Numerical methods for kinetic equations

Lecture 5: Asymptotic-preserving schemes

Lorenzo Pareschi

Department of Mathematics and Computer Science
University of Ferrara, Italy

http://www.lorenzopareschi.com

Imperial College, October 2-9, 2015

Lecture 5 Outline

Motivations

Many applications involve *multiscale differential problems*, like convection-diffusion systems

Convection-Diffusion Equations

$$\partial_t U + \partial_x F(U) = \partial_x (K(U)\partial_x U), \quad x \in \mathbb{R},$$

or hyperbolic balance laws with source terms of the form

Conservation Laws with Relaxation

$$\partial_t U + \partial_x F(U) = \frac{1}{\varepsilon} R(U), \quad x \in \mathbb{R},$$

where $U = U(x,t) \in \mathbb{R}^N$, and $\varepsilon > 0$ is called relaxation parameter. Several kinetic equations have the same structure with $U = F(U) = f(x,v,t) \geq 0$, $v \in \mathbb{R}$.

▶ The numerical discretization of such systems may be challenging in presence of multiple scales, typically when the diffusion or the source terms are stiff.

Numerical approaches

Method of lines (MOL) approach

- Discretize all spatial operators
- Obtain a system of ODEs

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

  with $\mathcal{F}$ non stiff and $\mathcal{G}$ a stiff term.
- Integrate ODEs system in time

Advantages

- Spatial discretization and time integration are treated separately
- Spatial discretization: easy to combine different schemes
- Time integration: free to choose suitable method (Runge-Kutta, multi-step, etc.)

Numerical approaches

Fully explicit methods

- Non stiff term: $\Delta t \leq \rho(\nabla_u F)\Delta x$ (CFL condition)
- Stiff term: $\Delta t \leq D^{-1}(\Delta x)^2$ or $\Delta t \leq C\varepsilon$.
  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[1].

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 [2].

[1] S.Gottlieb, C-W.Shu, E.Tadmor '01, R.Spiteri, S.Ruth, '02
[2] S.Jin '99

A toy example

Consider the *singularly perturbed problem*[3]

Singularly perturbed problem

$$P^\varepsilon : \begin{cases} u'(t) &= f(u,v), \\ \varepsilon v'(t) &= g(u,v), \qquad\qquad \varepsilon > 0. \end{cases}$$

As $\varepsilon \to 0$ we get the index 1 *differential algebraic equation* (DAE)

$$u'(t) = f(u,v), \qquad 0 = g(u,v).$$

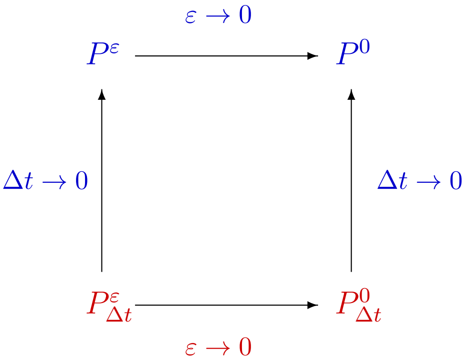
Assuming that $g(u,v) = 0 \Leftrightarrow v = E(u)$ we obtain

$$P^0 : \quad u'(t) = f(u, E(u)).$$

Explicit methods: restricted to $\Delta t \sim \varepsilon$.
Implicit methods: require the numerical inversion of $f(u,v)$ and $g(u,v)$, and as $\varepsilon \to 0$ must satisfy the algebraic condition $g(u,v) = 0 \Leftrightarrow v = E(u)$.

[3] E.Hairer, C.Lubich, M.Roche '89

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.

Space discretizations

Consider the case of the single hyperbolic equation

Conservation Law

$$U_t + \partial_x F(U) = 0.$$

- We can use any finite difference/volume or spectral method to approximate the spatial derivative, and use the standard (linear) stability analysis.
- In presence of shocks and discontinuities this stability analysis is not sufficient (nonlinear problems can develop discontinuous solutions in finite time even starting from a smooth solution).
- Build spatial discretizations which capture the shock structure and that satisfy some nonlinear stability properties. These methods include total variation diminishing (TVD) schemes and essentially non-oscillatory (ENO) or weighted ENO (WENO) schemes[4].

[4] A. Harten '87, T.Chan, X-D.Liu, S.Osher '94, G-S.Jang, C-W.Shu '95

Implicit-explicit methods

Splitting 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[5]

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.

