High-order Asymptotic-Preserving schemes for the Boltzmann equation and related problems

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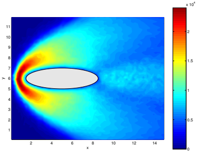
Motivations



The computation of *fluid-kinetic interfaces* and *asymptotic behaviors* involves multiple scales where most numerical methods lose their efficiency because they are forced to operate on a very short time scale.

- *Partitioned time discretizations* represent a powerful tool for the numerical treatment of stiff terms in PDEs. When necessary they can be designed in order to achieve suitable asymptotic preserving (*AP*) properties.
- Similar techniques can be adopted when dealing with kinetic equation of *Boltzmann-type*. Here, however, the major challenge is represented by the complicated nonlinear structure of the collisional operator which makes prohibitively expensive the use of implicit solvers for the stiff collision term.
- Additional difficulties are given by the need to preserve some relevant *physical properties* like conservation of mass, momentum and energy, nonnegativity of the solution, and entropy inequality.

Outline

The Implicit-Explicit (IMEX) paradigm

Many practical application involves systems of differential equations of the form

$$U' = \underbrace{\mathcal{F}(U)}_{\textit{non stiff term}} + \underbrace{\mathcal{G}(U)}_{\textit{stiff term}},$$

where $\mathcal{F}$ and $\mathcal{G}$, eventually obtained as suitable finite-difference or finite-element approximations of spatial derivatives (*method of lines*), induce considerably different time scales.

- The use of fully implicit solvers originates a nonlinear system of equations involving also the non stiff term $\mathcal{F}$.
- Thus it is highly desirable to have a combination of *implicit* and *explicit* discretization terms to resolve stiff and non–stiff dynamics accordingly.
- IMEX methods have been developed to deal with the numerical integration of *hyperbolic balance laws*, *kinetic equations*, *convection–diffusion equations* and *singular perturbed problems*.

A simple example

Consider the *singularly perturbed problem*[1]

Singularly perturbed problem

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

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

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

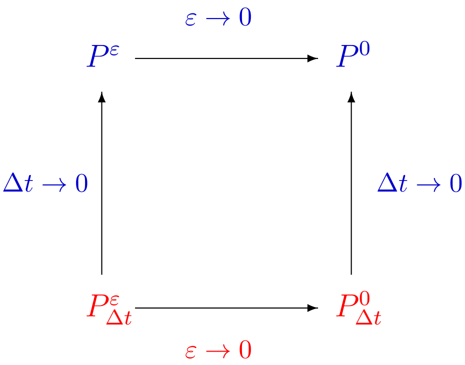
Assuming that $g(u,v) = 0 \Leftrightarrow v = E(u)$ we obtain

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

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

[1] 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.

Numerical approaches

- The simplest approach is based on *splitting methods* where we solved separately the subproblems

$$U' = F(U), \qquad U' = G(U).$$

  Easy to analyze and achieve AP property, possible to use existing solvers for the simplified problems and to preserve some relevant physical properties. Main drawback: order reduction in stiff regimes.
- Different approaches to achieve high-order AP schemes
  - *IMEX Runge-Kutta methods*
  - *Exponential methods*
  - *IMEX Multistep methods*
- All the different approaches share the difficulty of the inversion of the collision operator due to its implicit evaluation.
- Here we will not discuss problems related to the discretization of other variables in the systems (like space and velocity), we will just mention in the numerical results the different choices we used (both deterministic and DSMC).

Kinetic equations in the fluid-dynamic scaling

The density $f = f(x,v,t) \geq 0$ of particles follows[2]

Kinetic model

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

which is written in this form after the scaling $x \to x/\varepsilon$, $t \to t/\varepsilon$ where $\varepsilon > 0$ is a nondimensional parameter (*Knudsen number*) proportional to the mean free path. The structure of the collision operator $Q(f,f)$ depends on the particular model. For example, the classical *Boltzmann collision operator* reads

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

where B is a nonnegative kernel characterizing the binary interactions and

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

[2] C.Cercignani '88

Main properties

The collision operator satisfies local conservation properties

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

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

$$\int_{\mathbb{R}^{d_v}} Q(f,f)\log(f)dv \leq 0.$$

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

Maxwellian distribution

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

with ρ, u, T the *density*, the *mean velocity* and the gas *temperature*

$$(\rho, u, E) = \int_{\mathbb{R}^{d_v}} f\phi(v)dv, \quad T = \frac{1}{3\rho}(E - \rho|u|^2).$$

