Asymptotic-preserving schemes for kinetic equations and related problems with stiff sources

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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.
The Implicit-Explicit (IMEX) paradigm

Many practical application involves systems of differential equations of the form

\[ U' = \underbrace{\mathcal{F}(U)}_{\text{non stiff term}} + \underbrace{\mathcal{G}(U)}_{\text{stiff term}}, \]

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 \textit{implicit} and \textit{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.
IMEX Runge-Kutta methods

\[ U_i = U^n + \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} F(t_0 + \tilde{c}_j \Delta t, U_j) + \Delta t \sum_{j=1}^{\nu} a_{ij} G(t_0 + c_j \Delta t, U_j), \]

\[ U^{n+1} = U^n + \Delta t \sum_{i=1}^{\nu} \tilde{w}_i F(t_0 + \tilde{c}_i \Delta t, U_i) + \Delta t \sum_{i=1}^{\nu} w_i G(t_0 + c_i \Delta t, U_i). \]

**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 are $\tilde{c} = (\tilde{c}_1, \ldots, \tilde{c}_\nu)^T$, $\tilde{c}_i = \sum_{j=1}^{i-1} \tilde{a}_{ij}$, $\tilde{w} = (\tilde{w}_1, \ldots, \tilde{w}_\nu)^T$.

**Implicit scheme** characterized by the $\nu \times \nu$ matrix $A = (a_{ij})$, and the coefficient vectors are $c = (c_1, \ldots, c_\nu)^T$, $c_i = \sum_{j=1}^{\nu} a_{ij}$, $w = (w_1, \ldots, w_\nu)^T$.

▶ We restrict to *diagonally implicit (DIRK)* schemes, $a_{ij} = 0$, $j > i$ since they guarantee that $\mathcal{F}$ is evaluated explicitly.
The Implicit-Explicit (IMEX) paradigm

**IMEX Runge-Kutta methods**

- The schemes can be written in compact form using vector notation

\[
U^n = U^n e + \Delta t \tilde{A} \mathcal{F}(t_0 + \tilde{c} \Delta t, U) + \Delta t A \mathcal{G}(t_0 + c \Delta t, U),
\]

\[
U^{n+1} = U^n + \Delta t \tilde{w}^T \mathcal{F}(t_0 + \tilde{c} \Delta t, U) + \Delta t w^T \mathcal{G}(t_0 + c \Delta t, U).
\]

with \(e = (1, \ldots, 1)^T\) and are schematically summarized using a **double Butcher tableau** of the type

\[
\begin{array}{c|c|c|c}
\tilde{c} & \tilde{A} & c & A \\
\tilde{w}^T & \tilde{w}^T
\end{array}
\]

- In additions the scheme should satisfy
  - **order conditions** (if \(c = \tilde{c}\) and \(w = \tilde{w}\) mixed conditions are satisfied up to order 3)
  - **stability properties** (strong stability preserving, asymptotic preserving, \ldots)
  - **other requirements** (positivity, \ldots).
Some references on IMEX-RK


A simple example

Consider the *singularly perturbed problem*\(^1\)

### Singularly perturbed problem

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

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

\[ u'(t) = f(u, v) \]
\[ 0 = g(u, v). \]

Assuming that \( g(u, v) = 0 \iff v = E(u) \) 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 \( g(u, v) = 0 \iff v = E(u) \).

\(^1\)E.Hairer, C.Lubich, M.Roche ’89
In the diagram $P^\epsilon$ is the original singular perturbation problem and $P^\epsilon_{\Delta t}$ its numerical approximation characterized by a discretization parameter $\Delta t$. The \textit{asymptotic-preserving (AP) property} corresponds to the request that $P^\epsilon_{\Delta t}$ is a consistent discretization of $P^0$ as $\epsilon \to 0$ independently of $\Delta t$. 
Kinetic equations in the fluid-dynamic scaling

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

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

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

\[ \int_{\mathbb{R}^d} Q(f, f) \phi(v) \, dv = 0, \]

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

\[ \int_{\mathbb{R}^d} Q(f, f) \log(f) \, dv \leq 0. \]