[5] 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[6].

IMEX-RK	Number of coupling conditions			
Order	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

[6] 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 $\gamma = (1-\sqrt{2})/2$.

Application to hyperbolic relaxation systems

Consider the case of hyperbolic relaxation systems[7]

Hyperbolic system with relaxation (Full model)

$$\partial_t U + \partial_x F(U) = \frac{1}{\varepsilon} R(U), \quad x \in \mathbb{R}.$$

$R : \mathbb{R}^N \to \mathbb{R}^N$ is a relaxation operator if there exists a $n \times N$ matrix Q with rank$(Q) = n < N$ s.t. $QR(U) = 0 \quad \forall\, U \in \mathbb{R}^N$.
This gives n conserved quantities $u = QU$ that uniquely determine a local equilibrium $U = \mathcal{E}(u)$, s.t. $R(\mathcal{E}(u)) = 0$, and satisfy

$$\partial_t (QU) + \partial_x (QF(U)) = 0.$$

As $\varepsilon \to 0 \Rightarrow R(U) = 0 \Rightarrow U = \mathcal{E}(u) \Rightarrow$ (subcharacteristic condition on on $f(u)$)

Equilibrium system (Reduced model)

$$\partial_t u + \partial_x f(u) = 0, \qquad f(u) = QF(\mathcal{E}(u)).$$

[7] G.Chen, D.Levermore, T.P.Liu, '94

A simple example

A simple prototype example of relaxation system is given by[8]

Jin-Xin relaxation system

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

where $u = u(x,t)$, $v = v(x,t)$, $(x,t) \in \mathbb{R} \times \mathbb{R}_+$.
For small values of ε we get the local equilibrium

$$v = f(u)$$

and (subcharacteristic condition $a > f'(u)^2$) we obtain at $O(\varepsilon)$

$$\partial_t u + \partial_x f(u) = \varepsilon \partial_x ((a - f'(u)^2)\partial_x u).$$

[8] S.Jin, Z.Xin '95

AP schemes

Definition

An IMEX scheme for an hyperbolic system with relaxation is asymptotic preserving (AP) if in the limit $\epsilon \to 0$ the scheme becomes a consistent discretization of the limit system of conservation laws. We use the notation AP_k if the scheme is of order k in the limit $\epsilon \to 0$.

We can prove[9]

Theorem

If $\det A \neq 0$ *then in the limit* $\epsilon \to 0$*, the IMEX scheme applied to an hyperbolic system with relaxation becomes the explicit RK scheme characterized by* $(\tilde{A}, \tilde{w}, \tilde{c})$ *applied to the limit system of conservation laws.*

- The theorem guarantees that in the stiff limit the IMEX scheme becomes the explicit RK scheme applied to the equilibrium system.
- To satisfy $\det A \neq 0$ it is necessary that $c \neq \tilde{c}$. The corresponding scheme may be inaccurate if the initial condition is not "well prepared" (initial layer).

[9] L.P., G.Russo, '04

Stability

To study the A-stability of a IMEX-RK scheme, one may consider the problem[10]

Test problem

$$u' = \lambda u + \mu u, \quad u(0) = 1, \quad \lambda, \mu \in \mathbb{C}.$$

This test problem characterizes the stability properties also for linear systems

$$U' = AU + BU, \quad U(0) = U_0$$

with $U \in \mathbb{R}^m$, and $A, B \in \mathbb{R}^{m\times m}$ if A and B are normal, commuting matrices. In general the two matrices do not share the same eigenvectors, and can not be diagonalized simultaneously. This makes the stability analysis for systems extremely difficult. Only available results are for the case $m = 2$.

[10] L.P., G.Russo '00, L.P. G.Russo '08

Numerical examples

Broadwell model

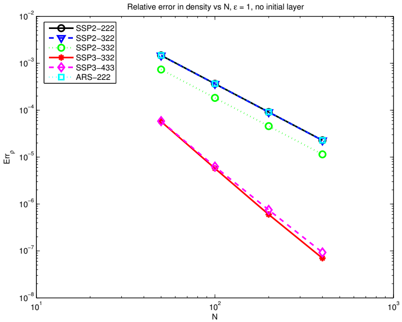
$$
\begin{aligned}
\partial_t \rho + \partial_x m &= 0, \\
\partial_t m + \partial_x z &= 0, \\
\partial_t z + \partial_x m &= \frac{1}{\varepsilon}(\rho^2 + m^2 - 2\rho z),
\end{aligned}
$$

with ε is the mean free path. The dynamical variables ρ and m are the density and the momentum respectively, while z represents the flux of momentum.
In the relaxation limit $\varepsilon \to 0$ we obtain

$$
\begin{aligned}
\partial_t \rho + \partial_x m &= 0 \\
\partial_t m + \frac{1}{2}\partial_x \left(\rho + \frac{m^2}{\rho}\right) &= 0
\end{aligned}
$$

