

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

Lecture 2: Asymptotic-preserving schemes (Part I)

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Lecture 2 Outline

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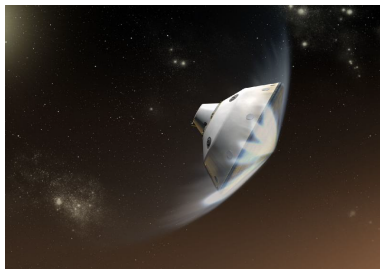
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Motivations

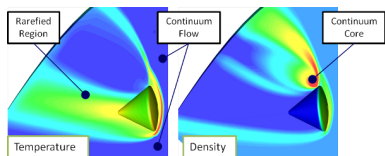


Intermediate Experimental Vehicle - ESA



NASA Mars Science Laboratory

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

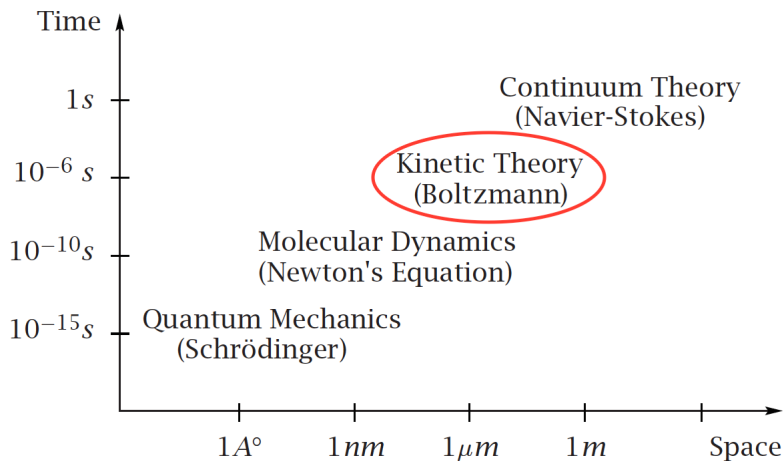


One of the most challenging phases of any space-planetary discovery mission is the stage of *hypersonic entering* into a planet's atmosphere. For the earth, reentry velocities range between 7.7 to 15 km/s.

- The spacecraft is exposed to various physical processes that is engendered by the synthesis of chemical kinetics, radiation physics, quantum mechanics and ablation effects with fluid dynamics.
- Due to the high altitude circumstances, the flow-regime characteristics are affected by the *breakdown of the continuum assumption*, which makes it impossible to simulate these cases with conventional CFD routines.
- Typically a model for a mixture of reacting gases is solved by DSMC (altitudes of 200 to 85 km) and coupled with a CFD solver for the *compressible Navier-Stokes equations* at low altitude (in the range 95 to 65 km) ¹.

¹G. Bird '94; J.N. Moss, C.E. Glassy, F.A. Greenz '06

Multiscale physics



The asymptotic-preserving (AP) property

- Numerically resolving the small scales may be computationally prohibitive and therefore one resorts on the use of some asymptotic analysis in order to derive *reduced models* which are valid in the small scales regime.
- Thus a *multi-physics* approach, that hybridizes the different models (and numerical methods) in a *domain-decomposition* framework, becomes necessary. This matching, however, is often very difficult.
- A different approach for such multiscale problems is the *asymptotic-preserving (AP)* method. The basic idea is to preserve the asymptotic procedure that lead to the reduced model in a discrete setting².
- The design of AP schemes needs special care for both time and space discretizations, but often, since we deal with *stiff problems*, the time discretization is more crucial.

²E.W. Larsen, J.E. Morel, W.F. Miller '87; F. Coron '91; S. Jin '99; L. P., G. Russo '11; P. Degond '11; G. Dimarco, L. P. '15

A simple illustrative example

A simple prototype example of *relaxation system* is given by³

Jin-Xin relaxation system

$$P^\varepsilon : \begin{cases} \partial_t u + \partial_x v & = 0, \\ \partial_t v + a \partial_x u & = -\frac{1}{\varepsilon}(v - f(u)), \end{cases} \quad (x, t) \in \mathbb{R} \times \mathbb{R}_+$$

The characteristic speeds are $\pm\sqrt{a}$. It corresponds to the original system in the *fluid scaling*: $t \rightarrow t/\varepsilon$, $x \rightarrow x/\varepsilon$. As $\varepsilon \rightarrow 0$ we get the *local equilibrium* $v = f(u)$ and we obtain

$$P^0 : \quad \partial_t u + \partial_x f(u) = 0.$$

Using the Chapman-Enskog expansion $v = f(u) + \varepsilon v_1$, under the *subcharacteristic condition* $a > |f'(u)|$, we obtain at $O(\varepsilon)$

