Numerical fluid dynamic limit of the Boltzmann equation and beyond

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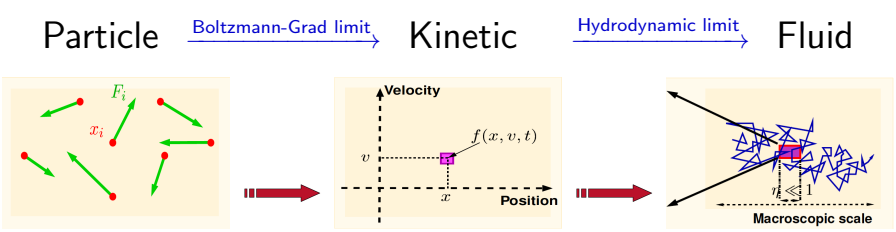
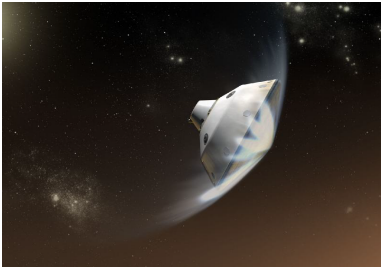
Motivations



- In *fluid regimes* the collision rate is large and particles interactions typically drive the underlying kinetic densities toward local equilibria.
- This fact allows solutions of the kinetic equation to be approximated by solutions of a reduced system, typically a fluid-dynamical system or diffusion equations, that can be solved efficiently by classical numerical methods.
- However there are *transition regimes*, where collisions are plentiful enough to make the kinetic equation stiff but not enough to drive the kinetic system close to local equilibria. These kind of problems are characterized by *breakdowns of fluid models*, either Euler or Navier-Stokes.

Motivations

Intermediate Experimental Vehicle - ESA



NASA Mars Science Laboratory

- Design of spacecraft heat shields
- Hypersonic cruise vehicles
- Granular gases
-

Outline

A toy example

Consider the *singularly perturbed problem*[1]

Singularly perturbed problem

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

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

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

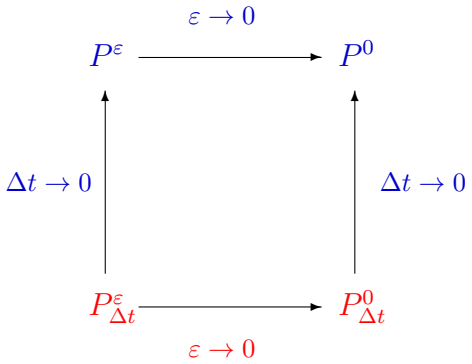
Assuming that $g(u,v) = 0 \Leftrightarrow v = E(u)$ we obtain

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

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 $g(u,v) = 0 \Leftrightarrow v = E(u)$.

[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.

The Boltzmann equation in the fluid-dynamic limit

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

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

Numerical approaches

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

$$\frac{\partial f}{\partial t} = \frac{1}{\varepsilon} Q(f, f), \qquad \frac{\partial f}{\partial t} + v \cdot \nabla_x f = 0.$$

  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*
  - *Hybrid decomposition methods*
- All the different approaches share the difficulty of the inversion of the collision operator if evaluated implicitly.
- Other major problems are related to the discretization of space and velocity, the latter in particular is related to the approximation of the collision integral.

Some references

- *Theoretical aspects:* Hilbert '12; Grad '62; Nishida '78; Caflisch '80; Caflisch, Nicolaenko '82; Bardos, Golse, Levermore '93', '98;...
- *Exponential splitting methods:* Gabetta, Pareschi, Toscani '97; Pareschi, Russo '00; Carlen, Salvarani '02; Pareschi, Dimarco '11;...
- *Non splitting exponential methods:* Li, Pareschi '13; Hu, Li, Pareschi '14;...
- *IMEX methods:* Jin '95; Asher, Ruuth, Spiteri '96; Caflisch, Jin, Russo '97; Carpenter, Kennedy '03; Pareschi, Russo '05; Boscarino, Russo '09;...
- *Penalized IMEX methods:* Jin, Filbet '10; Yan, Jin '11; Hu, Jin, Yan '12; Jin, Wang '13; Dimarco, Pareschi '13;...
- *Related Micro-macro approaches:* Klar '98; Bennoune, Lemou, Mieussens '08; Lemou '10; Lemou, Mehats '12;...
- *Hybrid decomposition methods:* Caflisch, Pareschi '99; Caflisch, Chen, Luo, '06; Dimarco, Pareschi '07,'08; Degond, Dimarco, Pareschi '10; Baker, Hadjiconstantinou '08;...