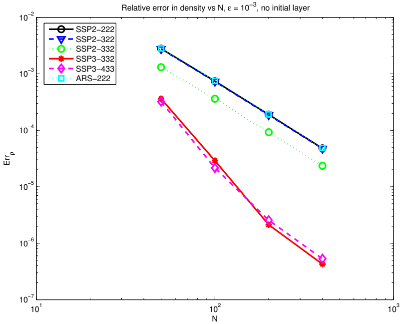
(1) Accuracy test for IMEX-RK schemes with smooth initial data and periodic b.c.
(2) Shock test for IMEX-RK schemes.

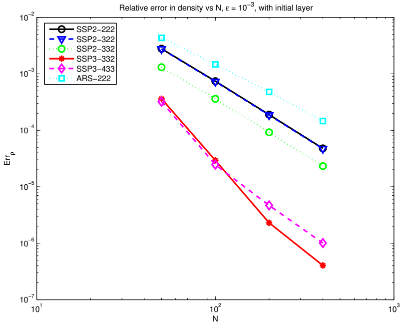
Convergence rates $\epsilon = 1$



Relative error for different second and third order IMEX-RK schemes for the Broadwell equations with $\epsilon = 1$. Left: no initial layer. Right: initial layer.

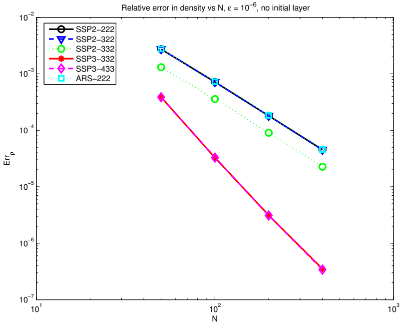
Convergence rates $\epsilon = 10^{-3}$

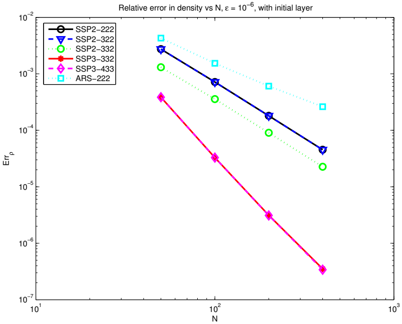




Relative error for different second and third order IMEX-RK schemes for the Broadwell equations with $\epsilon = 10^{-3}$. Left: no initial layer. Right: initial layer.

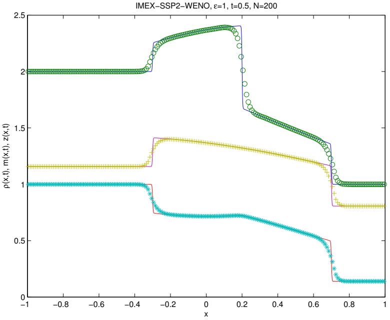
Convergence rates $\epsilon = 10^{-6}$

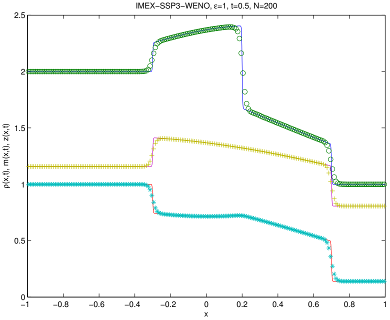




Relative error for different second and third order IMEX-RK schemes for the Broadwell equations with $\epsilon = 10^{-6}$. Left: no initial layer. Right: initial layer.

