Numerical methods for multiscale kinetic equations: asymptotic-preserving and hybrid methods

Lecture 3: Asymptotic-preserving schemes (Part II)

Lorenzo Pareschi

Department of Mathematics and Computer Science
University of Ferrara, Italy

http://www.lorenzopareschi.com

Beijing Computational Science Research Center, June 7-10, 2017

Lecture 3 Outline

1. AP schemes for Boltzmann equations
   - Penalized IMEX-RK schemes
   - Penalized IMEX-LM schemes
2. Exponential schemes
   - Exponential schemes for homogeneous equations
   - Extension to non homogeneous problems
3. The Navier-Stokes regime
   - Navier-Stokes asymptotics of IMEX-LM
   - Navier-Stokes asymptotics of IMEX-RK
4. Multiple scalings
   - The unified IMEX approach
   - A numerical example
5. Final considerations

Kinetic equations in the fluid-dynamic scaling

The density $f = f(x,v,t) \geq 0$ of particles follows

Kinetic model

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

where $\varepsilon > 0$ (*Knudsen number*) is proportional to the mean free path.
The collision operator satisfies local conservation properties

$$\int_{\mathbb{R}^{d_v}} Q(f)\phi(v)\, dv =: \langle Q(f)\phi \rangle = 0,$$

where $\phi(v) = (1, v, |v|^2/2)^T$ are the *collision invariants* and the entropy inequality

$$\langle Q(f) \log(f) \rangle \leq 0.$$

From this we get $Q(f) = 0 \Leftrightarrow f = M[f]$ where

$$M[f](v) = \frac{\rho}{(2\pi T)^{3/2}} \exp\left(-\frac{|u-v|^2}{2T} \right),$$

$$(\rho, \rho u, E)^T = \langle f\phi \rangle, \quad T = \frac{1}{3\rho}(E - \rho|u|^2).$$

Hydrodynamic equations

Integrating the kinetic equation against the collision invariants we get

$$\partial_t \langle f\phi \rangle + \langle v \cdot \nabla_x f\phi \rangle = 0,$$

corresponding to conservation of mass, momentum and energy. The differential system is *not closed* since it involves higher order moments of the function f. As $\varepsilon \to 0$ formally $Q(f) = 0$ implies $f = M[f]$ and we get the closed system [1]

Compressible Euler equations

$$\partial_t U + \mathrm{div}_x \mathcal{F}(U) = 0$$

$$U = \langle M[f]\phi \rangle = (\rho, \rho u, E)^T$$

$$\mathcal{F}(U) = \langle v \otimes \phi M[f] \rangle = \begin{pmatrix} \rho u \\ \rho u \otimes u + pI \\ Eu + pu \end{pmatrix}, \; p = \rho T, \; T = \frac{1}{3}\left(\frac{2E}{\rho} - |u|^2\right).$$

▷ The result is independent on the particular choice of $Q(f)$ provided it admits Maxwellian as local equilibrium functions.

[1] R. Caflisch '80

Hydrodynamic equations II

For small but non zero values of the Knudsen number, the evolution equation for the moments can be derived by the so-called *Chapman-Enskog expansion*. This originates the compressible Navier-Stokes equations as a second order approximation with respect to ε to the solution of the Boltzmann equation[2]

Compressible Navier-Stokes equations

$$\partial_t U + \mathrm{div}_x \mathcal{F}(U) = \varepsilon\, \mathrm{div}_x \mathcal{D}(\nabla_x U)$$

$$\mathcal{D}(\nabla_x U) = \begin{pmatrix} 0 \\ \nu\sigma(u) \\ \kappa\nabla_x T + \nu\sigma(u)\cdot u \end{pmatrix}, \ \sigma(u) = \frac{1}{2}\left(\nabla_x u + (\nabla_x u)^T - \frac{2}{3}\mathrm{div}_x u I\right),$$

and the viscosity ν and the thermal conductivity κ are defined according to the linearized Boltzmann operator. The *Prandtl number* is the ratio $Pr = 5\nu/(2\kappa)$.

▷ The choice of the collision operator $Q(f)$ influences the structure of the Navier-Stokes system in terms of the Prandtl number.

[2] F. Golse '05

Penalized IMEX methods in the Boltzmann case

- The goal is to construct AP schemes *avoiding the implicit solution* of the collision term of the Boltzmann equation[3].
- The main idea is to use the fact that when ε is small we do not really need to resolve the whole collision operator since we know that $f \approx M[f]$.
- When $f \approx M[f]$ the collision operator is well approximated by its linear counterpart or directly by a BGK relaxation operator.
- If we denote by $Q_P(f)$ the linear approximating operator we can write

Penalized setting

$$Q(f) = \underbrace{G_P(f)}_{explicit} + \underbrace{Q_P(f)}_{implicit}, \quad G_P(f) = Q(f) - Q_P(f).$$

▶ The penalized IMEX methods are implicit in the linear part $Q_P(f)$ and explicit in the deviations from equilibrium $G_P(f)$.

[3] E. Gabetta, L. P., G. Toscani '97, S. Jin, F. Filbet '11, G. Dimarco, L. P. '13

Penalized IMEX-RK schemes

We assume $Q_P(f) = \mu(M[f] - f)$, $\mu > 0$ and denote $L(f) = v \cdot \nabla_x f$.
In vector form, the penalized IMEX-RK scheme reads

Penalized IMEX-RK for Boltzmann

$$F = f^n\, e + \Delta t\, \tilde{A} \left(\frac{1}{\varepsilon} G_P(F) - L(F) \right) + \frac{\Delta t}{\varepsilon}\, A Q_P(F)$$

$$f^{n+1} = f^n + \Delta t\, \tilde{w}^T \left(\frac{1}{\varepsilon} G_P(F) - L(F) \right) + \frac{\Delta t}{\varepsilon}\, w^T Q_P(F),$$

where $F = (F^{(1)}, \dots, F^{(\nu)})^T$.

