)^T$, $w = (w_1, \ldots, w_\nu)^T$.

- We restrict to diagonally implicit (DIRK) scheme, $a_{ij} = 0$, $j > i$ since they guarantee that $\mathcal{F}$ is evaluated explicitly.

[4] U.Ascher, S.Ruth, R.Spiteri '97, L.P., G.Russo '00

Order conditions

- If $w_i = \tilde{w}_i$ and $c_i = \tilde{c}_i$ mixed conditions are automatically satisfied. This is not true for higher that third order accuracy
- IMEX-RK schemes are a particular case of additive Runge-Kutta (ARK) methods. Higher order conditions can be derived using a generalization of Butcher 1-trees to 2-trees.
- The number of coupling conditions increase dramatically with the order of the schemes[5].

IMEX-RK Order	**Number of coupling conditions**			
	General case	$\tilde{w}_i = w_i$	$\tilde{c} = c$	$\tilde{c} = c$ and $\tilde{w}_i = w_i$
1	0	0	0	0
2	2	0	0	0
3	12	3	2	0
4	56	21	12	2
5	252	110	54	15
6	1128	528	218	78

[5] M.Carpenter, C.Kennedy, '03

Design of IMEX-RK

Start with a p-order explicit SSP method and find the p-order DIRK method that matches the order conditions with good damping properties (L-stability).

Second order SSP IMEX-RK

$$\begin{aligned} U_1 &= U^n + \gamma \Delta t \mathcal{G}(U_1) \\ U_2 &= U^n + \Delta t \mathcal{F}(U^n) + (1-2\gamma)\Delta t \mathcal{G}(U_1) + \gamma \Delta t \mathcal{G}(U_2) \\ U^{n+1} &= U^n + \frac{1}{2}\Delta t(\mathcal{F}(U^n) + \mathcal{F}(U_1)) + \frac{1}{2}\Delta t(\mathcal{G}(U_1) + \mathcal{G}(U_2)), \end{aligned}$$

with $\gamma = (1-\sqrt{2})/2$.

Third order SSP IMEX-RK

$$\begin{aligned} U_1 &= U^n + \gamma \Delta t \mathcal{G}(U_1) \\ U_2 &= U^n + \Delta t \mathcal{F}(U^n) + (1-2\gamma)\Delta t \mathcal{G}(U_1) + \gamma \Delta t \mathcal{G}(U_2) \\ U_3 &= U^n + \frac{1}{4}\Delta t(\mathcal{F}(U^n) + \mathcal{F}(U_1)) + (1/2-\gamma)\Delta t \mathcal{G}(U_1) + \gamma \Delta t \mathcal{G}(U_3) \\ U^{n+1} &= U^n + \frac{1}{6}\Delta t(\mathcal{F}(U^n) + \mathcal{F}(U_1) + 4\mathcal{F}(U_2)) + \frac{1}{6}\Delta t(\mathcal{G}(U_1) + \mathcal{G}(U_2) + 4\mathcal{G}(U_3)), \end{aligned}$$

with $\gamma = (1-\sqrt{2})/2$.

Asymptotically preserving and accurate methods

Definition (Asymptotic preservation)

A consistent time discretization method, of stepsize Δt, for a kinetic equation is *asymptotic preserving (AP)* if, independently of the initial data and of the stepsize Δt, in the limit $\varepsilon \to 0$ becomes a consistent time discretization method for the corresponding fluid equations.

Definition (Asymptotic accuracy)

A consistent time discretization method, of stepsize Δt, for a kinetic equation is *asymptotic accurate (AA)* if, is asymptotic preserving and it preserves a given order of accuracy in time for all values of ε. In particular, in the limit $\varepsilon \to 0$, it is automatically reduced to a consistent high order time discretization method for the corresponding fluid equations.

IMEX Formulation

The general formulation of the IMEX schemes for kinetic equations is

$$\begin{aligned} F^{(i)} &= f^n - \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} v \cdot \nabla_x F^{(j)} + \Delta t \sum_{j=1}^{\nu} a_{ij} \frac{1}{\varepsilon} Q(F^{(j)}) \\ f^{n+1} &= f^n - \Delta t \sum_{i=1}^{\nu} \tilde{w}_i v \cdot \nabla_x F^{(i)} + \Delta t \sum_{i=1}^{\nu} w_i \frac{1}{\varepsilon} Q(F^{(i)}). \end{aligned}$$

$F^{(i)}$ are called stages and f^{n+1} the numerical solution. Using the vector notations

$$\begin{aligned} F &= f^n e + \Delta t \tilde{A}\, L(F) + \frac{\Delta t}{\varepsilon} A Q(F) \\ f^{n+1} &= f^n + \Delta t \tilde{w}^T L(F) + \frac{\Delta t}{\varepsilon} w^T Q(F), \end{aligned}$$

where $e = (1, 1, .., 1)^T \in \mathbb{R}^\nu$ and $L(F) = -v \cdot \nabla_x F$.

IMEX Formulation II

- The matrices $\tilde{A} = (\tilde{a}_{ij})$, $\tilde{a}_{ij} = 0$ for $j \geq i$ and $A = (a_{ij})$ are $\nu \times \nu$ matrices such that the resulting scheme is explicit in $v \cdot \nabla_x f$, and diagonally implicit ($a_{ij} = 0$, for $j > i$) in $Q(f)$.
- A Runge-Kutta method is characterized by the above defined matrices and by the coefficient vectors $\tilde{w} = (\tilde{w}_1, .., \tilde{w}_\nu)^T$, $w = (w_1, .., w_\nu)^T$.
- The use of a DIRK (Diagonally Implicit RK) scheme is enough to assure that the transport term $v \cdot \nabla_x f$ is evaluated explicitly.
- The order conditions can be simply derived by matching the schemes with a Taylor expansion of the solution.

The schemes can be represented by a double Butcher tableau

$$\begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{w}^T \end{array} \qquad \begin{array}{c|c} c & A \\ \hline & w^T \end{array}$$

IMEX definitions

Definition

We call an IMEX-RK method of *type A* if the matrix $A \in \mathbb{R}^{\nu \times \nu}$ is invertible, or equivalently $a_{ii} \neq 0$, $i = 1, \dots, \nu$. We call an IMEX-RK method of *type CK* if the matrix A can be written as

$$A = \begin{pmatrix} 0 & 0 \\ a & \hat{A} \end{pmatrix},$$

with the submatrix $\hat{A} \in \mathbb{R}^{(\nu-1) \times (\nu-1)}$ invertible.