Hydrodynamic equations

If we multiply the kinetic equation for its collision invariants 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.
As $\varepsilon \to 0$ formally $Q(f,f) = 0$ which implies $f = M[f]$ and we get the closed system

Compressible Euler equations

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

IMEX-RK for easy invertible collision operators

Let us first consider the BGK relaxation approximation $Q(f,f) = M[f] - f$.
A general IMEX schemes in vector form reads

IMEX-RK for BGK

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

with $F = (F^{(1)}, \ldots, F^{(\nu)})^T$, $M[F] = (M[F^{(1)}], \ldots, M[F^{\nu}])^T$, $e = (1, \ldots, 1)^T$.
Explicit scheme characterized by the $\nu \times \nu$ matrix $\tilde{A} = (\tilde{a}_{ij})$, $\tilde{a}_{ij} = 0$, $j \geq i$ and the coefficient vectors $\tilde{w} = (\tilde{w}_1, \ldots, \tilde{w}_\nu)^T$, $\tilde{c} = \tilde{A}e$.
Implicit scheme characterized by the $\nu \times \nu$ matrix $A = (a_{ij})$, and the coefficient vectors $w = (w_1, \ldots, w_\nu)^T$, $c = Ae$.

- The coefficient $\tilde{a}_{ij}$, a_{ij}, $\tilde{w}_j$, w_j must satisfy suitable order and stability conditions. Note that coupling an order p explicit RK method with and order p implicit RK method in general does not originate and order p IMEX-RK method.

AP-property

The scheme can be *implemented explicitly* since the Maxwellian term $M[F^{(i)}]$ depends only the moments of $F^{(i)}$ which can be explicitly evaluated.
If we multiply the IMEX scheme by the collision invariants $\phi(v) = 1, v, v^2$ and integrate in v we get a *moment scheme* characterized by the explicit method

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

Assuming A invertible from the original IMEX scheme we obtain

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

Thus, for $\varepsilon \to 0$ we get

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

which inserted into the moment scheme originates an *asymptotic– preserving scheme* for the Euler equations.

Asymptotically and stiffly accurate schemes

- As a result of the previous analysis as $\varepsilon \to 0$ we obtain the explicit Runge-Kutta scheme applied to the Euler equations. Therefore the method is not only consistent (AP) but also preserves the accuracy in the limit (*asymptotically accurate*).
- The numerical solution f^{n+1} is independent on ε and can be written as

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

In principle we can require a stronger property then AP, namely that

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

We call an IMEX method that satisfies this property *globally stiffly accurate*. It is guaranteed if $\tilde{w}_j = \tilde{a}_{\nu j}$ and $w_j = a_{\nu j}$, $j = 1, \ldots, \nu$.

Positivity and contractivity

Positivity of the numerical solution in the space non homogeneous case usually impose rather severe restriction on the time stepping[3]. If we restrict to space homogeneous BGK equations, we have[4]

Definition

Let us consider a DIRK method characterized by (A, w) satisfying

$$1 - w^T A^{-1} e \geq 0, \qquad w^T A^{-1} \geq 0.$$

The values of $z = \Delta t/\varepsilon$ such that

$$(I + zA)^{-1} e \geq 0, \qquad (I + zA)^{-1} c \geq 0,$$

defines the positivity region $R_{BGK}(z) \subseteq \mathbb{R}_+$ of the method.

- By convexity, since $H(M[f]) \leq H(f)$, where $H = \int f \log f$ is the *H-functional* the schemes are also entropic $H(f^{n+1}) \leq H(f^n)$.

[3] I. Higueras '07

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

Some references on IMEX-RK

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Design principles for the Boltzmann case

- The goal is to construct AP and asymptotically accurate schemes *avoiding the implicit solution* of the collision term of the Boltzmann equation.
- 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 $Q(M, f)$ or directly by a BGK/ES-BGK relaxation operator.
- If we denote by $L(f)$ the linear approximating operator we can write [5]

Penalized setting

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

▶ The idea now is to be implicit (or exact) in the linear part $L(f)$ and explicit in the deviations from equilibrium $G(f)$.