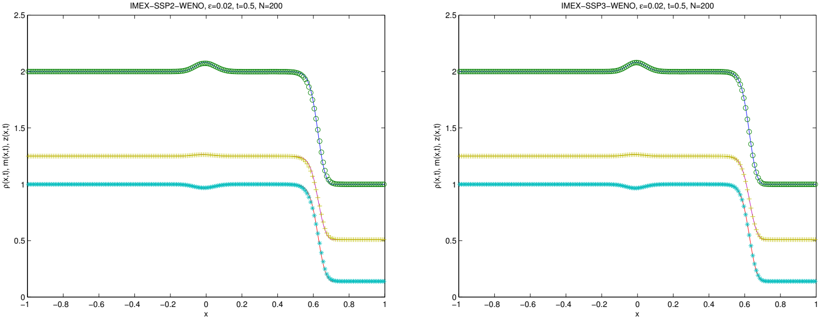
Shock test $\epsilon = 1$





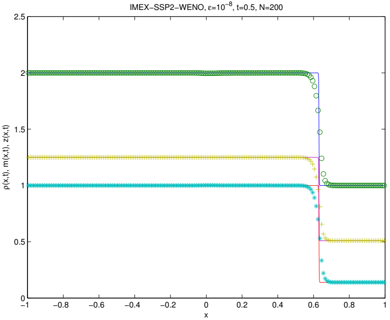
Numerical solution for second and third order SSP IMEX-RK schemes for the Broadwell equations with $\epsilon = 1$

Shock test $\epsilon = 10^{-3}$



Numerical solution for second and third order SSP IMEX-RK schemes for the Broadwell equations with $\epsilon = 10^{-3}$

Shock test $\epsilon = 10^{-6}$



Numerical solution for second and third order SSP IMEX-RK schemes for the Broadwell equations with $\epsilon = 10^{-6}$

Design principles for kinetic equations

- AP schemes *avoiding the implicit solution* of the collision term $Q(f,f)$

Boltzmann-like equations

$$\partial_t f + \partial_x f = \frac{1}{\varepsilon} Q(f,f), \quad x \in \mathbb{R},$$

where $f = f(x,v,t)$ and $Q(f,f) = 0$ implies $f = M[f]$ the local Maxwellian.

- When $f \approx M[f]$ the collision operator is well approximated by its linear counterpart $Q(M,f)$ or directly by a BGK relaxation operator $\mu(M[f] - f)$.
- If we denote by $L_P(f)$ the linear approximating operator we can write [11]

Penalized setting

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

[11] S.Jin, F.Filbet '11

Penalized IMEX Runge-Kutta methods

In the sequel we assume $L_P(f) = \mu(M[f] - f)$, $\mu > 0$. The IMEX-RK scheme take the form [12]

Penalized IMEX-RK for Boltzmann

$$F = f^n\, e + \Delta t\, \tilde{A} \left(\frac{1}{\varepsilon} G(F) - v \cdot \nabla_x F \right) + \frac{\mu \Delta t}{\varepsilon}\, A(M[F] - F)$$
$$f^{n+1} = f^n + \Delta t\, \tilde{w}^T \left(\frac{1}{\varepsilon} G(F) - v \cdot \nabla_x F \right) + \frac{\mu \Delta t}{\varepsilon}\, w^T (M[F] - F).$$

- Clearly the scheme being implicit only in the linear part, which can be easily inverted and computed, can be *implemented explicitly*.
- Note however that here the problem is stiff as a whole. The hope is that applying the same design principles we used for hyperbolic systems with relaxation we get an *AP-scheme* for the full Boltzmann model.

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

AP-property

First let us point out that since the linear operator enjoys the same conservation property of the full Boltzmann operator we have the same associated *moment scheme* characterized by $(\tilde{A}, \tilde{w})$ of the explicit method

$$\int_{\mathbb{R}^3} F\phi(v)\,dv = \int_{\mathbb{R}^3} f^n\, e\phi(v)\,dv - \Delta t\tilde{A}\int_{\mathbb{R}^3} v\cdot\nabla_x F\phi(v)\,dv$$

$$\int_{\mathbb{R}^3} f^{n+1}\phi(v)\,dv = \int_{\mathbb{R}^3} f^n\phi(v)\,dv - \Delta t\,\tilde{w}^T\int_{\mathbb{R}^3} v\cdot\nabla_x F\phi(v)\,dv.$$

Consider now an invertible matrix A and solve the IMEX scheme for $(M[F]-F)$

$$\Delta t(M[F]-F) = \frac{\varepsilon}{\mu}A^{-1}\left[F - f^n\,e + \Delta t\tilde{A}\left(v\cdot\nabla_x F - \frac{1}{\varepsilon}G(F)\right)\right]$$