Recent review: G.Dimarco, L.Pareschi, *Acta Numerica* '14.

IMEX Runge-Kutta for simple 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 $F = (F^{(1)}, \dots, F^{(\nu)})^T$, $M[F] = (M[F^{(1)}], \dots, M[F^{\nu}])^T$, $e = (1, \dots, 1)^T$.
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 $\tilde{w} = (\tilde{w}_1, \dots, \tilde{w}_\nu)^T$, $\tilde{c} = \tilde{A}e$.
Implicit scheme characterized by the $\nu \times \nu$ matrix $A = (a_{ij})$, and the coefficient vectors $w = (w_1, \dots, w_\nu)^T$, $c = Ae$.

- 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

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

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

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 $L_P(f)$ the linear approximating operator we can write [3]

Penalized setting

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

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

[3] 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 [4]

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.

[4] G.Dimarco, L.Pareschi '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

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

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

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

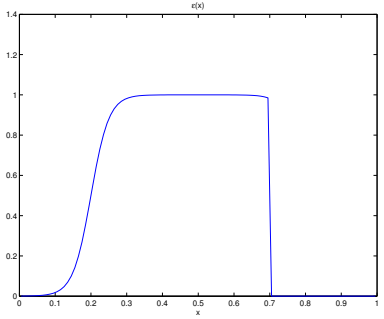
and so as $\varepsilon \to 0$

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

- 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.

Mixing regimes problem

Collision term approximated by the *Fast Fourier-Galerkin method* [5]. Second and third order *WENO* is used in space [6]

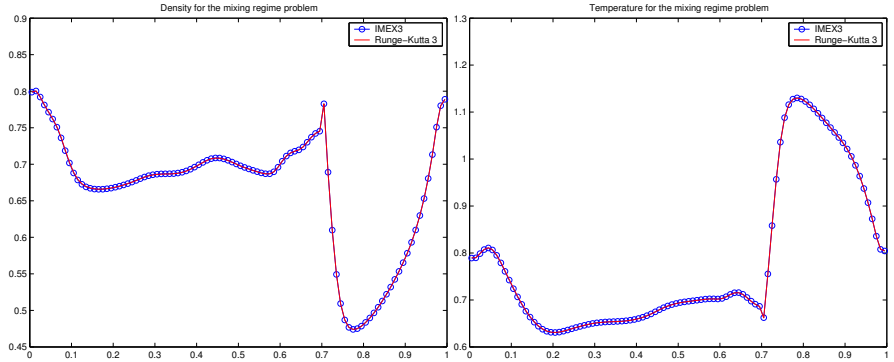


Knudsen number value for the mixed regime test with $\varepsilon_0 = 10^{-4}$

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

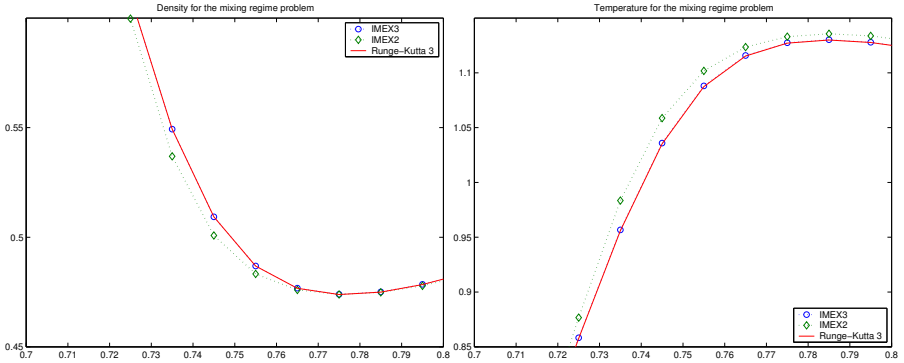
[5] L.Pareschi, B.Perthame '96, C.Mouhot, L.Pareschi '06
[6] C-W.Shu '97

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 $x \in [0.7, 0.8]$.