- Clearly the scheme being implicit only in the linear part, which can be easily inverted and computed, can be *implemented explicitly*.
- Again, since the problem is stiff as a whole, the hope is that we can still find conditions for the AP property.
- In the penalized case, the *globally stiffly accurate* property, is required to have a stable AP scheme. It corresponds to have $\tilde{w}_j = \tilde{a}_{\nu j}$ and $w_j = a_{\nu j}$, $j = 1, \dots, \nu$ which implies $f^{n+1} = F^{(\nu)}$.

AP-property

First let us point out that we have the same associated *moment scheme* characterized by $(\tilde{A}, \tilde{w})$ of the explicit method

$$\langle F\phi\rangle = \langle f^n\phi\rangle\, e - \Delta t\, \tilde{A}\langle L(F)\phi\rangle$$
$$\langle f^{n+1}\phi\rangle = \langle f^n\phi\rangle - \Delta t\, \tilde{w}^T\langle L(F)\phi\rangle.$$

Consider now an invertible matrix A and solve the IMEX scheme for $Q_P(F)$

$$Q_P(F) = \frac{\varepsilon}{\Delta t}A^{-1}\left[F - f^n\, e + \Delta t\tilde{A}\left(L(F) - \frac{1}{\varepsilon}G_P(F)\right)\right]$$

As $\varepsilon \to 0$ we get

$$Q_P(F^{(i)}) = 0 \quad \Rightarrow \quad F^{(i)} = M[F^{(i)}], \quad i = 1, \ldots, \nu.$$

In fact $\widetilde{A}$ is lower triangular with $\widetilde{a}_{ii} = 0$ and we have a hierarchy of equations

$$G_P(F^{(i)}) = Q(F^{(i)}) - Q_P(F^{(i)}) = 0, \quad i = 1, .., \nu.$$

Further requirements

Now the last level still depends on ε. After some manipulations it reads

$$f^{n+1} \quad = \quad f^n \left(1 - w^T A^{-1} e\right) + \Delta t \left(w^T A^{-1} \tilde{A} - \tilde{w}^T\right) \left(L(F) - \frac{1}{\varepsilon} G_P(F)\right) + w^T A^{-1} F.$$

For small values of ε the scheme turns out to be unstable since f^{n+1} is not bounded.
A remedy, is to consider *globally stiffly accurate schemes* for which $f^{n+1} = F^{(\nu)}$. This is guaranteed if

$$\tilde{w}^T = w^T A^{-1} \tilde{A}, \quad w^T A^{-1} = e_\nu^T, \quad e_\nu^T = (0, \ldots, 1),$$

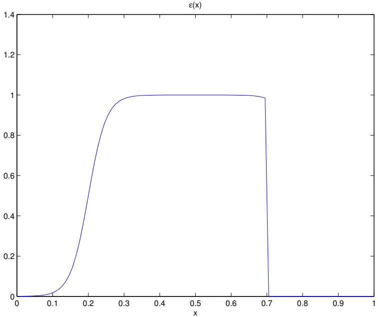
which implies $\tilde{w}_j = \tilde{a}_{\nu j}$ and $w_j = a_{\nu j}$, $j = 1, \ldots, \nu$.
So as $\varepsilon \to 0$ we get

$$F^{(\nu)} = M[F^{(\nu)}] \Rightarrow f^{n+1} = M[f^{n+1}].$$

- In the penalized case, the stiffly accurate property is required to have a stable AP scheme.

Mixing regimes problem

Collision term approximated by the *Fast Fourier-Galerkin method* [4]. Second and third order *WENO* is used in space [5]



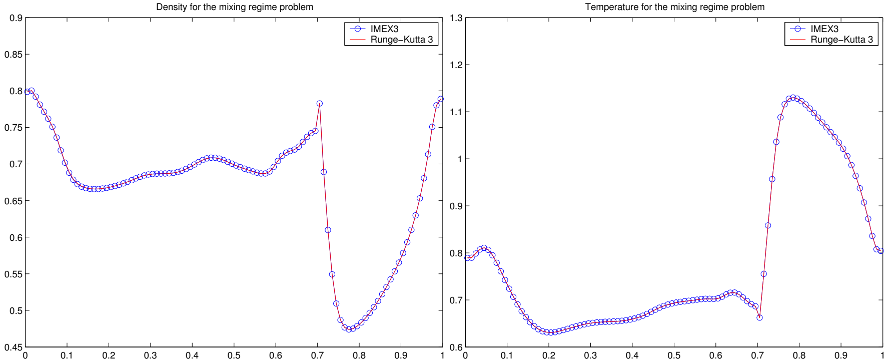
Knudsen number value for the mixed regime test with $\varepsilon_0 = 10^{-4}$

$$\begin{cases} \varepsilon = \varepsilon_0 + \frac{1}{2}(\tanh(16 - 20x) + \tanh(-4 + 20x)), & x \leq 0.7 \\ \varepsilon = \varepsilon_0, & x > 0.7 \end{cases}$$