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

Penalized IMEX-RK for the Boltzmann equation

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

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* exactly as in the BGK case.
- Note however that here the problem is stiff as a whole. The hope is that applying the same design principles we used for the BGK we get an *AP-scheme* for the full Boltzmann model.

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 BGK model, 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 $\varepsilon \to 0$

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

- On the contrary to the BGK case, for the Boltzmann case the stiffly accurate property is required to have a stable AP and asymptotically accurate scheme.

Positivity

Conditions for non homogenous positive schemes are extremely restrictive due to the penalization procedure. We restrict to the space homogeneous case and take $\mu > 0$ such that[6]

$$P(f,f) = Q(f,f) + \mu f \geq 0.$$

Definition

Let us consider a globally stiffly accurate IMEX method characterized by (A, w), $(\tilde{A}, \tilde{w})$. The values of $z = \Delta t/\varepsilon$ such that

$$(I + \mu z A)^{-1} e \geq 0, \qquad (I + \mu z A)^{-1} \tilde{A} \geq 0, \qquad (I + \mu z A)^{-1} (c - \tilde{c}) \geq 0,$$

define the positivity region $R_B(z) \subseteq \mathbb{R}_+$ of the method.

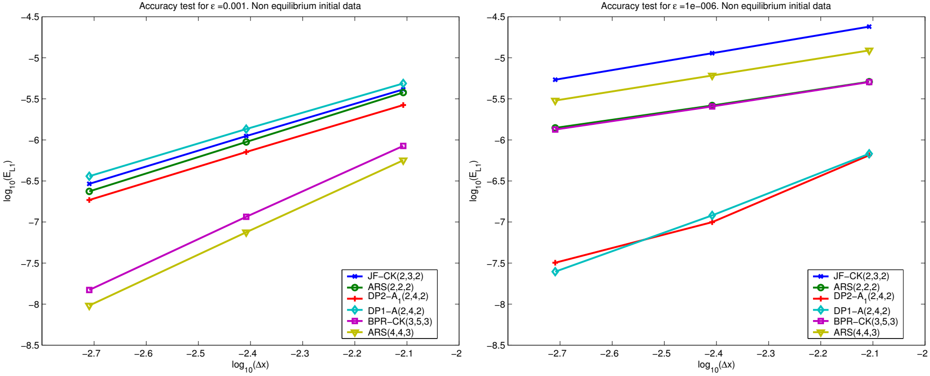
- From the above properties it follows that the schemes are also entropic provided we have an estimate of the type[7] $H(P(f,f) \leq H(f)$.

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

[7] C.Villani '98, G.Toscani, C.Villani '99

Homogeneous relaxation

Collision term approximated by the *fast Fourier-Galerkin method* [8].

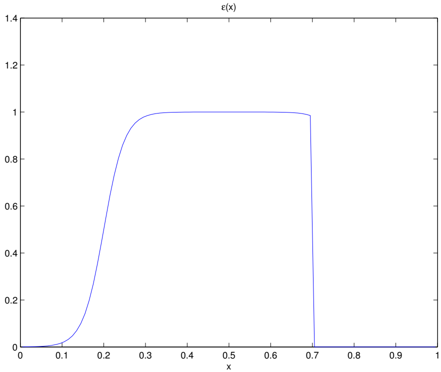


L_1-error of second and third order penalized IMEX-RK for $\varepsilon = 10^{-3}$ (left) and $\varepsilon = 10^{-6}$ (right). Nonequilibrium data.

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

Mixing regimes problem

Second and third order *WENO* is used in space [9]

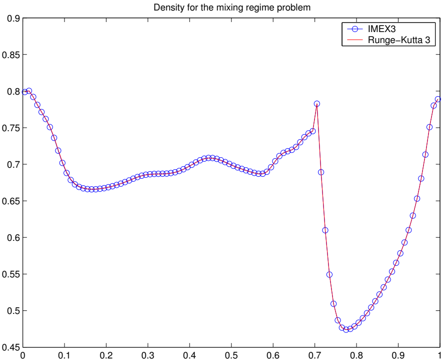


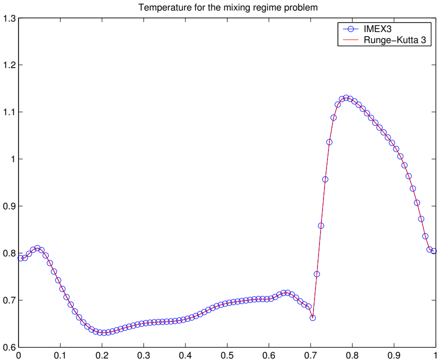
Knudsen number value for the mixed regime test with $\varepsilon_0 = 10^{-4}$