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

**Maxwellian distribution**

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

with \( \rho, u, T \) the density, the mean velocity and the gas temperature

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

\[
\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i} (\rho u_i) = 0, \\
\frac{\partial}{\partial t} (\rho u_j) + \sum_{i=1}^{3} \frac{\partial}{\partial x_i} (\rho u_i u_j) + \frac{\partial}{\partial x_j} p = 0, \quad j = 1, 2, 3 \\
\frac{\partial E}{\partial t} + \sum_{i=1}^{3} \frac{\partial}{\partial x_i} (E u_i + p u_i) = 0, \quad p = \rho T.
\]
IMEX-RK for easy invertible collision operators

For the sake of simplicity let us consider the BGK relaxation approximation $Q(f, f) = M[f] - f$. A general IMEX schemes has the form

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

- Although implicit the scheme can be *implemented explicitly* since the only implicit part is a diagonal linear term $F^{(i)}$ and a Maxwellian term $M[F^{(i)}]$ depending on the moments of $F^{(i)}$ which can be explicitly evaluated\(^3\).

- It can be shown that applying the same design principles used for hyperbolic relaxation systems, we obtain *AP-schemes* for the BGK model.

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\(^3\)S.Pieraccini, G.Puppo ’07
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.
**Stiffly accurate schemes**

The numerical solution $f^{n+1}$ is independent on $\varepsilon$ and can be written as

$$
f^{n+1} = f^n (1 - w^T A^{-1} e) - \Delta t \tilde{w}^T v \cdot \nabla_x F + \Delta t w^T A^{-1} \tilde{A} v \cdot \nabla_x F + w^T A^{-1} F.
$$

In principle we can require a stronger property than 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**. Thus we require

$$
w^T A^{-1} e = 1, \quad w^T A^{-1} \tilde{A} = \tilde{w}^T, \quad w^T A^{-1} F = M[f^{n+1}].
$$

This is guaranteed independently of $f$ if

$$
w_i = a_{vi}, \quad \tilde{w}_i = \tilde{a}_{vi}, \quad \forall i = 1, \ldots, \nu,
$$

since it implies that $f^{n+1} = F(\nu)$. 

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Positivity and contractivity

The determination of general conditions for positivity of the numerical solution in the space non homogeneous case usually impose rather severe restriction on the time stepping\(^4\). If we restrict to space homogeneous BGK equations, we have\(^5\)

**Definition**

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

\[
1 - w^T A^{-1} e \geq 0, \quad w^T A^{-1} \geq 0.
\]

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

\[
(I + zA)^{-1} e \geq 0, \quad (I + zA)^{-1} c \geq 0,
\]

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

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

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\(^4\)I. Higuera's '07

\(^5\)G. Dimarco, L.P. '12
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 \( \varepsilon \) is small we do not really need to resolve the whole collision operator since we know that \( f \approx M[f] \).

On the other hand when \( f \approx M[f] \) we know that the collision operator is well approximated by its linear counterpart

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

or directly by a BGK or an improved \textit{ES-BGK} relaxation operator.

If we denote by \( L(f) \) the selected linear approximating operator we can write

\[
Q(f, f) = G(f) + L(f), \quad G(f) = Q(f, f) - L(f).
\]

The idea now is to be implicit (or exact) in the linear part \( L(f) \) and explicit in the deviations from equilibrium \( G(f) \).
Some references for the Boltzmann case


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

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

\[
f^{n+1} = f^n + \Delta t \tilde{w}^T \left( \frac{1}{\varepsilon} G(F') - v \cdot \nabla_x F' \right) + \frac{\mu \Delta t}{\varepsilon} w^T (M[F] - F').
\]

- 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.
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 $\tilde{A}$ is lower triangular with $\tilde{a}_{ii} = 0$ and we have a hierarchy of equations such that

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

As opposite to the BGK model, now the last level still depends on $\varepsilon$. After some manipulations it reads

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

$$+ \Delta t w^T A^{-1} \tilde{A} \left(v \cdot \nabla_x F - \frac{1}{\varepsilon} G(F)\right) + w^T A^{-1} F.$$ 

Now for small values of $\varepsilon$ the scheme turns out to be unstable since $f^{n+1}$ is not bounded. A remedy to this fact, is to consider globally stiffly accurate schemes for which

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

and so as $\varepsilon \to 0$

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

Note that on the contrary to the BGK case, for the Boltzmann case the stiffly accurate property is required to have a stable AP scheme.
Positivity

The determination of a non homogenous positive scheme seems extremely difficult due to the penalization procedure. Thus we restrict to the space homogeneous case and take $\mu > 0$ such that

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

**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

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

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 $^7 H(P(f, f) \leq H(f)$.