[4] L.P., B.Perthame '96, C.Mouhot, L.P. '06

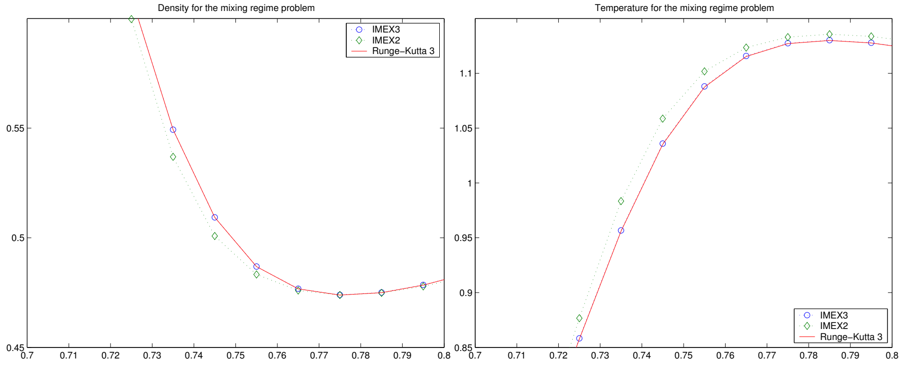
[5] C-W. Shu '97

Mixing regimes: third order scheme



Density (left) and temperature (right) profiles for the mixing regime problem. Time $t = 0.5$, $N_x = 100$ using third order WENO. Reference solution computed using a third order Runge-Kutta. Here $\Delta t_{IMEX}/\Delta t_{RK} = 7$.

Mixing regimes: second vs third order



Density (left) and temperature (right) profiles for the mixing regime problem at $t = 0.5$ for $x \in [0.7, 0.8]$.

Penalized IMEX-LM schemes

In the penalized setting, using vector notations, an IMEX-LM scheme reads

Penalized IMEX-LM for Boltzmann

$$f^{n+1} = -a^T \cdot F + \Delta t b^T \cdot \left(\frac{1}{\varepsilon} G_P(F) - L(F) \right) + \frac{\Delta t}{\varepsilon} c^T \cdot Q_P(F) + \frac{\Delta t}{\varepsilon} c_{-1} Q_P(f^{n+1}),$$

where $F = (f^n, \dots, f^{n-\nu+1})^T$.

- The scheme is implicit only in the penalization term $Q_P(f)$, therefore it can be *implemented explicitly*.
- To avoid a fully implicit solver we are integrating explicitly the stiff term $G_p(f)/\varepsilon$, a particular care is then needed to avoid instabilities.
- To satisfy the AP property, at variance with the non penalized case, also IMEX-BDF schemes require the initial vector to be *well-prepared*.

AP property

Taking the moment system of the penalized IMEX-LM scheme we obtain the explicit multistep method

$$\langle \phi f^{n+1} \rangle = -a^T \langle \phi F \rangle - \Delta t\, b^T \langle \phi L(F) \rangle.$$

Now we can write the penalized IMEX-LM scheme in the form

$$\varepsilon f^{n+1} = -\varepsilon a^T \cdot F + \Delta t\, b^T \cdot (G_P(F) - \varepsilon L(F)) + \Delta t\, c^T \cdot Q_P(F) + \Delta t\, c_{-1} Q_P(f^{n+1}),$$

which as $\varepsilon \to 0$ yields

$$0 = b^T \cdot G_P(F) + c^T \cdot Q_P(F) + c_{-1} Q_P(f^{n+1}).$$

If the initial steps are well prepared, as $\varepsilon \to 0$ we get $F = M[F]$ which implies $Q_P(F) \equiv 0$, $G_P(F) \equiv 0$ and therefore since $c_{-1} \neq 0$ we have

$$Q(f^{n+1}) = 0 \quad \Rightarrow \quad f^{n+1} = M[f^{n+1}].$$

Thus we have the explicit multistep method for the Euler equations.
▷ Note that, at variance with the non penalized case, also IMEX-BDF schemes require the initial vector to be well-prepared.

Accuracy test

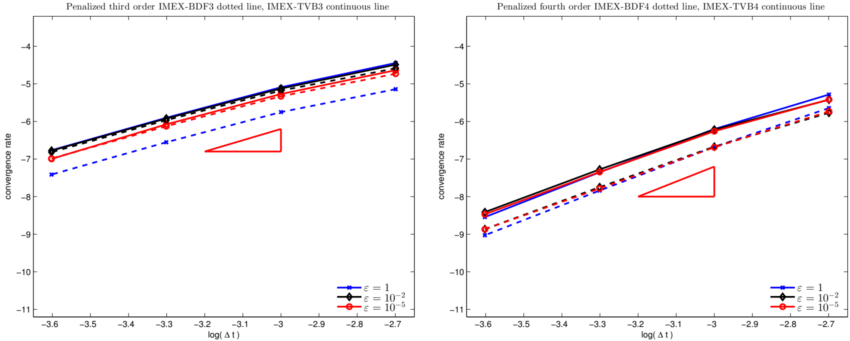


Figure: L_1 error for the density ρ. Left IMEX-BDF3 and IMEX-TVB3, Right IMEX-BDF4 and IMEX-TVB4.

Stability

- High order IMEX-LM methods are very sensitive to the choice of the penalization factor and may lead to instabilities unless the eigenvalues of the stiff part are estimated with enough accuracy.

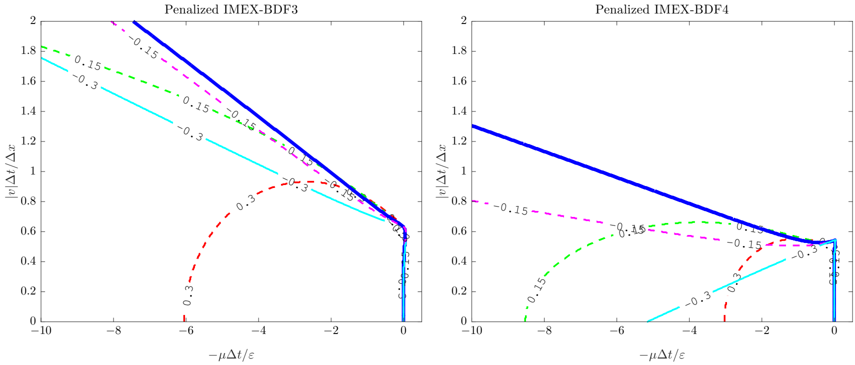


Figure: Stability regions in the BGK model for various relative errors in the penalization parameter. Left IMEX-BDF3, Right IMEX-BDF4.