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

[9] C-W. Shu '97

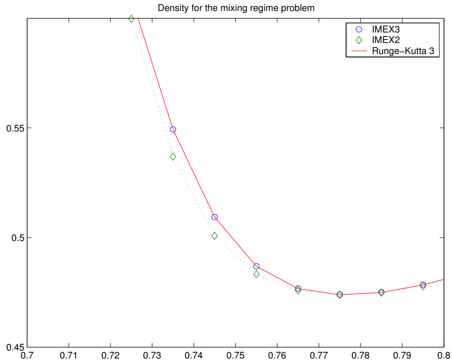
Mixing regimes: third order scheme





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 $x \in [0.7, 0.8]$.

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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[10]

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

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

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

AP Exponential Runge-Kutta methods

A different approach consist in taking an explicit Runge-Kutta discretization of the transformed problem and then reverting back to the original variables [11]

Exponential Runge-Kutta

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

$$f^{n+1} = e^{-\mu\frac{\Delta t}{\varepsilon}} f^n + (1 - e^{-\mu\frac{\Delta t}{\varepsilon}})M[f^n] + \Delta t \sum_{i=1}^{\nu} W_i\left(\mu\frac{\Delta t}{\varepsilon}\right) G(F^{(i)}),$$

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

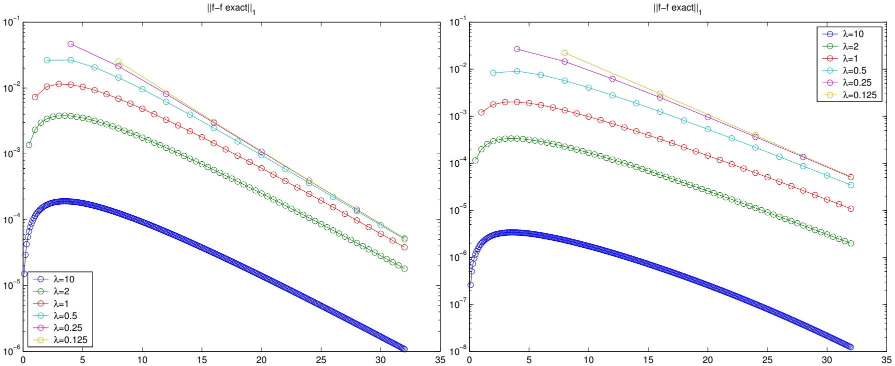
$$A_{ij}\left(\mu\frac{\Delta t}{\varepsilon}\right) = a_{ij} e^{-(c_i - c_j)\mu\frac{\Delta t}{\varepsilon}}, \quad i,j = 1,\dots,\nu, \quad j > i$$

$$W_i\left(\mu\frac{\Delta t}{\varepsilon}\right) = w_i e^{-(1-c_i)\mu\frac{\Delta t}{\varepsilon}}, \quad i = 1,\dots,\nu.$$

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

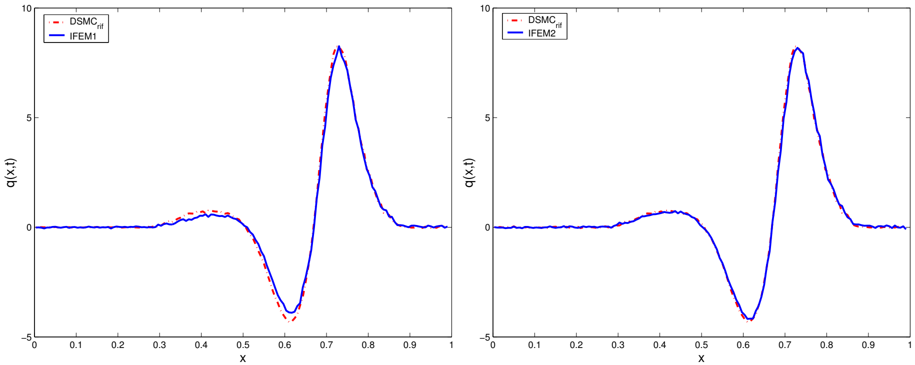
[11] G.Dimarco, L.P. '11, S.Maset, M.Zennaro '09