Definition

We call an IMEX-RK method *implicitly stiffly accurate (ISA)* if

$$a_{\nu i} = w_i, \quad i = 1, \dots, \nu.$$

If in addition the explicit method satisfies

$$\tilde{a}_{\nu i} = \tilde{w}_i, \quad i = 1, \dots, \nu$$

the IMEX-RK method is said to be *globally stiffly accurate (GSA)* or simply *stiffly accurate*.

Asymptotic Preserving and Asymptotic Accurate IMEX schemes for A type matrix

The following theorem shows that type A IMEX schemes are asymptotic preserving and asymptotic accurate.

Theorem

If the IMEX method is of type A then in the limit $\varepsilon \to 0$, it becomes the explicit Runge Kutta scheme characterized by $(\tilde{A}, \tilde{w}, \tilde{c})$ applied to the limit Euler system.

In fact, multiplying the IMEX method by the collision invariants and integrating in velocity space we obtain the explicit Runge-Kutta methods applied to the moment system

$$\begin{aligned} \langle \varphi F \rangle &= \langle \varphi f^n e \rangle + \Delta t \tilde{A} \langle \varphi L(F) \rangle \\ \langle \varphi f^{n+1} \rangle &= \langle \varphi f^n \rangle + \Delta t \tilde{w}^T \langle \varphi L(F) \rangle. \end{aligned}$$

Since A is invertible we can solve for $Q(F)$ to get

$$\Delta t Q(F) = \varepsilon A^{-1} \left(F - f^n e - \Delta t \tilde{A} L(F) \right) \Rightarrow \varepsilon \to 0 \; \Delta t Q(F) = 0 \Rightarrow F = M[F].$$

Asymptotic Preserving and Asymptotic Accurate IMEX schemes for A type matrix II

Replacing $F = M[F]$ in the moment system leads to an explicit Runge-Kutta method applied to the limiting Euler system

$$\begin{aligned} \mathcal{U} &= U^n e - \Delta t \tilde{A} \nabla_x \cdot \mathcal{F}(\mathcal{U}) \\ U^{n+1} &= U^n + \Delta t \tilde{w}^T \nabla_x \cdot \mathcal{F}(\mathcal{U}), \end{aligned}$$

$\mathcal{U} = (\mathcal{U}^{(1)}, \dots, \mathcal{U}^{(\nu)})^T$, $\mathcal{F}(\mathcal{U}) = (\mathcal{F}(\mathcal{U}^{(1)}), \dots, \mathcal{F}(\mathcal{U}^{(\nu)}))^T$, $\mathcal{U}^{(i)} = \langle \varphi M[F^{(i)}] \rangle$ and $\mathcal{F}(\mathcal{U}^{(i)}) = \langle \varphi L(M[F^{(i)}]) \rangle$.

Another property we can demand is that in the limit $\varepsilon \to 0$ the distribution function is projected over the equilibrium $f^{n+1} \to M[f^{n+1}]$. One possibility is

Theorem

If the IMEX scheme is of type A and Globally Stiffly Accurate (GSA) then

$$\lim_{\varepsilon \to 0} f^{n+1} = M[f^{n+1}].$$

AP-AA IMEX schemes for CK-type matrix

The request that the matrix A is invertible is highly restrictive for high order methods. We search then for AP and AA even when the matrix is of type CK. We need the notion of initial data consistent with the limit problem.

Definition

The initial data for the Boltzmann kinetic equation are said *consistent* or *well prepared* if

$$f_0(x,v) = M[f_0(x,v)] + g^\varepsilon(x,v), \qquad \lim_{\varepsilon\to 0} g^\varepsilon(x,v) = 0.$$

We can then state the following result

Theorem

If the IMEX scheme is of type CK and GSA then for consistent initial data, in the limit $\varepsilon \to 0$, the IMEX scheme becomes the explicit RK scheme characterized by $(\tilde{A}, \tilde{w}, \tilde{c})$ applied to the limit Euler system.

Penalization of the collision integral

We rewrite the collision operator in the form

$$Q_B(f) = (Q_B(f) - Q_P(f)) + Q_P(f) = G_P(f) + Q_P(f),$$

where $Q_P(f)$ is a general operator which will be used to penalize the original Boltzmann operator $Q_B(f)$. The corresponding kinetic equation reads

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} G_P(f) + \frac{1}{\varepsilon} Q_P(f).$$

Recalling that $Q_B(f) = P(f) - \mu f$ where $P(f)$ is the so-called gain part of the operator and μ an estimate of the largest value of the loss part and taking $Q_P(f) = \mu(M - f)$ leads to

$$\partial_t f + v \cdot \nabla_x f = \frac{\mu}{\varepsilon}\left(\frac{P(f)}{\mu} - M\right) + \frac{\mu}{\varepsilon}(M - f).$$

Penalization of the collision integral II

- We use now a numerical scheme in which only the simpler operator $Q_P(f)$ is treated implicitly.
- This means that the term $G_P(f)$ describing the deviations of the true Boltzmann operator $Q_B(f)$ from the simplified operator $Q_P(f)$ and the convection term $v \cdot \nabla_x f$ are treated explicitly.
- This approach introduces some additional stability requirements in order for the IMEX schemes to preserve the asymptotic behavior of the equation.

The penalized IMEX Runge-Kutta schemes read

$$F^{(i)} = f^n + \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} \left(\frac{1}{\varepsilon} G_P(F^{(j)}) - v \cdot \nabla_x F^{(j)} \right) + \Delta t \sum_{j=1}^{\nu} a_{ij} \frac{1}{\varepsilon} Q_P(F^{(j)})$$

$$f^{n+1} = f^n + \Delta t \sum_{i=1}^{\nu} \tilde{w}_i \left(\frac{1}{\varepsilon} G_P(F^{(i)}) - v \cdot \nabla_x F^{(i)} \right) + \Delta t \sum_{j=1}^{\nu} w_i \frac{1}{\varepsilon} Q_P(F^{(i)}).$$

Properties of the penalized IMEX schemes

We have the following results

Theorem

If the penalized IMEX method is of type A *and satisfies*

$$\tilde{w}^T = w^T A^{-1} \tilde{A},$$

then in the limit $\varepsilon \to 0$*, it becomes the explicit RK scheme characterized by* $(\tilde{A}, \tilde{w}, \tilde{c})$ *applied to the limit Euler system. The above condition is automatically satisfied if the IMEX scheme is GSA. Moreover, in this case we have*

$$\lim_{\varepsilon \to 0} f^{n+1} = M[f^{n+1}].$$

In the case of penalized IMEX schemes of type CK, we can state an analogous result if in addition consistent initial data are considered.

L_1 error for the density for different second and third order IMEX schemes on smooth solution I

- 3rd order WENO space discretization
- Fast spectral method for the collision integral.
- Time step $\Delta t = \Delta x/(2v_{\max})$.