Exponential schemes for homogeneous equations

For positivity a more robust approach is based on the exact integration of the penalization term which permits to write the homogeneous equation as

$$\frac{\partial}{\partial t}\left[(f - M[f])e^{\frac{\mu t}{\varepsilon}}\right] = \frac{1}{\varepsilon}G(f)e^{\frac{\mu t}{\varepsilon}} = \frac{1}{\varepsilon}(P(f,f) - \mu M[f])e^{\frac{\mu t}{\varepsilon}}.$$

Taking a truncated Taylor expansion along $\tau = 1 - e^{-\frac{\mu t}{\varepsilon}}$ and using the bilinearity of $P(f,f)$ we derive a class of unconditionally positive schemes of order m as[6]

Time relaxed methods

$$f^{n+1} = e^{-\mu\frac{\Delta t}{\varepsilon}} f^n + e^{-\mu\frac{\Delta t}{\varepsilon}} \sum_{k=0}^{m} (1 - e^{-\mu\frac{\Delta t}{\varepsilon}})^k f_k^n + (1 - e^{-\mu\frac{\Delta t}{\varepsilon}})^{m+1} M[f^n],$$

where the functions f_k are given by the recurrence formula

$$f_{k+1}(v) = \frac{1}{k+1}\sum_{h=0}^{k}\frac{1}{\mu}P(f_h, f_{k-h})(v), \quad k = 0, 1, \dots.$$

[6] E.Gabetta, L.P., G.Toscani '97

AP Exponential Runge-Kutta methods

A different approach consist in taking an explicit Runge-Kutta discretization with $\nu \geq m$ stages of the transformed problem and then reverting back to the original variables [7]

Exponential Runge-Kutta

$$\begin{aligned} F^{(i)} &= e^{-c_i\mu\frac{\Delta t}{\varepsilon}}f^n + (1 - e^{-c_i\mu\frac{\Delta t}{\varepsilon}})M[f^n] + \Delta t \sum_{j=1}^{i-1} A_{ij}\left(\mu\frac{\Delta t}{\varepsilon}\right) G(F^{(j)}), \\ f^{n+1} &= e^{-\mu\frac{\Delta t}{\varepsilon}}f^n + (1 - e^{-\mu\frac{\Delta t}{\varepsilon}})M[f^n] + \Delta t \sum_{i=1}^{\nu} W_i\left(\mu\frac{\Delta t}{\varepsilon}\right) G(F^{(i)}), \end{aligned}$$

where $c_i \geq 0$, and the coefficients A_{ij} and the weights W_i are

$$\begin{aligned} A_{ij}\left(\mu\frac{\Delta t}{\varepsilon}\right) &= a_{ij}e^{-(c_i - c_j)\mu\frac{\Delta t}{\varepsilon}}, \quad i,j = 1,\ldots,\nu, \quad j > i \\ W_i\left(\mu\frac{\Delta t}{\varepsilon}\right) &= w_i e^{-(1-c_i)\mu\frac{\Delta t}{\varepsilon}}, \quad i = 1,\ldots,\nu. \end{aligned}$$

- Unconditionally positive schemes can be constructed up to fourth order.

[7] G.Dimarco, L.P. '11, S.Maset, M.Zennaro '09

Extension to non homogeneous problems

Let us now consider the non homogeneous case and compute

$$
\begin{aligned}
& \partial_t \left[(f - M) e^{\mu t/\varepsilon} \right] \\
= \;& \partial_t (f - M) e^{\mu t/\varepsilon} + (f - M) \frac{\mu}{\varepsilon} e^{\mu t/\varepsilon} \\
= \;& \left[\frac{1}{\varepsilon}(Q + \mu f - \mu M) - \partial_t M - v \cdot \nabla_x f \right] e^{\mu t/\varepsilon} \\
= \;& \left[\frac{1}{\varepsilon}(P - \mu M) \underbrace{- \partial_t M - v \cdot \nabla_x f}_{\text{new terms}} \right] e^{\mu t/\varepsilon}.
\end{aligned}
$$

Note that the equation above is equivalent to the original Boltzmann equation even when M is not the local Maxwellian.
In the simplified case of the BGK collision operator $Q = \mu(M - f)$, where M is the local Maxwellian, the problem reformulation just described applies with $P = \mu M$ and the first term on the RHS vanishes.

AP exponential Runge-Kutta

Thus we have the following scheme[8]

Exponential Runge-Kutta non homogeneous case

Step i:

$$
\begin{aligned}
&(F^{(i)} - M^{(i)})e^{c_i \mu \frac{\Delta t}{\varepsilon}} \\
=\ & (f^n - M^n) + \sum_{j=1}^{i-1} a_{ij} \frac{\Delta t}{\varepsilon} \left[P^{(j)} - \mu M^{(j)} - \varepsilon v \cdot \nabla_x F^{(j)} - \varepsilon \partial_t M^{(j)} \right] e^{c_j \mu \frac{\Delta t}{\varepsilon}},
\end{aligned}
$$

Final Step:

$$
\begin{aligned}
&(f^{n+1} - M^{n+1})e^{\mu \frac{\Delta t}{\varepsilon}} \\
=\ & (f^n - M^n) + \sum_{i=1}^{\nu} w_i \frac{\Delta t}{\varepsilon} \left[P^{(i)} - \mu M^{(i)} - \varepsilon v \cdot \nabla_x F^{(i)} - \varepsilon \partial_t M^{(i)} \right] e^{c_i \mu \frac{\Delta t}{\varepsilon}}.
\end{aligned}
$$

- How to compute $M^{(j)}$ and $\partial_t M^{(j)}$, $j = 1, \ldots, \nu$?