Again as $\varepsilon\to 0$ we get

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

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

$$G(F^{(i)}) = Q(F^{(i)},F^{(i)}) - \mu(M[F^{(i)}]-F^{(i)}) = 0,\quad i=1,..,\nu.$$

Further requirements

As opposite to the case of hyperbolic systems with relaxation, now the last level still depends on ε. After some manipulations it reads

$$\begin{aligned} f^{n+1} &= f^n\left(1 - w^T A^{-1} e\right) - \Delta t\, \tilde{w}^T \left(v \cdot \nabla_x F - \frac{1}{\varepsilon} G(F)\right) \\ &+ \Delta t\, w^T A^{-1} \tilde{A} \left(v \cdot \nabla_x F - \frac{1}{\varepsilon} G(F)\right) + w^T A^{-1} F. \end{aligned}$$

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

$$f^{n+1} = F^{(\nu)},$$

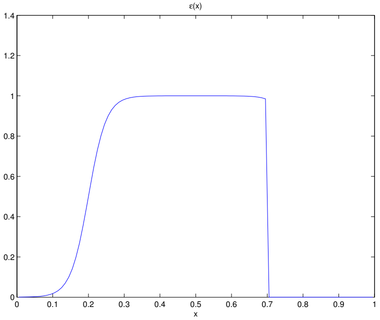
and so as $\varepsilon \to 0$

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

- For the Boltzmann case the stiffly accurate property is required to have a stable AP and asymptotically accurate scheme.

Mixing regimes problem

Collision term approximated by the *Fast Fourier-Galerkin method* [13]. Second and third order *WENO* is used in space [14]



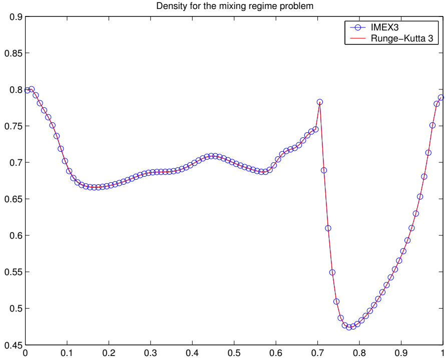
Knudsen number value for the mixed regime test with $\varepsilon_0 = 10^{-4}$

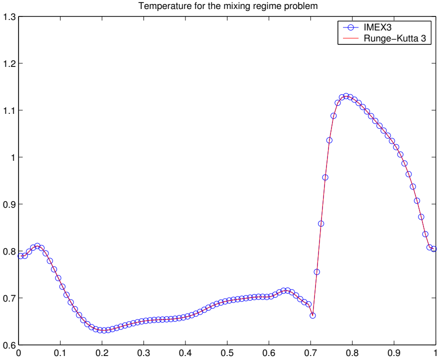
$$\begin{cases} \varepsilon = \varepsilon_0 + \frac{1}{2}(\tanh(16-20x) + \tanh(-4+20x)), & x \leq 0.7 \\ \varepsilon = \varepsilon_0, & x > 0.7 \end{cases}$$

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

[14] C-W.Shu '97

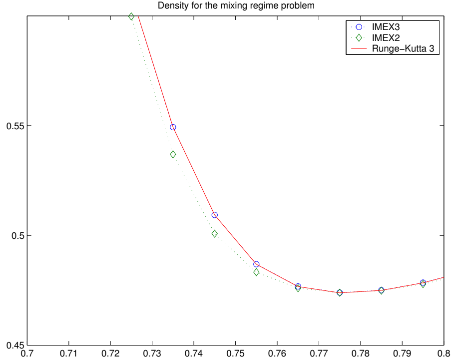
Mixing regimes: third order scheme

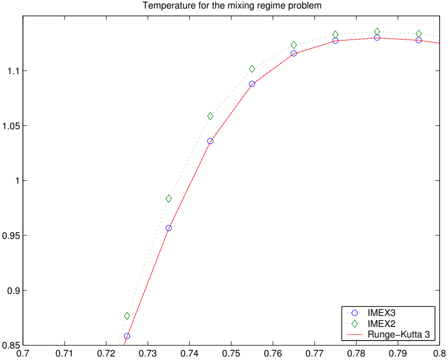




Density (left) and temperature (right) profiles for the mixing regime problem. Time $t = 0.5$, $N_x = 100$ using third order WENO. Reference solution computed using a third order Runge-Kutta. Here $\Delta t_{IMEX}/\Delta t_{RK} = 7$.

Mixing regimes: second vs third order





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

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.
- 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).