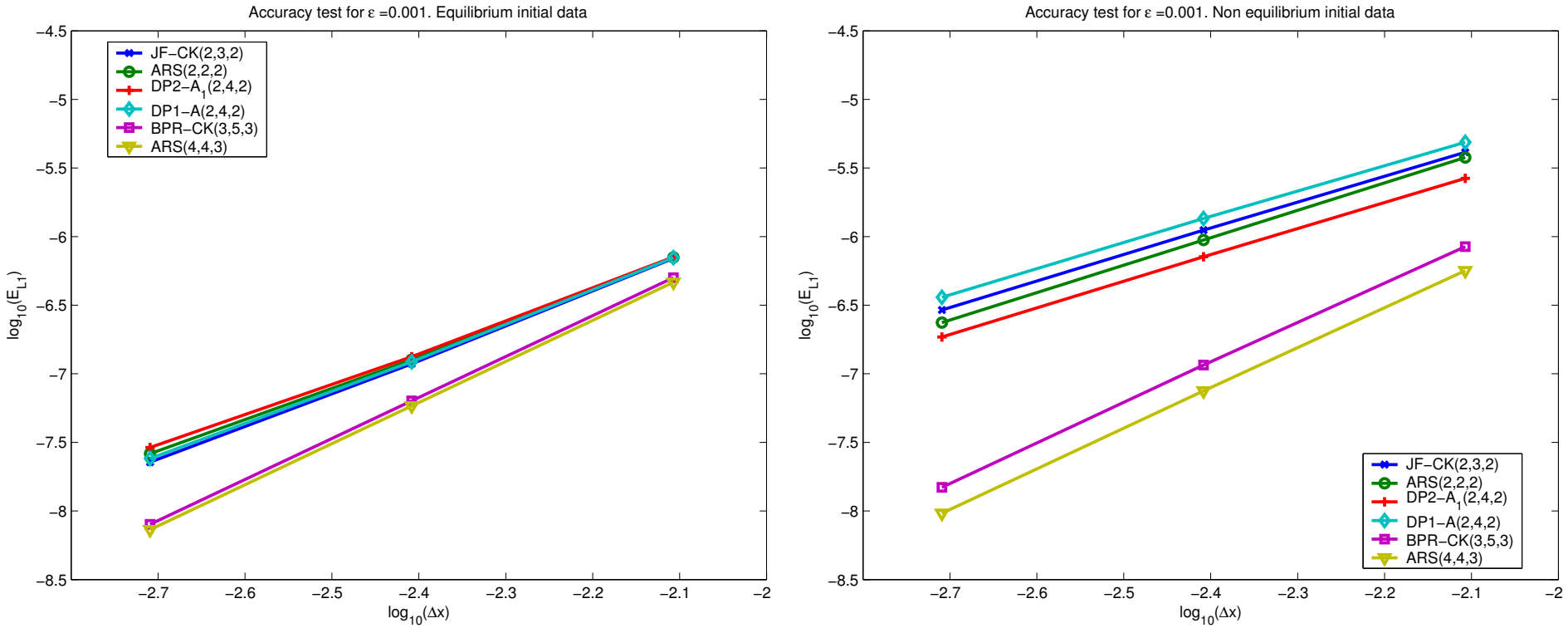


Figure: Left equilibrium initial data, right non equilibrium initial data, $\varepsilon = 10^{-3}$.

L_1 error for the density for different second and third order IMEX schemes on smooth solution II

- 3rd order WENO space discretization
- Fast spectral method for the collision integral.
- Time step $\Delta t = \Delta x/(2v_{\max})$.

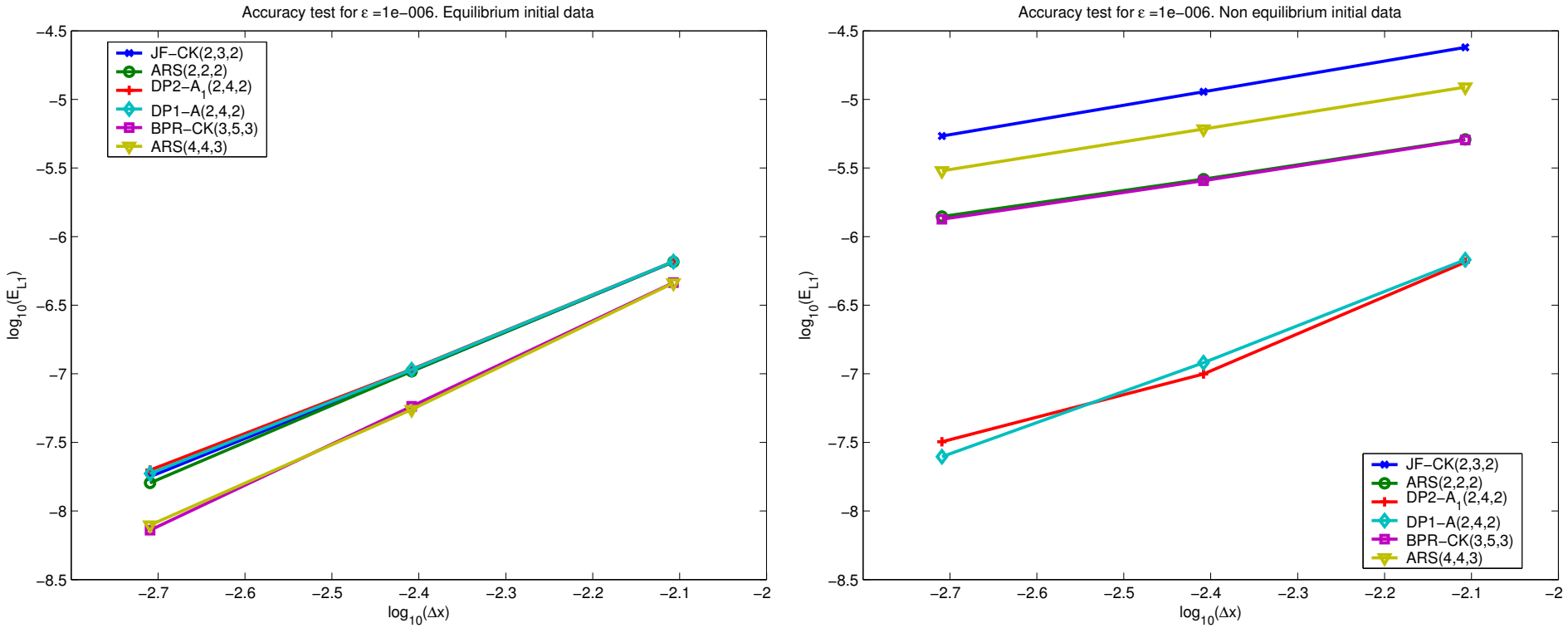


Figure: Left equilibrium initial data, right non equilibrium initial data, $\varepsilon = 10^{-6}$.