Homogeneous relaxation



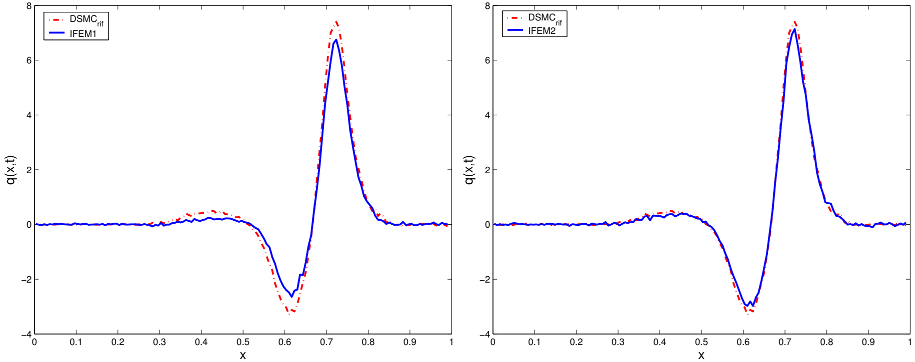
L_1-error of second order (left) and third order (right) EXP-RK for different time steps, $\lambda = \varepsilon/(\mu\Delta t)$.

Sod shock tube: Heat flux $\varepsilon = 0.001$



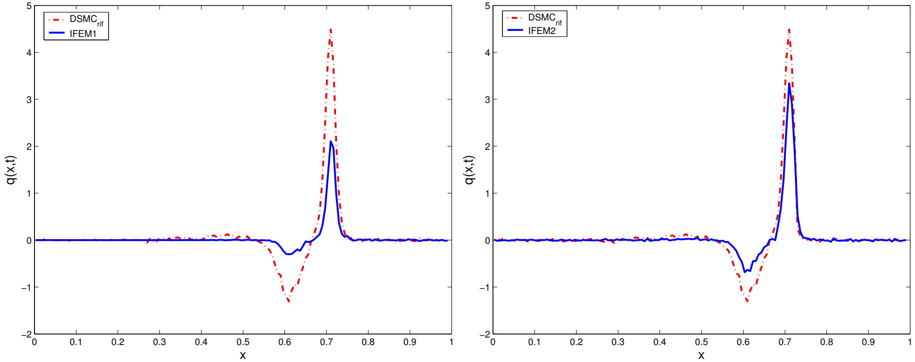
Monte Carlo solution using first (left) and second order (right) AP EXP-RK. First and second order splitting is used with $\Delta t_{EXP-RK}/\Delta t_{DSMC} = 1$

Sod shock tube: Heat flux $\varepsilon = 0.0005$



Monte Carlo solution using first (left) and second order (right) AP EXP-RK. First and second order splitting is used with $\Delta t_{EXP-RK}/\Delta t_{DSMC} = 2$

Sod shock tube: Heat flux $\varepsilon = 0.0001$



Monte Carlo solution using first (left) and second order (right) AP EXP-RK. First and second order splitting is used with $\Delta t_{EXP-RK}/\Delta t_{DSMC} = 10$

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[12]

Exponential Runge-Kutta non homogeneous case

Step i:

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

Final Step:

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

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

[12] 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 [13] 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.

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

Convergence test

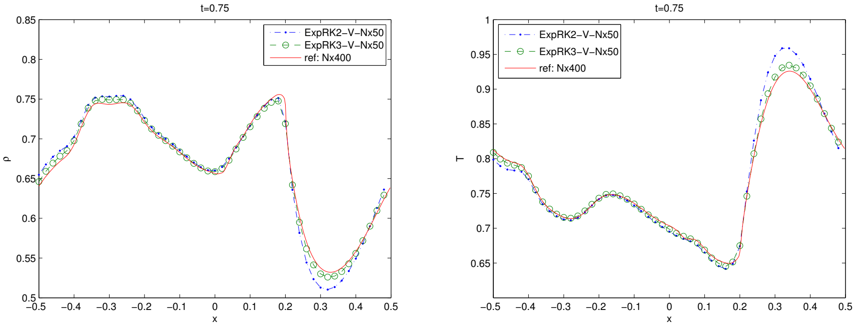
Initial data sum of two Maxwellians in space solved using WENO3-5[14] in space and the fast Fourier-Galerkin method[15] in velocity.