[8] Q.Li, L.P. '13

Computation of $M^{(j)}$ and $\partial_t M^{(j)}$

- The computation of $M^{(j)}$ follows from the associated moment scheme which gives an explicit Runge-Kutta method applied to the moment equations.
- To compute $\partial_t M^{(j)}$ in d-dimension use relations

$$\partial_t M^{(j)} = \partial_\rho M^{(j)} \partial_t \rho^{(j)} + \nabla_u M^{(j)} \cdot \partial_t u^{(j)} + \partial_T M^{(j)} \partial_t T^{(j)},$$

with

$$\partial_\rho M^{(j)} = \frac{M^{(j)}}{\rho^{(j)}}, \quad \nabla_u M^{(j)} = M^{(j)} \frac{v - u^{(j)}}{T^{(j)}}, \quad \partial_T M^{(j)} = M^{(j)} \left[\frac{(v - u^{(j)})^2}{2(T^{(j)})^2} - \frac{d}{2T^{(j)}} \right].$$

Then substitute

$$\begin{aligned}
\partial_t \rho^{(j)} &= -\int v \cdot \nabla_x F^{(j)} dv, \\
\partial_t u^{(j)} &= \frac{1}{\rho^{(j)}} \left(u^{(j)} \int v \cdot \nabla_x F^{(j)} dv - \int v \otimes v \cdot \nabla_x F^{(j)} dv \right), \\
\partial_t T^{(j)} &= \frac{1}{d\rho^{(j)}} \left(-\frac{2E^{(j)}}{\rho^{(j)}} \partial_t \rho^{(j)} - 2\rho^{(j)} u^{(j)} \partial_t u^{(j)} - \int v^2 v \cdot \nabla_x F^{(j)} dv \right).
\end{aligned}$$

Properties

At variance with IMEX RK thanks to the positivity of the coefficients using the Shu-Osher [9] representation of Runge-Kutta methods it is possible to prove

Theorem

There exist $h_* > 0$ *and* $\mu_* > 0$ *such that* $f^{n+1} \geq 0$ *provided that* $f^n \geq 0$, $\mu \geq \mu_*$ *and* $0 < h \leq h_*$.

In addition the same AP-property as for the homogeneous schemes is obtained

Theorem

The non homogeneous ExpRK-F method is AP and asymptotically accurate for general explicit Runge-Kutta method with $0 \leq c_1 \leq c_2 \leq \cdots \leq c_\nu < 1$.

Runge-Kutta methods that satisfy the above condition can be constructed up to fourth order.

[9] C-W.Shu, S.Osher '89

Convergence test

Initial data sum of two Maxwellians in space solved using WENO3-5[10] in space and the fast Fourier-Galerkin method[11] in velocity.

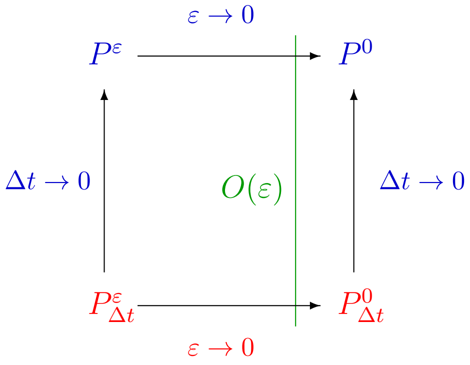
		Maxwellian Initial		*Non-Maxwellian Initial*	
$\varepsilon = 1$	ExpRK2	2.416	2.023	2.677	2.054
	ExpRK3	5.025	4.403	5.135	4.790
$\varepsilon = 0.1$	ExpRK2	2.414	2.022	2.566	2.058
	ExpRK3	5.022	4.396	5.138	4.792
$\varepsilon = 10^{-3}$	ExpRK2	2.023	1.859	1.474	1.754
	ExpRK3	3.868	3.032	2.591	2.803
$\varepsilon = 10^{-6}$	ExpRK2	2.561	2.045	2.563	2.048
	ExpRK3	5.088	4.567	4.919	3.806

Convergence rates for ExpRK methods with different initial data, in different regimes.

[10] C-W.Shu '97

[11] C.Mouhot, L.P. '06

The Navier-Stokes regime



Most of the results in the literature refer to low order methods and the AP property. Here we will focus on high order methods and their behavior in the more difficult case of the $O(\varepsilon)$ term, corresponding to a consistency condition with the *compressible Navier-Stokes limit*.

Navier-Stokes asymptotics of IMEX-LM

In order to do this we consider the simplified case of the *BGK model*, $Q(f) = (M[f] - f)$, and *IMEX-BDF* schemes. We rewrite the IMEX-BDF scheme as

$$\frac{f^{n+1} + a^T \cdot F}{\Delta t} + b^T \cdot L(F) = \frac{1}{\varepsilon} c_{-1}(M[f^{n+1}] - f^{n+1}).$$

Next, we consider the *Chapman-Enskog expansion* taking

$$f^{n+1} = M[f^{n+1}] + \varepsilon g^{n+1}, \quad F = M[F] + \varepsilon G,$$

where $\langle \phi g^{n+1} \rangle = 0$ and $\langle \phi G \rangle \equiv 0$ with $G = (g^n, \ldots, g^{n-s+1})^T$.
Inserting the above expansions in the numerical method yields

$$\begin{aligned}\frac{M[f^{n+1}] + a^T \cdot M[F]}{\Delta t} &+ b^T \cdot L(M[F]) \\ &+ \varepsilon \left(\frac{g^{n+1} + a^T \cdot G}{\Delta t} + b^T \cdot L(G) \right) = -c_{-1} g^{n+1}.\end{aligned}$$