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[7]

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

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

[7] E.Gabetta, L.Pareschi, 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 [8]

Exponential Runge-Kutta

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

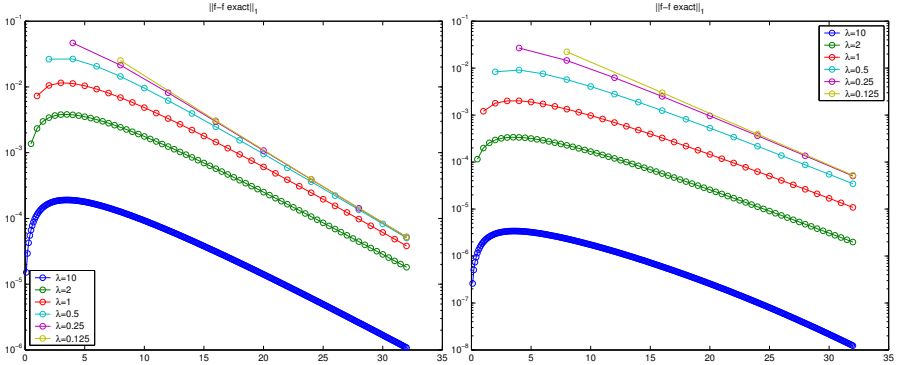
where $c_i \geq 0$, and the coefficients A_{ij} and the weights W_i are

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

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

[8] G.Dimarco, L.Pareschi '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, $\lambda = \varepsilon/(\mu\Delta t)$.

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[9]

Exponential Runge-Kutta non homogeneous case

Step i:

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

Final Step:

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

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

[9] Q.Li, L.Pareschi '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 [10] 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.

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

Convergence test

Initial data sum of two Maxwellians in space solved using WENO3-5[11] in space and the fast Fourier-Galerkin method[12] 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.

[11] C-W.Shu '97
[12] C.Mouhot, L.Pareschi '06

The Landau-Fokker-Planck equation

The Landau-Fokker-Planck model is a common kinetic model in plasma physics characterized by the nonlinear integro-differential diffusion operator [13]

$$Q_L(f,f)(v) = \nabla_v \cdot \int_{\mathbb{R}^3} A(v-v_*)[f(v_*)\nabla_v f(v) - f(v)\nabla_{v_*} f(v_*)]\, dv_*$$

where $A(v-v_*) = \Psi(|v-v_*|)\Pi(v-v_*)$ is a 3×3 nonnegative symmetric matrix and

$$\Pi(v-v_*) = I - \frac{(v-v_*)(v-v_*)}{|v-v_*|^2}.$$

We have $\Psi(|v-v_*|) = \Lambda|v-v_*|^{\alpha+2}$ for inverse-power laws, with $\alpha \geq -3$ and $\Lambda > 0$.
The case $\alpha = -3$ corresponds to the *Coulombian case*, of primary importance for applications. In such case the Boltzmann collision operator has no meaning, due to the divergence of the integral, even for smooth functions, and the Landau equation can be derived in the so-called *grazing collision limit* [14].

[13] L.Landau '81
[14] C.Villani '02; L.Pareschi, G.Toscani, C.Villani '03

Choice of the penalization operator

- Since conservation of mass, momentum, and energy, as well as H-theorem for the entropy are satisfied, equilibrium states are Maxwellians.
- For the Landau equation, however, one has the additional difficulty of the diffusive nature of the operator $Q_L(f,f)$, which introduces a parabolic stiffness relating the time step to the square of the velocity mesh.
- The simple BGK-like penalization is not capable to avoid such a stiffness. A better choice in this case is given by the Fokker-Planck operator [15]

$$L_P(f) = \nabla_v \cdot \left(M[f] \nabla_v \left(\frac{f}{M[f]} \right) \right).$$

Note that, the use of a diffusive penalization term is essential in removing the parabolic stiffness.

[15] S.Jin, B.Yan '11; Q.Li, L.Pareschi, B.Yan '14

Principles of hybrid decomposition methods

- Couplings of atomistic or molecular, and more generally microscopic stochastic models, to macroscopic deterministic models is highly desirable in many applications. Similar arguments apply to numerical methods[16].
- This coupling play an important role in the case of kinetic equations. IMEX and exponential methods based on splitting represent a natural framework for such coupling since the homogeneous step can be written in the general form