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$^6$ G.Dimarco, L.P. '12  
$^7$ C.Villani '98, G.Toscani, C.Villani '99
Exponential schemes for the Boltzmann equation

When positivity is required a more robust approach is based on the exact integration of the penalization term which permits to write the homogeneous step

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

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

Time relaxed methods

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

where the functions \( f_k \) are given by the recurrence formula

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

\[^8\text{E.Gabetta, L.P., G.Toscani '97}\]
A different approach consists in taking an explicit Runge-Kutta discretization of the transformed homogeneous problem and then reverting back to the original variables. In this way we obtain an explicit exponential Runge-Kutta method.

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

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

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

\[ A_{ij}(\mu \Delta t) = a_{ij} e^{-(c_i - c_j) \mu \Delta t}, \quad i, j = 1, \ldots, \nu, \quad j > i \]

\[ W_i(\mu \Delta t) = w_i e^{-(1-c_i) \mu \Delta t}, \quad i = 1, \ldots, \nu. \]

Unconditionally positive schemes can be constructed up to fourth order.

\[ G.Dimarco, L.P. '11, S.Maset, M.Zennaro '09, Q.Li, L.P. '12 \]

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9 AP Exponential Runge-Kutta methods
Kinetic equations
Exponential schemes for the Boltzmann equation

Homogeneous relaxation: second order schemes

$L_1$-error of second order AP IMEX-RK and EXP-RK for different time steps.
Homogeneous relaxation: third order schemes

$L_1$-error of third order AP IMEX-RK and EXP-RK for different time steps.
A comparison of penalized IMEX schemes

$L_1$-error of second and third order penalized IMEX-RK for $\varepsilon = 10^{-3}$ (left) and $\varepsilon = 10^{-6}$ (right). Nonequilibrium data.
Knudsen number value for the mixed regime test
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 for the continuous line, third order IMEX computed solution dotted line with $(\Delta t)_{IMEX}/(\Delta t)_{RK3} = 7$. 
Density (left) and temperature (right) profiles for the mixing regime problem at $t = 0.5$ for $x \in [0.7, 0.8]$. 
Kinetic equations in the diffusive scaling

We consider the multidimensional transport equation under the diffusive scaling.

Transport equation

\[ \varepsilon \partial_t f + v \nabla_x f = \frac{1}{\varepsilon} \left( \frac{\sigma_s}{S} \int_{\Omega} f dv' - \sigma f \right) + \varepsilon Q, \]

where \( \sigma = \sigma(x) \) is the total cross section, \( \sigma_s = \sigma_s(x) \) is the scattering coefficient. Here \( Q = Q(x) \) is a source term and \( \varepsilon \) the mean free path. Typically, \( \sigma_s = \sigma - \varepsilon^2 \sigma_A \) where \( \sigma_A = \sigma_A(x) \) is the absorption coefficient.

Setting \( f = r + \varepsilon j \), with \( \int j dv = 0 \) and \( (1/S) \int r dv = \rho \) we can write the equation in the form\(^{10}\)

\[
\begin{align*}
\partial_t r + v \nabla_x j &= -\frac{\sigma_s}{\varepsilon^2} (r - \rho) - \sigma_A r + Q, \\
\partial_t j + \frac{v}{\varepsilon^2} \nabla_x r &= -\frac{\sigma_s}{\varepsilon^2} j - \sigma_A j,
\end{align*}
\]