Outline

The Boltzmann equation in the drift-diffusion limit

Let consider the Boltzmann equation under the diffusive scaling which describes the time evolution of electrons inside semiconductor devices

$$\varepsilon\,\partial_t f + v\cdot\nabla_x f - \frac{q}{m}E\cdot\nabla_v f = \frac{1}{\varepsilon}Q(f) + \varepsilon\widehat{G}\,.$$

$\widehat{G} = \widehat{G}(t,x,v)$ models the generation and recombination process, while $Q(f)$ the collisions, $E(t,x) = -\nabla_x\Phi(t,x)$ is the electric field computed through Φ

$$\gamma\Delta_x\Phi = \rho - \rho_d,$$

where γ is the scaled Debye length and $\rho_d(x)$ is given. Now, defining the total mass $\rho = \rho(t,x)$ as

$$\rho = \int f(v)\,dv\,,$$

one can show that when $\varepsilon\to 0$, ρ satisfies the drift-diffusion equation

$$\partial_t\rho = \nabla_x\cdot(D\nabla_x\rho + \eta\rho E) + \widetilde{G}.$$

where D is the diffusion coefficient defined implicitly in terms of the cross section, $\eta = qD/m\theta$ is the so-called mobility and $\widetilde{G}$ is the integral of the generation recombination function.

Even and odd parities

Let split the Boltzmann equation into two equations, one for v and one for $-v$

$$\varepsilon\,\partial_t f + v\cdot\nabla_x f - \frac{q}{m}E\cdot\nabla_v f = \frac{1}{\varepsilon}Q(f)(v) + \varepsilon\widehat{G},$$
$$\varepsilon\,\partial_t f - v\cdot\nabla_x f + \frac{q}{m}E\cdot\nabla_v f = \frac{1}{\varepsilon}Q(f)(-v) + \varepsilon\widehat{G}.$$

Introducing the so called even parity r and odd parity j defined by

$$r(t,x,v) = \frac{1}{2}\Big(f(t,x,v) + f(t,x,-v)\Big),$$
$$j(t,x,v) = \frac{1}{2\varepsilon}\Big(f(t,x,v) - f(t,x,-v)\Big).$$

Adding and subtracting the two above equations we get

$$\partial_t r + v\cdot\nabla_x j - \frac{q}{m}E\cdot\nabla_v j = \frac{1}{\varepsilon^2}Q(r) + \widehat{G},$$
$$\partial_t j + \frac{1}{\varepsilon^2}\left(v\cdot\nabla_x r - \frac{q}{m}E\cdot\nabla_v r\right) = -\frac{1}{\varepsilon^2}\,\lambda j\,,$$

A suitable reformulation

The scheme should solve, in the limit $\varepsilon \to 0$, the drift-diffusion equation with an *implicit treatment* of the diffusion term. This ensures a *stability condition* for the time step of the order : $\Delta t = O(\Delta x)$. We add to both sides of the equation for r the following term

$$v \cdot \nabla_x \left(\mu \frac{v}{\lambda} \cdot \nabla_x r \right),$$

where $\mu = \mu(\varepsilon)$ is a positive function such that $\mu(0) = 1$. The modified system reads

$$\partial_t r + v \cdot \nabla_x \left(j + \mu \frac{v}{\lambda} \cdot \nabla_x r \right) - E \cdot \nabla_v j = \frac{1}{\varepsilon^2} Q(r) + v \cdot \nabla_x \left(\mu \frac{v}{\lambda} \cdot \nabla_x r \right) + \widehat{G},$$

$$\partial_t j = -\frac{1}{\varepsilon^2} \left(v \cdot \nabla_x r - E \cdot \nabla_v r \right) - \frac{1}{\varepsilon^2} \lambda j \,.$$

The reformulated system can be rewritten in a compact form as

$$\partial_t r = f_1(r, j) + \frac{1}{\varepsilon^2} Q(r) + f_2(r),$$

$$\partial_t j = -\frac{1}{\varepsilon^2} g(r, j)$$

where

IMEX Runge-Kutta scheme

$$
\begin{aligned}
f_1(r,j) &= -v\cdot\nabla_x\left(j+\mu\frac{v}{\lambda}\cdot\nabla_x r\right)+E\cdot\nabla_v j+\widehat{G},\\
f_2(r) &= \mu\, v\cdot\nabla_x\left(\frac{v}{\lambda}\cdot\nabla_x r\right),\ g(r,j)=\lambda j+(v\cdot\nabla_x r-E\cdot\nabla_v r)\,.
\end{aligned}
$$

Now, an IMEX Runge-Kutta scheme reads for the internal stages $k=1,\dots,\nu$ as

$$
\begin{aligned}
R^{(k)} &= r^n+\Delta t\sum_{j=1}^{k-1}\widetilde{a}_{kj}\, f_1\left(R^{(j)},J^{(j)}\right)+\Delta t\sum_{j=1}^{k}a_{kj}\left(\frac{1}{\varepsilon^2}Q\left(R^{(j)}\right)+f_2\left(R^{(j)}\right)\right)\\
J^{(k)} &= j^n-\frac{\Delta t}{\varepsilon^2}\sum_{j=1}^{k}a_{kj}\, g\left(R^{(j)},J^{(j)}\right)
\end{aligned}
$$

while the numerical solution is given by

$$
\begin{aligned}
r^{n+1} &= r^n+\Delta t\sum_{k=1}^{\nu}\widetilde{w}_k f_1\left(R^{(k)},J^{(k)}\right)+\Delta t\sum_{k=1}^{\nu}w_k\left(\frac{1}{\varepsilon^2}Q\left(R^{(k)}\right)+f_2\left(R^{(k)}\right)\right)\\
j^{n+1} &= j^n-\frac{\Delta t}{\varepsilon^2}\sum_{k=1}^{\nu}w_k\, g\left(R^{(k)},J^{(k)}\right).
\end{aligned}
$$

A linearization technique for the implicit collision term

- In the numerical method described the collision operator, which could be costly to compute or even more to invert, has to be implicitly computed.
- A solution is represented by the penalization. We add and subtract to the collision term Q an operator L and then we combine the implicit and the explicit solvers.

$$\underbrace{Q(r)}_{Implicit} \quad \rightarrow \quad \underbrace{\Big(Q(r) - L(r)\Big)}_{Explicit} + \underbrace{L(r)}_{Implicit} .$$