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

³S.Jin, Z.Xin '95

The Boltzmann equation in the fluid-dynamic scaling

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

Kinetic model

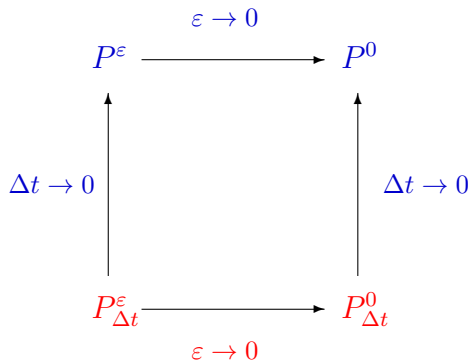
$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} Q(f), \quad x \in \Omega \subset \mathbb{R}^{d_x}, v \in \mathbb{R}^3,$$

which is written in this form after the scaling $x \rightarrow x/\varepsilon$, $t \rightarrow t/\varepsilon$ where $\varepsilon > 0$ is a nondimensional parameter (*Knudsen number*) proportional to the mean free path.

- As $\varepsilon \rightarrow 0$ formally $Q(f) = 0$ which implies $f = M[f]$. Therefore, the associated moment system is closed and corresponds to the *compressible Euler equations*. This result is independent of the choice of $Q(f)$ provided it admits Maxwellian as local equilibrium functions.
- For small but non zero values of ε , closed evolution equations for the moments can be derived by the *Chapman-Enskog expansion* $f = M[f] + \varepsilon f_1$. This leads to the *compressible Navier-Stokes equations* as a second order approximation in ε to the Boltzmann equation⁴. The choice of $Q(f)$ influences the Navier-Stokes system in terms of the *Prandtl number*.

⁴F. Golse '05

The AP diagram



In the diagram P^ε is the original singular perturbation problem and $P_{\Delta t}^\varepsilon$ its numerical approximation characterized by a discretization parameter Δt .

The *asymptotic-preserving (AP) property* corresponds to the request that $P_{\Delta t}^\varepsilon$ is a good (consistent and stable) discretization of P^0 as $\varepsilon \rightarrow 0$.

Numerical approaches

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

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

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*
 - ▶ *IMEX linear multistep methods*
 - ▶ *Exponential methods*
- All the different approaches share the difficulty of the inversion of the collision operator if evaluated implicitly.

The Implicit-Explicit (IMEX) paradigm

Consider a systems of differential equations in the form

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

where \mathcal{F} and \mathcal{G} , eventually obtained as finite-difference/element approximations of spatial derivatives, induce considerably different time scales.

- Fully **explicit solvers** suffer from a time step restriction induced by the stiff term \mathcal{G} . Since the problem is stiff as a whole implicit methods should be used.
- Fully **implicit solvers**, however, originate a nonlinear system of equations involving also the non stiff term \mathcal{F} .
- One may combine different time approximations to resolve stiff and non-stiff terms efficiently. These methods are referred to as **Implicit-explicit (IMEX)**⁵.
- A related approach, based on **Explicit exponential integrators**⁶, aim at solving exactly the linear stiff operator while keeping the nonlinear term explicit.

⁵U. Asher, S. Ruth, R. Spiteri, B. Wetton '95,'97; M. Carpenter, C. Kennedy '03; L. P., G. Russo '00,'05

⁶M.Hochbruck, A.Ostermann '12, L.P., G. Dimarco '11, L.P., Q. Li '15

Numerical requirements

The combination of the implicit and explicit method should satisfy suitable order conditions. For **Runge-Kutta (RK)** schemes additional mixed compatibility conditions are required.

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) property⁷.

Implicit method

- Stable for stiff systems, and good damping properties.
 - Computationally feasible in term of cost.
- ▶ The resulting scheme should be *Asymptotic Preserving (AP)* namely it should be consistent with the model reduction that occur in stiff regimes.