Navier-Stokes asymptotics

Consistency with the *Navier-Stokes* equations is obtained if the vector of initial steps satisfies [12] for $j = 0, \ldots, s-1$

$$\langle \phi\, L(g^{n-j}) \rangle \;=\; -\left\langle \phi\, L\left(\left(\frac{\partial M[f]}{\partial t} + L(M[f])\right)\right)\Big|_{t=t^{n-j}} \right\rangle + O(\varepsilon + \Delta t^q),\; q \geq 1.$$

In order for the scheme to be consistent with the Navier-Stokes limit in time it is crucial that at the next time step g^{n+1} satisfies a consistency relation as we assumed on g^n. From the scheme we have

$$g^{n+1} = -\frac{1}{c_{-1}}\left(\frac{M[f^{n+1}] + a^T \cdot M[F]}{\Delta t} + b^T \cdot L(M[F])\right) + O\left(\frac{\varepsilon}{\varepsilon + \mu^{n+1} c_{-1} \Delta t}\right).$$

Since by construction the IMEX-BDF coefficients are such that

$$\frac{1}{c_{-1}}\left(\frac{M[f^{n+1}] + a^T \cdot M[F]}{\Delta t} + b^T \cdot L(M[F])\right) = \left(\frac{\partial M[f]}{\partial t} + L(M[f])\right)\Big|_{t=t^{n+1}} + O(\Delta t^p)$$

we get the desired result.

[12] F. Bouchut, B. Perthame '93; F. Golse '05

Navier-Stokes asymptotics

More in general we can prove the following [13]

Theorem

If the vector of initial steps is well-prepared with respect to the Navier-Stokes limit, then, for small values of ε *and with* $\varepsilon\Delta t^q + \Delta t^p = o(\varepsilon)$, *the IMEX multistep scheme becomes the explicit multistep scheme for the Navier-Stokes system, with* $q = p$ *for the IMEX-BDF methods and* $q = 1$ *for the other IMEX multistep methods.*

- The result shows that the schemes are capable, in principle, to capture the Navier-Stokes asymptotics without resolving the small scale ε.
- The analysis just performed can be carried on in a similar way also for the full *Boltzmann equation*. The conclusions one obtains for the various IMEX multistep schemes are exactly the same as for the BGK model.

[13] G. Dimarco, L. P. '16

Convergence rates: IMEX-LM for BGK model

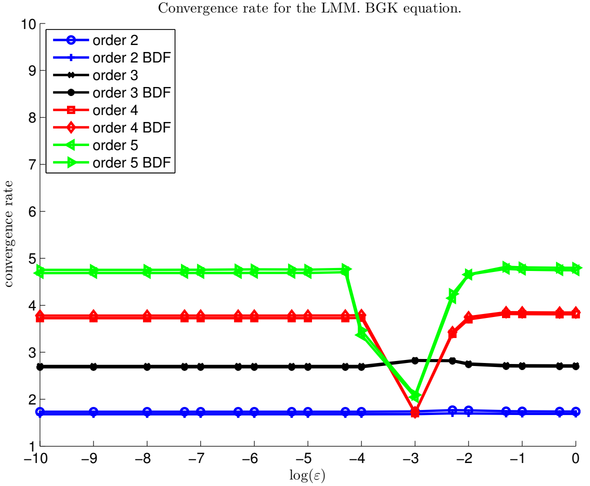


Figure: Convergence rates for the L_1 error for the density ρ in the BGK model.

The $O(\varepsilon)$ behavior

To illustrate this we consider the *Jin-Xin model* in the linear case $f(u) = bu$

$$\begin{cases} \partial_t u + \partial_x v &= 0 \\ \partial_t v + a^2 \partial_x u &= -\dfrac{1}{\varepsilon}(v - bu), \end{cases}$$

which at $O(\varepsilon)$ yields $v = bu - \varepsilon(a^2 - b^2)\partial_x u$, and then for $a^2 > b^2$

$$\partial_t u + b\partial_x u = \varepsilon(a^2 - b^2)\partial_{xx} u.$$

In vector form a general IMEX scheme for the system above can be written as

$$\begin{aligned} \mathbf{u} &= u^n e - \Delta t \tilde{A}\, \partial_x \mathbf{v} \\ \mathbf{v} &= v^n e - \Delta t \tilde{A} a^2 \partial_x \mathbf{u} - \Delta t A \frac{1}{\varepsilon}(\mathbf{v} - b\mathbf{u}) \\ u^{n+1} &= u^n - \Delta t \tilde{w}^T \partial_x \mathbf{v}, \\ v^{n+1} &= v^n - \Delta t \tilde{w}^T a^2 \partial_x \mathbf{u} - \Delta t w^T \frac{1}{\varepsilon}(\mathbf{v} - b\mathbf{u}). \end{aligned}$$

The $O(\varepsilon)$ behavior

Similarly to the continuos case we now consider the initial data well-prepared $v^n = bu^n + \varepsilon v_1^n$ and expand

$$\mathbf{v} = b\mathbf{u} + \varepsilon \mathbf{v}_1.$$

Using this we can compute from the IMEX-RK scheme

$$\mathbf{v}_1 = A^{-1}\tilde{A}\left(b^2 - a^2\right)\mathbf{u}_x + O(\varepsilon).$$

We therefore obtain the following Runge-Kutta scheme for the $O(\varepsilon)$ limit

$$\begin{aligned} \mathbf{u} &= u^n e - \Delta t \tilde{A}\, b\partial_x \mathbf{u} + \varepsilon \Delta t \tilde{A} A^{-1}\tilde{A}\left(a^2 - b^2\right)\partial_{xx}\mathbf{u} \\ u^{n+1} &= u^n - \Delta t \tilde{w}^T b\partial_x \mathbf{u} + \varepsilon \Delta t \tilde{w}^T A^{-1}\tilde{A}\left(a^2 - b^2\right)\partial_{xx}\mathbf{u}. \end{aligned}$$

The above scheme represents an *additive Runge-Kutta method* for the $O(\varepsilon)$ limit based on the coefficient matrices $\tilde{A}$, $\tilde{A}A^{-1}\tilde{A}$ and the weights $\tilde{w}^T$, $\tilde{w}^T A^{-1}\tilde{A}$.