Different choices for L are possible : linearized operators, relaxation operators.. Regardless from the choice of L, we apply the IMEX schemes to get

$$\begin{aligned}
\partial_t r &= \underbrace{-v \cdot \nabla_x \left(j + \mu \frac{v}{\lambda} \cdot \nabla_x r \right) + E \cdot \nabla_v j + \frac{1}{\varepsilon^2} \Big(Q(r) - L(r) \Big) + \widehat{G}}_{\text{Explicit}} \\
&+ \underbrace{\frac{1}{\varepsilon^2} L(r) + v \cdot \nabla_x \left(\mu \frac{v}{\lambda} \cdot \nabla_x r \right)}_{\text{Implicit}}, \\
\partial_t j &= \underbrace{-\frac{1}{\varepsilon^2} \Big(\lambda\, j + v \cdot \nabla_x r - E \cdot \nabla_v r \Big)}_{\text{Implicit}} .
\end{aligned}$$

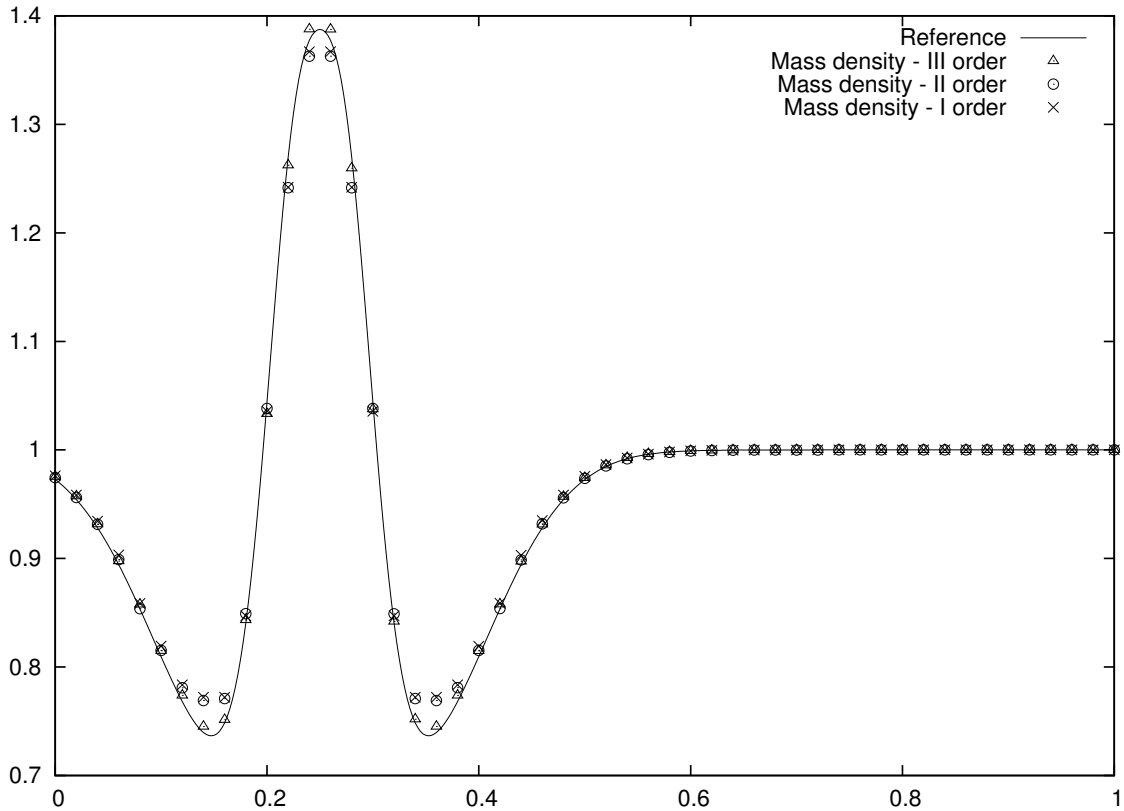
Properties of the IMEX schemes

- *Computing implicitly* the operator L stabilizes the non-linear collision operator, without changing the asymptotic behavior of the solution.
- *This stabilization is not straightforward*, in order to stabilize the reformulated system it is necessary that the coefficients of the scheme used for the time integration of the linearized collision operator dominate those used for the time integration of the original operator.
- *Type A IMEX schemes* are Asymptotic Preserving and Asymptotically Accurate. If in addition they are GSA the distribution function is projected over the equilibrium at each time step.
- *Two sufficient conditions* for type CK IMEX schemes which guarantee the AP and AA properties are be GSA and have the initial data are close to the equilibrium state (we say in this case that the initial data are consistent with the limit problem).
- In this case, we get also sufficient conditions to assure that the *distribution function is projected* over the equilibrium state at each time step.

Kinetic regime

We compare a fourth order explicit RK scheme with $N_x = 400$, with the first, second and third order IMEX approximations using 50 grid points, $\varepsilon = 1$ and $\Delta t = \Delta t_H = 0.5\,\varepsilon\,\Delta x / v_{\max}$. The explicit integrator require

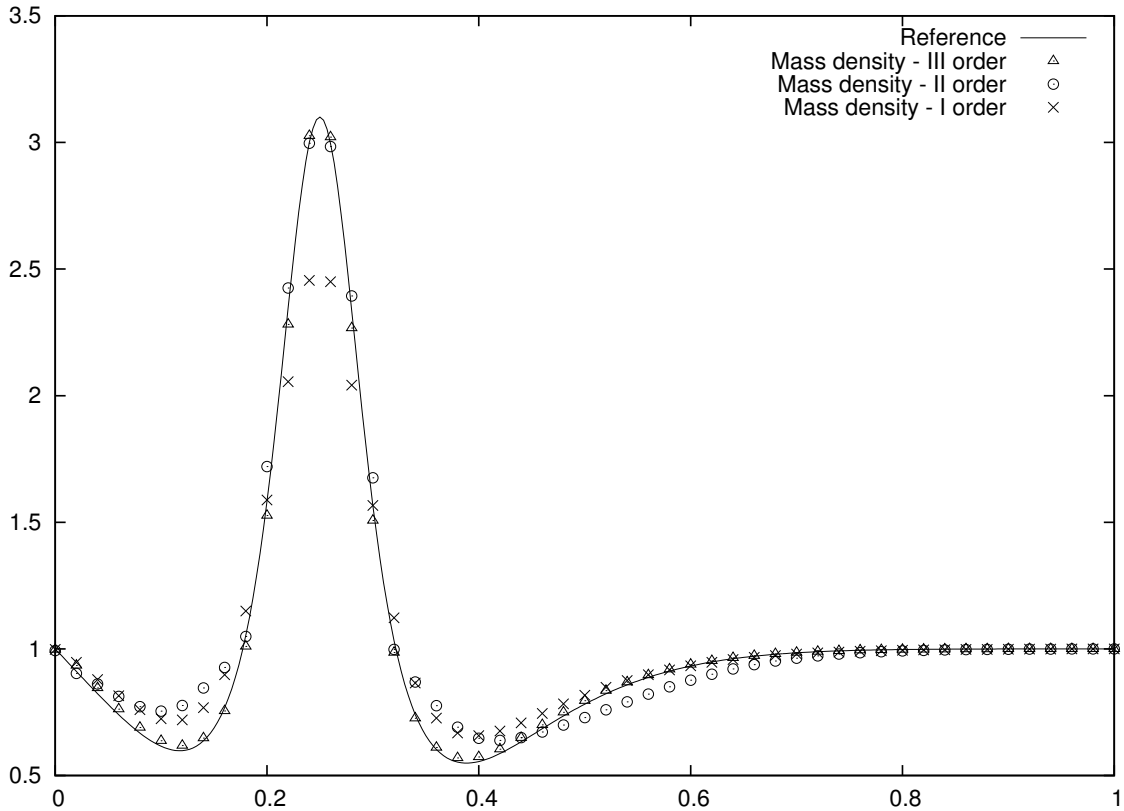
$$\Delta t = \min\left\{\Delta t_P = \frac{\Delta x^2}{2},\ \Delta t_H = c_H\,\varepsilon\,\Delta x / v_{\max}\right\}$$