⁷S.Gottlieb, C-W.Shu, E.Tadmor '01, R.Spiteri, S.Ruth, '02

The simplest IMEX-AP scheme

Consider the Jin-Xin relaxation system solved by the simple IMEX scheme

IMEX Euler scheme

$$P_{\Delta t}^\varepsilon : \begin{cases} \frac{u^{n+1} - u^n}{\Delta t} + \partial_x v^n & = 0, \\ \frac{v^{n+1} - v^n}{\Delta t} + a \partial_x u^n & = -\frac{1}{\varepsilon}(v^{n+1} - f(u^{n+1})), \end{cases}$$

For small values of ε we get the **local equilibrium**

$$v^{n+1} = f(u^{n+1})$$

which substituted into the first equation gives

$$P_{\Delta t}^0 : \frac{u^{n+1} - u^n}{\Delta t} + \partial_x f(u^n) = 0.$$

IMEX Runge-Kutta methods⁸

IMEX Runge-Kutta

$$U^{(i)} = U^n + \Delta t \sum_{j=1}^{i-1} \tilde{a}_{ij} \mathcal{F}(U^{(j)}) + \Delta t \sum_{j=1}^{\nu} a_{ij} \mathcal{G}(U^{(j)}),$$

$$U^{n+1} = U^n + \Delta t \sum_{i=1}^{\nu} \tilde{w}_i \mathcal{F}(U^{(i)}) + \Delta t \sum_{i=1}^{\nu} w_i \mathcal{G}(U^{(i)}).$$

$\tilde{A} = (\tilde{a}_{ij})$, $\tilde{a}_{ij} = 0$, $j \geq i$ and $A = (a_{ij})$: $\nu \times \nu$ matrices and $\tilde{c} = (\tilde{c}_1, \dots, \tilde{c}_\nu)^T$, $\tilde{w} = (\tilde{w}_1, \dots, \tilde{w}_\nu)^T$, $c = (c_1, \dots, c_\nu)^T$, $w = (w_1, \dots, w_\nu)^T$.

- For *diagonally implicit schemes* (DIRK), $a_{ij} = 0$, $j > i$. They they guarantee that \mathcal{F} is evaluated explicitly.
- Schemes for which $\tilde{w}_j = \tilde{a}_{\nu j}$ and $w_j = a_{\nu j}$, $j = 1, \dots, \nu$ are called *globally stiffly accurate* (GSA).

⁸U. Ascher, S. Ruth, R. Spiteri '97, L.P., G. Russo '00

Order conditions

- IMEX-RK schemes are a particular case of *additive Runge-Kutta (ARK)* methods⁹. Further generalization are also possible¹⁰.
- Order conditions can be derived using a generalization of *Butcher 1-trees* to 2-trees.
- If $w_i = \tilde{w}_i$ and $c_i = \tilde{c}_i$ *mixed conditions* are automatically satisfied. This is not true for higher than third order accuracy

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

⁹M. Carpenter, C. Kennedy, '03

¹⁰A. Sandu, M. Günther '13

Design of IMEX-RK

Start with a p -order explicit SSP method and find the 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 $\gamma = (1 - \sqrt{2})/2$.

IMEX Linear Multistep Methods¹¹

IMEX Linear Multistep

$$U^{n+1} = \sum_{j=0}^{\nu-1} a_j U^{n-j} + \Delta t \sum_{j=0}^{\nu-1} b_j \mathcal{F}(U^{n-j}) + \Delta t \sum_{j=-1}^{\nu-1} c_j \mathcal{G}(U^{n-j}),$$

with starting values U^0, U^1, \dots, U^n .

- The schemes are characterized by the coefficients $a = (a_0, \dots, a_{\nu-1})^T$, $b = (b_0, \dots, b_{\nu-1})^T$, $c = (c_0, \dots, c_{\nu-1})^T$ and $c_{-1} \neq 0$.
- Methods for which $c_0 = c_1 = \dots = c_{\nu-1} = 0$ are referred to as implicit-explicit backward differentiation formula, *IMEX-BDF* in short.
- Note that *coupling conditions* in IMEX-LM can be easily satisfied (in contrast to IMEX Runge Kutta methods).
- Stability constraints usually increase with the order of the schemes. A-stable schemes have accuracy $p \leq 2$.

¹¹U.Ascher, S.Ruth, B.Wetton '95, W.Hundsdorfer, S.Ruth '07

Design of IMEX-LMM

Again we can start from an explicit SSP method and find the corresponding implicit method with good damping properties ($A(\alpha)$ -stability). Or we can start from an implicit method (BDF) and use the corresponding explicit scheme.