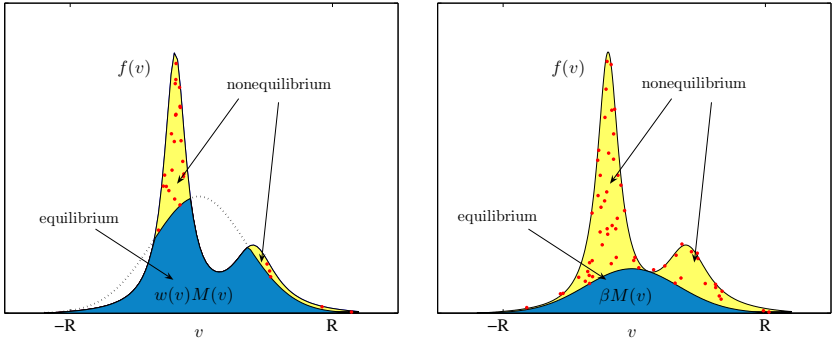
$$
\begin{aligned}
F^{(i)} &= a_i f^n + \sum_{j=1}^{i-1} A_{ij} \frac{P(F^{(j)})}{\mu} + \left(1 - a_i - \sum_{j=1}^{i-1} A_{ij}\right) M[f^n], \\
f^{n+1} &= \underbrace{w f^n + \sum_{i=1}^{\nu} W_i \frac{P(F^{(j)})}{\mu}}_{\textit{non equilibrium part}} + \underbrace{\left(1 - w - \sum_{i=1}^{\nu} W_i\right) M[f^n]}_{\textit{equilibrium part}}.
\end{aligned}
$$

- The main idea therefore is to treat the non equilibrium part by *stochastic particle methods* and the equilibrium part with *deterministic methods*.

[16] W.E, B.Engquist '03

Hybrid representation

The solution is represented at each space point as a combination of a nonequilibrium part (microscale) and an equilibrium part (macroscale)



Definition - hybrid function

Given a probability density $f(v)$, $v \in \mathbb{R}^d$ (i.e. $f(v) \geq 0$, $\int f(v)dv = 1$) and a probability density $M(v)$, $v \in \mathbb{R}^d$ called equilibrium density, we define $w(v) \in [0,1]$ and $\tilde{f}(v) \geq 0$ in the following way

$$w(v) = \begin{cases} \dfrac{f(v)}{M(v)}, & f(v) \leq M(v) \neq 0 \\ 1, & f(v) \geq M(v) \end{cases}$$

and $\tilde{f}(v) = f(v) - w(v)M(v)$. Thus $f(v)$ can be represented as

$$f(v) = \tilde{f}(v) + w(v)M(v).$$

Taking $\beta = \min_v\{w(v)\}$, and $\tilde{f}(v) = f(v) - \beta M(v)$, we have

$$\int \tilde{f}(v)dv = 1 - \beta.$$

Let us define for $\beta \neq 1$ the probability density

$$f_p(v) = \frac{\tilde{f}(v)}{1-\beta}.$$

The case $\beta = 1$ is trivial since it implies $f \equiv M$. Thus we recover the hybrid representation[17] as

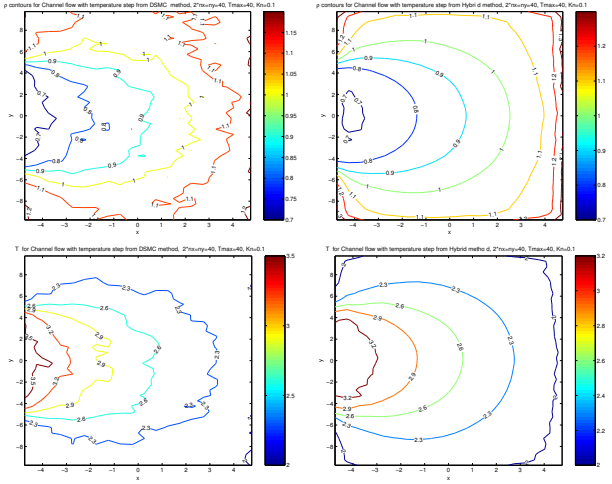
$$f(v) = (1-\beta)f_p(v) + \beta M(v).$$

Remark: Typically the procedure is applied only in a finite region Ω of the velocity domain leaving the tails represented by particles.

[17] R.Caflisch, L.Pareschi '99

Boltzmann equation: 2D channel flow

Comparison of results for ρ (left), T (right), DSMC (left), HM1 (right)[18].



[18] R.Caflisch, H.Chen, E. Luo, L.Pareschi AIAA '06

Thank you!

&

Happy 60th birthday Russ!