\(^{10}\) A. Klar '98, S.Jin, L.P., G.Toscani '00
Partitioned IMEX methods

In the limit $\varepsilon \to 0$ we get

$$r = \frac{\rho}{S}, \quad j = \frac{v}{\sigma} \nabla_x r.$$ 

Applying this in the first equation and integrating over $v$ we get the diffusion equation

$$\partial_t \rho = \frac{1}{S} \int_\Omega v \cdot \nabla_x \left( \frac{v}{\sigma} \cdot \nabla_x \rho \right) \, dv - \sigma_A \rho + Q.$$ 

Setting $U = (r, j)^T$ the IMEX paradigm

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

can be applied by partitioning the system as

$$\mathcal{F}(U) = (-v \nabla x j - \sigma_A r + Q, -\sigma_A j)^T, \quad \mathcal{G}(U) = \sigma_s \frac{1}{\varepsilon^2} \left( -r + \frac{\rho}{S}, -\frac{v}{\sigma_s} \nabla_x r - j \right)^T.$$ 

The use of stiffly accurate IMEX schemes gives an AP method that can be implemented explicitly, but for a given space discretization when $\varepsilon \to 0$ leads to a parabolic stability constraint of the type $\Delta t \approx (\Delta x)^2$. 

▶
Some references on schemes for the diffusive limit


Let us rewrite the system in the form ($\sigma_A = 0, Q = 0$)

\[
\begin{align*}
\partial_t r &= -v \nabla_x \left( j + \mu(\varepsilon) \frac{v}{\sigma_s} \nabla_x r \right) - \frac{\sigma_s}{\varepsilon^2} \left( r - \frac{\rho}{S} \right) + \mu(\varepsilon) v \nabla_x \left( \frac{v}{\sigma_s} \nabla_x r \right), \\
\quad \text{explicit} & \quad \quad & \quad \text{implicit} \\
\partial_t j &= -\frac{\sigma_s}{\varepsilon^2} \left( \frac{v}{\sigma_s} \nabla_x r + j \right), \\
\quad \text{implicit} & \quad \quad & \quad \text{implicit}
\end{align*}
\]

where $\mu(\varepsilon) \in [0, 1]$ is such that $\mu(0) = 1$.

- Stiffly accurate IMEX schemes are AP and require only the numerical inversion of the implicit "green" term. This has the same cost of the solution of an implicit solver for the limiting diffusion equation.
- The space discretization of the second order derivatives in the implicit "green" term can be done using a suitable space discretization for the limiting diffusion equation.
- The stability constraint now is related only to the non stiff transport part, thus typically is of the form $\Delta t \approx \Delta x$. 

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AP schemes for kinetic equations 
Porquerolles, May 19-25, 2012
On the left-hand side the mass density $\rho$, on the right-hand side the flux $\rho u$. Here $\sigma_s = 1$, $\sigma_A = 0$, $Q = 0$, $\varepsilon = 10^{-8}$. JPT ($\circ$), $\Delta x = 0.025$, $\Delta t = 0.0002$, $N_s = 50, 250, 750$. Third order IMEX-RK ($\Diamond$), $\Delta t = \lambda \Delta x$, with $\lambda = 0.035$, $N_s = 11, 57, 171$. The exact diffusive solution is represented by the solid line.
The AP IMEX-RK cooking recipe

**Step 1.** Partition your system into stiff and non-stiff terms, by correctly identifying the terms that contribute to your reduced limiting equilibrium system.

**Step 2.** If the implicit terms are easy to invert simply adopt a suitable IMEX scheme with AP-properties. Remember that for well-prepared data the problem is simpler and even non AP IMEX method works provided they are stiffly accurate.

**Step 3.** Whenever inversion is difficult you can try to avoid it by suitable penalization techniques, like penalizing the stiff terms by asymptotic linearization around the local equilibrium state. In this case being stiffly accurate is mandatory.

**Step 4.** If some degree of implicitness is required also in the reduced limiting equilibrium system (like in diffusion limit) you can reformulate your problem by suitably embedding the implicit limiting discretization into your IMEX scheme.
Further developments

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
- Construction of multistep AP IMEX schemes
- Development of hybrid strategies
- ...

Open problems

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