Diffusive regime

We compare a fourth order explicit RK scheme with $N_x = 400$, with the first, second and third order IMEX approximations using 50 grid points, $\varepsilon = 0.002$ and $\Delta t = \Delta t_H = 0.5\,\Delta x / v_{\max}$. The explicit integrator require

$$\Delta t = \min\left\{\Delta t_P = \frac{\Delta x^2}{2},\ \Delta t_H = c_H\,\varepsilon\,\Delta x / v_{\max}\right\}$$



Outline

Quasi neutral Vlasov Poisson system

We consider the so-called collisional Vlasov equation

$$\partial_t f + v \cdot \nabla_x f + \nabla_x \varphi \cdot \nabla_v f = \frac{1}{\varepsilon} Q(f).$$

The electric potential φ is coupled to f through the Poisson equation

$$\Delta \varphi = \frac{e}{\varepsilon_0}(\rho - 1), \quad \text{with} \quad \rho = \int f dv.$$

where e is the electric charge and ϵ_0 is the vacuum permittivity. A classical rescaling of the Vlasov-Poisson system leads to

$$\gamma^2 \Delta \varphi = \rho - 1, \quad \text{with} \quad \rho = \int f dv.$$

where we denoted by $\gamma = \left(\frac{\varepsilon_0 k_B T_0}{e^2 n_0} \right)^{1/2}$ the scaled Debye length, with k_B the Boltzmann constant, with n_0 the plasma density scale and T_0 the plasma temperature scale.

The reformulated quasi neutral Vlasov Poisson system

In order to recover an equation for the potential φ , we assume that the quasineutrality constraint is satisfied initially and we derive with respect to time the continuity equation. This leads to

$$\partial_{tt}\rho + \partial_t \nabla_x \cdot (\rho u) = 0.$$

Then, taking the divergence of momentum equation

$$\nabla_x \cdot \partial_t(\rho u) + \nabla_x^2 : S = \nabla_x \cdot (-\rho \nabla_x \varphi)$$

where $S = \int f v \otimes v dv$. Making the difference between the above two equations

$$\partial_{tt}\rho - \nabla_x^2 : S = \nabla_x \cdot (\rho \nabla_x \varphi).$$

Finally, using the Poisson equation to replace gives the Reformulated Poisson Equation (RPE)

$$-\gamma^2 \partial_{tt} \Delta\varphi - \nabla_x^2 : S = \nabla_x \cdot (\rho \nabla_x \varphi).$$

which is equivalent to the original one if initially the Poisson equation and its time derivative are satisfied.

The limit systems

Thus the reformulated system reads

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \nabla \varphi \cdot \nabla_v f = \frac{1}{\varepsilon} Q(f),$$

$$-\gamma^2 \partial_{tt} \Delta \varphi - \nabla_x^2 : S = \nabla_x \cdot (\rho \nabla_x \varphi)$$

The quasi-neutral limit of Vlasov-Poisson system reads

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + \nabla \varphi \cdot \nabla_v f = \frac{1}{\varepsilon} Q(f),$$

$$-\nabla_x^2 : S = \nabla_x \cdot (\rho \nabla_x \varphi).$$

The Reformulated Vlasov-Poisson system in the fluid limit reads

$$\partial_t U + \nabla_x \cdot F(U) = G(U),$$

$$-\gamma^2 \partial_{tt} \Delta \varphi - \nabla_x^2 : S = \nabla_x \cdot (\rho \nabla_x \varphi).$$

and the Euler-Poisson quasi-neutral system reads

$$\partial_t U + \nabla_x \cdot F(U) = G(U),$$

$$-\nabla_x^2 : S = \nabla_x \cdot (\rho \nabla_x \varphi).$$

A first order splitting

The initial condition satisfies the quasi-neutral limit: $\rho^n = 1$ and $\nabla_x \cdot (\rho u)^n = 0$

$$f^* = f^n - \Delta t \nabla_x \varphi \cdot \nabla_v f^n,$$
$$f^{n+1} = f^* - \Delta t\, v \cdot \nabla_x f^*.$$

This gives for the density and the momentum

$$\rho^* = \rho^n = 1,$$
$$(\rho u)^* = (\rho u)^n + \Delta t \rho^n \nabla_x \varphi,$$

so that $\nabla_x \cdot (\rho u)^* = \Delta t \nabla_x \cdot (\rho^n \nabla_x \varphi)$. The second step gives

$$\rho^{n+1} = \rho^* - \Delta t \nabla_x \cdot (\rho u)^* = \rho^n - \Delta t^2 \nabla_x \cdot (\rho^n \nabla_x \varphi),$$
$$(\rho u)^{n+1} = (\rho u)^* - \Delta t \nabla_x \cdot S^*.$$

First order splitting and high order splitting

And, then

$$\nabla_x \cdot (\rho u)^{n+1} = \nabla_x \cdot (\rho u)^* - \Delta t \nabla_x^2 : S^* = \Delta t (\nabla_x \cdot (\rho^n \nabla_x \varphi) - \nabla_x^2 : S^*).$$

- This means that in principle, we can choose an electric potential which ensures that $\nabla_x \cdot (\rho u)^{n+1} = 0$,
- This is the case if φ is the solution of $\nabla_x \cdot (\rho^n \nabla_x \varphi) = \nabla_x^2 : S^*$.
- However, in the general case, there is no choice of the electric potential which ensures the propagation of the quasi-neutral state $\rho^{n+1} = \rho^n = 1$.
- If we repeat the same analysis for a second order splitting as for instance the Strang splitting we realize that quasi neutrality is lost for any choice of the initial step.
- There is no easy solution for the construction of high order schemes preserving quasi-neutral states when splitting methods are used.