- The explicit additive Runge-Kutta method for the $O(\varepsilon)$ limit should satisfy suitable additional *order conditions* [14].

[14] S.Boscarino, L.P. '16

Convergence rates: IMEX-RK for BGK model

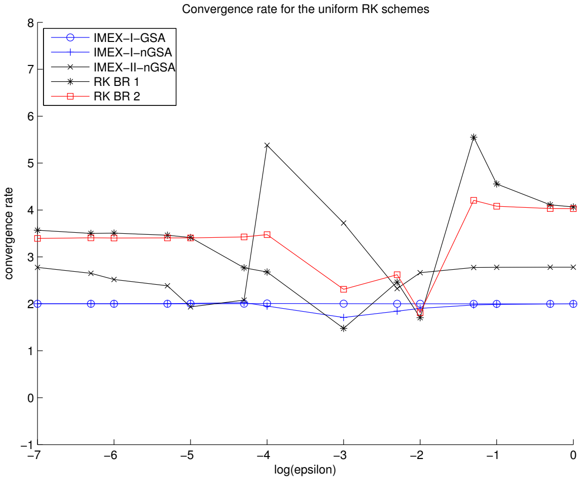


Figure: Convergence rates for the L_1 error for the density ρ in the BGK model.

Multiple scalings

Prototype hyperbolic system of balance laws with multiple scalings

Hyperbolic balance laws with multiple scalings

$$\begin{cases} \partial_t u + \partial_x v = 0, \\ \partial_t v + \dfrac{1}{\varepsilon^{2\alpha}} \partial_x p(u) = -\dfrac{1}{\varepsilon^{1+\alpha}} \left(v - f(u)\right), \quad \alpha \in [0,1]. \end{cases}$$

System has characteristics speeds $\pm\sqrt{p'(u)}/\varepsilon^{\alpha}$, $p'(u) > 0$. It corresponds to the scaling : $t \to t/\varepsilon^{1+\alpha}$, $x \to x/\varepsilon^{\alpha}$. For small values of ε we have

$$v = f(u) - \varepsilon^{1-\alpha} \partial_x p(u) + O(\varepsilon^{1+\alpha})$$

and using the first equation

$$\partial_t u + \partial_x f(u) = \varepsilon^{1-\alpha} \partial_{xx} p(u) + O(\varepsilon^{1+\alpha}).$$

The above space-time scaling for $\alpha = 0$ corresponds to the *compressible Euler limit*, for $\alpha \in (0,1)$ to the *incompressible Euler limit*, whereas for $\alpha = 1$ to the *incompressible Navier-Stokes limit* is obtained[15].

[15] C. Cercignani, R. Illner, M. Pulvirenti '94

A standard IMEX approach

Using the standard IMEX Euler approach we obtain

Standard IMEX Euler

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\Delta t} + \partial_x v^n = 0, \\ \dfrac{v^{n+1}-v^n}{\Delta t} + \dfrac{1}{\varepsilon^{2\alpha}} \partial_x p(u^n) = -\dfrac{1}{\varepsilon^{1+\alpha}} \left(v^{n+1} - f(u^{n+1}) \right), \quad \alpha \in [0,1]. \end{cases}$$

For small values of ε we get for $\alpha > 0$

$$v^{n+1} = f(u^{n+1}) - \varepsilon^{1-\alpha} \partial_x p(u^n) + O(\varepsilon^{1+\alpha})$$

and therefore using the first equation we have the explicit three time level scheme

$$\frac{u^{n+1}-u^n}{\Delta t} + \partial_x f(u^n) = \varepsilon^{1-\alpha} \partial_{xx} p(u^{n-1}) + O(\varepsilon^{1+\alpha})$$

Questions: Can we obtain a standard two time level method which avoids the parabolic stiffness? How can we deal with the indefinite grow of the characteristic speeds?

The unified IMEX approach

We introduce a different IMEX Euler approach [16]

Unified IMEX Euler

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\Delta t} + \partial_x v^{n+1} = 0, \\ \dfrac{v^{n+1}-v^n}{\Delta t} + \dfrac{1}{\varepsilon^{2\alpha}}\partial_x p(u^{n+1}) = -\dfrac{1}{\varepsilon^{1+\alpha}}\left(v^{n+1} - f(u^n)\right), \quad \alpha \in [0,1]. \end{cases}$$

We can rewrite the above scheme in the equivalent form

Reformulated unified IMEX Euler

$$\begin{cases} \dfrac{u^{n+1}-u^n}{\Delta t} + \dfrac{\varepsilon^{1+\alpha}}{\varepsilon^{1+\alpha}+\Delta t}\partial_x v^n + \dfrac{\Delta t}{\varepsilon^{1+\alpha}+\Delta t}\partial_x f(u^n) = \dfrac{\Delta t \varepsilon^{1-\alpha}}{\varepsilon^{1+\alpha}+\Delta t}\partial_{xx} p(u^{n+1}), \\ \dfrac{v^{n+1}-v^n}{\Delta t} + \dfrac{1}{\varepsilon^{1+\alpha}+\Delta t}\partial_x p(u^n) = -\dfrac{1}{\varepsilon^{1+\alpha}+\Delta t}\left(v^n - f(u^n)\right). \end{cases}$$