		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.

[14] C-W.Shu '97
[15] C.Mouhot, L.P. '06

Mixing regimes: second vs third order scheme



Density (left) and temperature (right) profiles for the mixing regime problem. Time $t = 0.75$, $N_x = 50$ using third order WENO. Reference solution computed using a third order Runge-Kutta for the continuos line with $N_x = 400$.

Multistep IMEX schemes

In the penalized setting an IMEX multistep scheme takes the form [16]

Penalized IMEX-Multistep for Boltzmann

$$
\begin{aligned}
f^n &= \sum_{j=1}^{k} a_j f^{n-j} + \Delta t \sum_{j=1}^{k} \tilde{b}_j \left(\frac{1}{\varepsilon} G(f^{n-j}) - v \cdot \nabla_x f^{n-j} \right) \\
&+ \frac{\mu \Delta t}{\varepsilon} \sum_{j=0}^{k} b_j (M^{n-j} - f^{n-j})
\end{aligned}
$$

where a_j, $\tilde{b}_j$ and b_j are the coefficients of the scheme.

- Again since the scheme is implicit only in the linear part it can be *implemented explicitly*.
- The schemes need a suitable starting procedure to compute the values f^{n-j}, $j = 1, \dots, k$. An AP IMEX-RK or EXP-RK of the same order of accuracy can be used.

[16] W. Hundsdorfer, S.J. Ruuth '07, G. Dimarco, L.P. '13

AP property

If we multiply the scheme by the collision invariants $\phi(v) = 1, v, v^2$ and integrate in v we get a *moment scheme* characterized by the explicit multistep method

$$\int_{\mathbb{R}^3} f^n \phi(v)\, dv \;=\; \sum_{j=1}^{k} a_j \int_{\mathbb{R}^3} f^{n-j}\phi(v)\, dv - \Delta t \sum_{j=1}^{k} \tilde{b}_j \int_{\mathbb{R}^3} v \cdot \nabla_x f^{n-j} \phi(v)\, dv.$$

We can write the scheme in the form

$$\begin{aligned} f^n \;&=\; \frac{\varepsilon}{\varepsilon + b_0 \mu \Delta t} \left[\sum_{j=1}^{k} a_j f^{n-j} + \Delta t \sum_{j=1}^{k} \tilde{b}_j \left(\frac{1}{\varepsilon} G(f^{n-j}) - v \cdot \nabla_x f^{n-j} \right) \right] \\ &+\; \frac{\mu \Delta t}{\varepsilon + b_0 \mu \Delta t} \left(\sum_{j=1}^{k} b_j (M^{n-j} - f^{n-j}) + b_0 M^n \right) \end{aligned}$$

and therefore as $\varepsilon \to 0$ we get if $b_0 \neq 0$

$$f^n = \frac{1}{\mu b_0} \sum_{j=1}^{k} \tilde{b}_j G(f^{n-j}) + \frac{1}{b_0} \sum_{j=1}^{k} b_j (M^{n-j} - f^{n-j}) + M^n.$$

AP, order conditions and efficiency

If the starting procedure is strongly AP we have as $\varepsilon \to 0$

$$f^{n-j} = M^{n-j}, \quad j = 1, \ldots, k$$

and then, since $G(f^{n-j}) = 0$, we get

$$\lim_{\varepsilon \to 0} f^n = M^n,$$

and the strong AP property.

- In contrast with IMEX-RK methods, conditions for the individual explicit and implicit method to be of order p are sufficient to generate an IMEX-Multistep combination of order p as well.
- Independently of the order, the computational cost of the IMEX-Multistep method is due to the evaluation of *one single collision term* at time level $n-1$. This is a remarkable advantage for Boltzmann-type equations.

Final considerations

Some work in progress

- Other asymptotic limits: Drift-diffusion for semiconductors, Incompressible Navier-Stokes, Diffusion limit for chemotaxis (with G.Dimarco, V.Rispoli)
- Construction of embedded IMEX-RK for adaptive time-stepping
- Analysis of multistep AP IMEX schemes
- Development of hybrid strategies/domain decomposition strategies
- ...

Open problems

- What happens when ε is small but not zero? Compressible Navier-Stokes limit (with S.Boscarino, G.Dimarco, G.Russo)
- What happens for large times? Well-balanced schemes
- ...