A new stable scheme for quasi neutrality

Let us first consider the quasi-neutral system and assume quasi-neutral initial conditions *i.e.* $\rho^n = 1$ and $\nabla_x \cdot (\rho u)^n = 0$, then we have

$$f^{n+1} = f^n - \Delta t\, v \cdot \nabla_x f^n - \Delta t \nabla_x \varphi^{n+1} \cdot \nabla_v f^n + \frac{\Delta t\, \nu}{\varepsilon}(M[f^{n+1}] - f^{n+1}),$$

$$\nabla_x \cdot (\rho^n \nabla_x \varphi^{n+1}) = \nabla_x^2 : S^n.$$

Taking the velocity moments leads to

$$\rho^{n+1} = \rho^n - \Delta t \nabla_x \cdot (\rho u)^n,$$
$$(\rho u)^{n+1} = (\rho u)^n - \Delta t \nabla_x \cdot S^n + \Delta t \rho^n \nabla_x \varphi^{n+1},$$

which gives

$$\rho^{n+1} = \rho^n, \quad \text{and} \quad \nabla_x \cdot (\rho u)^{n+1} = -\Delta t(\nabla_x^2 : S^n - \nabla_x \cdot (\rho^n \nabla_x \varphi^{n+1})) = 0.$$

Thus quasi-neutrality constraint is propagated in time.

Reformulation of the new scheme

Now, let conside the reformulated BGK-Vlasov-Poisson system and

$$\lambda^2 \frac{\Delta\varphi^{n+1} - 2\Delta\varphi^n + \Delta\varphi^{n-1}}{\Delta t} + \Delta t\, \nabla_x \cdot \Big(\rho^n\, \nabla_x \varphi^{n+1}\Big) = \Delta t\, \nabla_x^2 : S^n, \quad \forall\, n \geq 2.$$

Initially two resolutions of the constrained Poisson equation must be done to compute φ^{n+1}, φ^n.
To bypass this limitation, let us remark that the following reformulation holds

$$\lambda^2 \frac{\Delta\varphi^{n+1} - 2\Delta\varphi^n + \Delta\varphi^{n-1}}{\Delta t} - \frac{\rho^{n+2} - 2\,\rho^{n+1} + \rho^n}{\Delta t} = 0.$$

So, we can write

$$\lambda^2\, \Delta\varphi^{n+1} = \rho^{n+2} - 1.$$

By rearranging the above equation we finally get

$$f^{n+1} = f^n - \Delta t\, v \cdot \nabla_x f^n - \Delta t \nabla_x \varphi^{n+1} \cdot \nabla_v f^n + \frac{\Delta t\, \nu}{\varepsilon}(M[f^{n+1}] - f^{n+1}),$$
$$\nabla_x \cdot \big[(\lambda^2 + \Delta t^2 \rho^n)\nabla_x \varphi^{n+1}\big] = \rho^{n+1} - 1 - \Delta t \nabla_x \cdot (\rho u)^n + \Delta t^2\, \nabla_x^2 : S^n.$$

Analysis of the new stable scheme

Let us now analyze the behavior of the above scheme.

- If we let $\lambda \to 0$ we immediately get, if the initial data are consistent with the quasi neutral limit that the scheme is AP in the quasi neutral limit.
- On the other hand if $\lambda = 0$ at $t = 0$, but the initial data are not consistent with the quasi neutral limit we get

$$\rho^1 = \rho^0 - \Delta t \nabla_x \cdot (\rho u)^0,$$

and

$$\begin{aligned} \nabla_x \cdot (\rho u)^1 &= \nabla_x \cdot (\rho u)^0 - \Delta t \nabla_x^2 : S^0 + \Delta t \left(\nabla_x^2 : S^0 + \frac{2\rho^1 - \rho^0 - 1}{\Delta t^2} \right), \\ &= \nabla_x \cdot (\rho u)^0 - \nabla_x \cdot (\rho u)^0 + \frac{\rho^1 - 1}{\Delta t} = \frac{\rho^1 - 1}{\Delta t}. \end{aligned}$$

Analysis of the new stable scheme II

- The second time step leads to

$$\rho^2 = \rho^1 - \Delta t \nabla_x \cdot (\rho u)^1 = \rho^1 - \Delta t \frac{\rho^1 - 1}{\Delta t} = 1,$$

and

$$\begin{aligned} \nabla_x \cdot (\rho u)^2 &= \nabla_x \cdot (\rho u)^1 - \Delta t \nabla_x^2 : S^1 + \Delta t \left(\nabla_x^2 : S^1 + \frac{2\rho^2 - \rho^1 - 1}{\Delta t^2} \right), \\ &= \nabla_x \cdot (\rho u)^1 - \nabla_x \cdot (\rho u)^1 + \frac{\rho^2 - 1}{\Delta t} = \frac{\rho^2 - 1}{\Delta t} = 0, \end{aligned}$$

- Moreover, if at a given instant of time t^n, the Debye length becomes zero, at the time step t^{n+2} the quasi neutrality is obtained and then propagated for all times.
- A linear stability result for above described scheme in the fluid limit $\varepsilon \to 0$ can be done. which proves that the scheme proposed is stable for all values of λ to small perturbations of the quasi neutral equilibrium state.

Outline

The Vlasov-BGK-Poisson system

We consider a two species plasma: $x \in \Omega \subset \mathbb{R}^d$, $v \in \mathbb{R}^d$ and time $t > 0$

$$\partial_t f_i + v \cdot \nabla_x f_i + E \cdot \nabla_v f_i = \frac{1}{\varepsilon_i}(M_{f_i} - f_i),$$

$$\partial_t f_e + v \cdot \nabla_x f_e - E \cdot \nabla_v f_e = \frac{1}{\varepsilon_e}(M_{f_e} - f_e),$$

together with a Poisson equation for the electric potential

$$-\gamma^2 \Delta \varphi = \rho_i - \rho_e$$

with γ the Debye length and $E = -\nabla_x \varphi$. We divide for each species the physical domain Ω into $\mathcal{B}_t^K$, $\mathcal{B}_t^H$ and $\mathcal{B}_t$ and accordingly we define a cut-off function $h = h(x,t) \in \mathcal{C}(\mathbb{R})$ for each of the two species

$$h(x,t) = \begin{cases} 1, & \text{if } x \in \mathcal{B}_t^K \\ 0, & \text{if } x \in \mathcal{B}_t^H \\ 0 \le h(x,t) \le 1, & \text{if } x \in \mathcal{B}_t \end{cases}$$