[16] S. Boscarino, L.P., G. Russo '17

The unified IMEX approach

Now, up to $O(\Delta t)$ the left hand side corresponds to an hyperbolic system with characteristic speeds

$$\lambda_{\pm}^{\alpha}(\Delta t, \varepsilon) = \frac{\xi_\alpha}{2}\left(c \pm \sqrt{c^2 + \frac{4\varepsilon^{1+\alpha}}{(\Delta t)^2}}\right),$$

with $\xi_\alpha = \Delta t/(\varepsilon^{1+\alpha} + \Delta t) \in [0,1]$, $c = f'(u)$ and for simplicity we have set $p'(u) = 1$.

We now observe that the characteristic speed do not diverge as $\varepsilon \to 0$ since we have

$$\lambda_{\pm}^{\alpha}(\Delta t, 0) = \frac{1}{2}(c \pm |c|).$$

On the othe hand, if we fix ε and send $\Delta t \to 0$ we obtain the usual characteristic speeds

$$\lambda_{\pm}^{\alpha}(0, \varepsilon) = \pm\frac{1}{\varepsilon^{\alpha}}.$$

Remark: A similar analysis can be carried out for higher order IMEX methods. The GSA property is essential to obtain the correct behavior for all $\alpha \in [0,1]$.

A numerical example

We consider the nonlinear Ruijgrok-Wu model [17]

Standard IMEX Euler

$$\begin{cases} \partial_t \rho + \partial_x j = 0\,, \\ \partial_t j + \dfrac{1}{\varepsilon^{2\alpha}} \partial_x \rho = \dfrac{1}{\varepsilon^{1+\alpha}} \left\{ -j + \dfrac{1}{2}\left(\rho^2 - \varepsilon^2 j^{2\alpha}\right) \right\}. \end{cases}$$

For small values of ε and $\alpha > 1/3$ the model behaviour can be derived by the Chapman-Enskog expansion and is characterized by the viscous Burgers equation

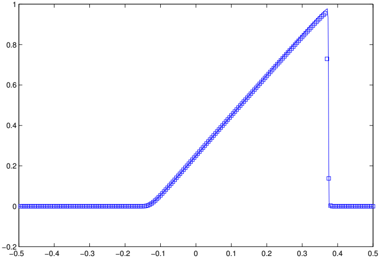
$$j = \frac{1}{2}\rho^2 - \varepsilon^{1-\alpha}\partial_x \rho + O(\varepsilon^{2\alpha})$$

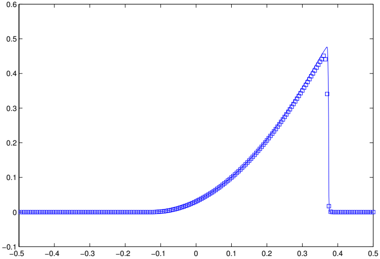
$$\partial_t \rho + \partial_x \left(\frac{\rho^2}{2}\right) = \varepsilon^{1-\alpha}\partial_{xx}\rho + O(\varepsilon^{2\alpha}).$$

[17] W.Ruijgrok, T.T.Wu '82

$\alpha = 0.5$

We use classical hyperbolic-type schemes, like WENO schemes, for the space derivatives characterized the hyperbolic part while for the second order term we used standard central differences.

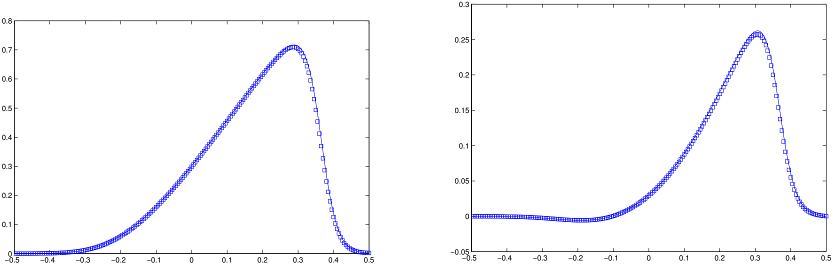




Third order IMEX. Propagation of a square wave at $t = 0.5$ for $\varepsilon = 10^{-8}$, $\Delta t = 0.8 \Delta x$, $\Delta x = 0.005$

$\alpha = 0.75$

We use classical hyperbolic-type schemes, like WENO schemes, for the space derivatives characterized the hyperbolic part while for the second order term we used standard central differences.



Third order IMEX. Propagation of a square wave at $t = 0.5$ for $\varepsilon = 10^{-8}$, $\Delta t = 0.8\Delta x$, $\Delta x = 0.005$

Final considerations

- *Penalization techniques* represent a powerful tool for the time discretization of the Boltzmann equation close to fluid regimes.
- *Penalized IMEX-LM schemes* have some advantages over the corresponding IMEX-RK methods. Easy to achieve high-order (up to order 5), greater efficiency in terms of computational cost, better uniform accuracy.
- *Penalized IMEX-RK schemes* on the other hand are easier to implement and have better stability properties, in particular in the penalized setting.
- *Exponential methods* are an interesting alternative to IMEX methods especially when nonnegativity of the solution is mandatory.
- Some recent references
  - G. Dimarco, L. Pareschi, SIAM J. Num. Anal. 2017
  - S. Boscarino, L. Pareschi, J. Comp. App. Math. 2017
  - S. Boscarino, L. Pareschi, G. Russo, SIAM J. Num. Anal (to appear)