The coupling strategy

Let us set for all $x \in \Omega$ define two new functions for each species

$$\begin{cases} f_K = h\, f \\ f_H = (1-h)\, f. \end{cases}$$

We then have for the time derivative of the defined new functions

$$\begin{aligned} \partial_t f_K \quad &= \partial_t (hf) \quad &&= f\,\partial_t h + h\partial_t f \\ \partial_t f_H \quad &= \partial_t \Big((1-h) f \Big) \quad &&= -f\,\partial_t h + (1-h)\partial_t f \end{aligned}$$

which give using the Vlasov-BGK equation

$$\partial_t f_K + h\, v \cdot \nabla_x f_K + h\, v \cdot \nabla_x f_H + E \cdot \nabla_v f_K = \frac{h}{\varepsilon} \Big(M_f - f \Big) + f \partial_t h,$$

$$\partial_t f_H + (1-h)\, v \cdot \nabla_x f_H + f_K + E \cdot \nabla_v f_H = \frac{1-h}{\varepsilon} \Big(M_f - f \Big) - f \partial_t h$$

The coupling strategy and the macroscopic equations

- Suppose now that in some part of the domain the ions or respectively the electrons are in equilibrium while in rest of the domain we are far from it
- This permits to replace f_H by M_{f_H} for one of both species at the same time.

We then get a system for the moments of M_{f_H} : $(\rho_H, \rho_H u_H, \mathcal{E}_H)$ which reads

$$\partial_t \rho_H + (1-h)\nabla_x \cdot (\rho_H u_H) = -(1-h)\nabla_x \cdot \left(\int_{\mathbb{R}^d} v f_K \, dv \right) - g \partial_t h,$$

$$\partial_t (\rho_H u_H) + (1-h)\nabla_x \cdot (\rho_H u_H \otimes u_H + p_H I) = \rho_H E$$
$$-(1-h)\nabla_x \cdot \left(\int_{\mathbb{R}^d} v^2 f_K \, dv \right) - g u \partial_t h,$$

$$\partial_t \mathcal{E}_H + (1-h)\nabla_x \cdot \Big((\mathcal{E}_H + p_H) u_H \Big) = \rho_H u_H E$$
$$-(1-h)\nabla_x \cdot \left(\int_{\mathbb{R}^d} v \frac{|v|^2}{2} f_K \, dv \right) - \mathcal{E} \partial_t h,$$

Key points

Correctly dividing the domain is a crucial step for this method:

- *accuracy:* use proper model everywhere ("positivity") issues
- *efficiency:* kinetic only if necessary, computational speedup
- *dynamically generate* kinetic or hydrodynamic regions
- *coupling functions* for different species *evolve independently*

Test 1 : Temperature for one specie expansion

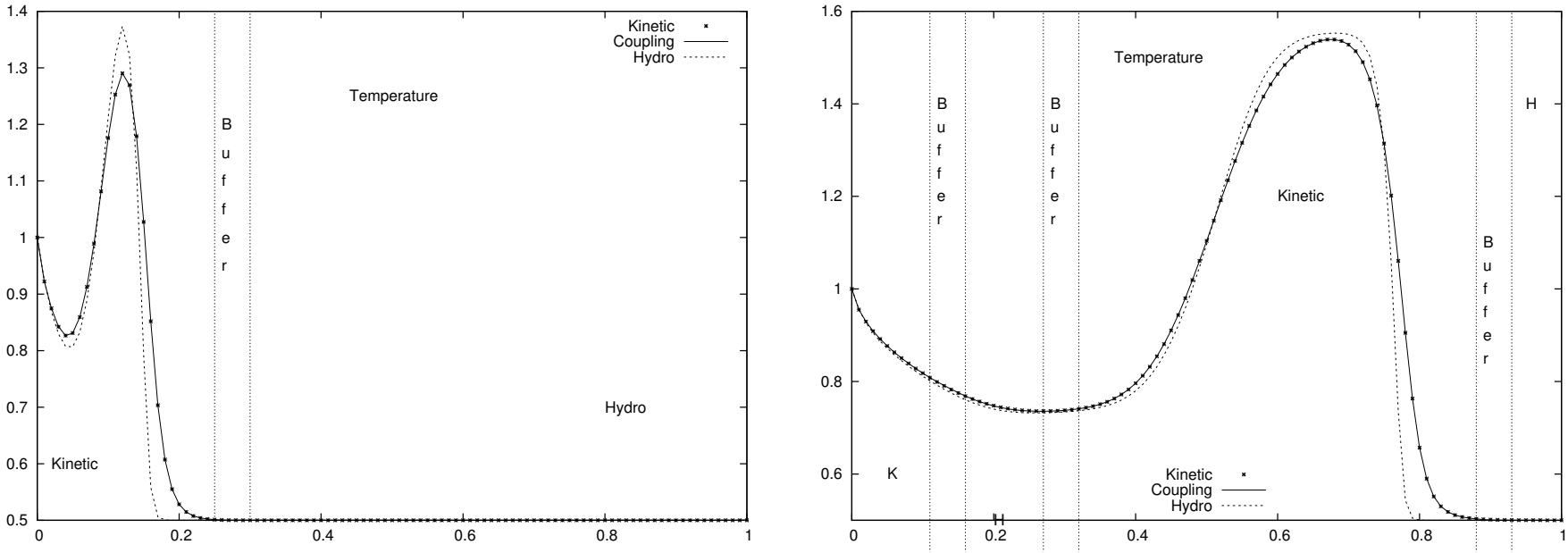


Figure: Temperature profiles at different times.

Remarks and further reading

- IMEX schemes represent a powerful tool for the time discretization of partial differential equations where convection and stiff sources/diffusion are present.
- However they are not a universal cure for all problems. It is not difficult to imagine a situation where a fully explicit (or implicit) method is preferable.
- The most critical case is the application to (nonlinear) PDEs where the stiff scales originate a model reduction. In such cases AP methods are essential in order to capture the correct physical behavior.
- The material for this part is mostly based on the recent survey G.D., L. Pareschi, Acta Numerica, 2014.
- Further surveys on AP schemes can be found in
  - S. Jin, 'Asymptotic preserving (AP) schemes for multiscale kinetic and hyperbolic equations: a review.', *Riv. Mat. Univ. Parma* **3**, (2012), 177–216.
  - P. Degond, 'Asymptotic-preserving schemes for fluid models of plasmas', *Panoramas et Syntheses*, (2014).