Second order IMEX-BDF

$$U^{n+1} = \frac{4}{3}U^n - \frac{1}{3}U^{n-1} + \frac{4}{3}\Delta t\mathcal{F}(U^n) - \frac{2}{3}\Delta t\mathcal{F}(U^{n-1}) + \frac{2}{3}\Delta t\mathcal{G}(U^{n+1}).$$

Third order SSP IMEX-LM

$$\begin{aligned} U^{n+1} &= \frac{3909}{2048}U^n - \frac{1367}{1024}U^{n-1} + \frac{873}{2048}U^{n-2} \\ &+ \frac{18463}{12288}\Delta t\mathcal{F}(U^n) - \frac{1271}{768}\Delta t\mathcal{F}(U^{n-1}) + \frac{8233}{12288}\Delta t\mathcal{F}(U^{n-2}) \\ &+ \frac{1089}{2048}\Delta t\mathcal{G}(U^{n+1}) - \frac{1139}{12288}\Delta t\mathcal{G}(U^n) - \frac{367}{6144}\Delta t\mathcal{G}(U^{n-1}) + \frac{1699}{12288}\Delta t\mathcal{G}(U^{n-2}). \end{aligned}$$

Hyperbolic relaxation systems

Consider the case of hyperbolic relaxation systems¹²

Hyperbolic system with relaxation (Full model)

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

$R: \mathbb{R}^N \rightarrow \mathbb{R}^N$ is a **relaxation operator** if there exists a $n \times N$ matrix Q with $\text{rank}(Q) = n < N$ 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 $\varepsilon \rightarrow 0 \Rightarrow R(U) = 0 \Rightarrow U = \mathcal{E}(u) \Rightarrow$ (subcharacteristic condition on $f(u)$)

Equilibrium system (Reduced model)

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

¹²G.Chen, D.Levermore, T.P.Liu, '94

AP property

In the case of hyperbolic system with relaxation we have the following result ¹³

Theorem (IMEX-RK)

If $\det A \neq 0$ then in the limit $\epsilon \rightarrow 0$, the IMEX-RK 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.

- To satisfy $\det A \neq 0$ it is necessary that $c \neq \tilde{c}$ (Type A schemes).
- The simplification assumption $c = \tilde{c}$ is possible if the matrix A can be written as (Type CK schemes)

$$\begin{pmatrix} 0 & 0 \\ a & \hat{A} \end{pmatrix}$$

with $\det(\hat{A}) \neq 0$ where \hat{A} is a $(\nu - 1) \times (\nu - 1)$ submatrix of A . However, the corresponding scheme may be inaccurate if the initial condition is not “well prepared” (initial layer).

¹³L.Pareschi, G.Russo, '05

AP property

In the case of IMEX-LM methods one has the following result ¹⁴

Theorem (IMEX-LM)

For arbitrary initial steps in the limit $\varepsilon \rightarrow 0$ an IMEX-BDF scheme ($w_j = 0, j = 0, \dots, s-1$) after s time steps becomes the explicit multistep scheme characterized by $a_j, \tilde{w}_j, j = 0, \dots, s-1$ applied to the limit system of conservation laws.

- Note that, if the initial steps are well-prepared it can be shown that any IMEX-LM scheme satisfy the above theorem.
- Of course, both for IMEX-RK and IMEX-LM these AP results do not guarantee any stability property of the method for fixed but non zero ε .

¹⁴G. Dimarco, L.Pareschi, '15

Stability

The A -stability of a IMEX scheme may be studied using the problem¹⁵

Test problem

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

This test problem characterizes the stability properties for linear systems

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

only 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 very difficult.

► Recent nonlinear stability and contractivity results by Higuera et al. '04-'09, Sandu and Günther '13, L.P. and Dimarco '13.

¹⁵U.Asher, S.Ruuth, R.Spiteri '97, J.Frank, W.Hundsdorfer, J.Verwer '97, L.P., G.Russo '00

Accuracy

Simple uniform error estimates can be based on the following argument.
 If $P_{\Delta t}^\varepsilon$ is a p -order approximation of P^ε then classical analysis gives

$$E_1 = \|P_{\Delta t}^\varepsilon - P^\varepsilon\| = O(\Delta t^p / \varepsilon^r), \quad 1 \leq r \leq p.$$

The AP-property typically gives

$$\|P_{\Delta t}^\varepsilon - P_{\Delta t}^0\| = O(\varepsilon), \quad \|P_{\Delta t}^0 - P^0\| = O(\Delta t^p).$$

From the previous estimates one gets immediately

$$E_2 = \|P_{\Delta t}^\varepsilon - P^\varepsilon\| = O(\varepsilon + \Delta t^p).$$

Taking the minimum between E_1 and E_2 one gets the *uniform estimate* ¹⁶

$$\|P_{\Delta t}^\varepsilon - P^\varepsilon\| = O(\Delta t^{p/(r+1)}).$$

¹⁶F.Golse, S.Jin, D.Levermore '99

A numerical example

Broadwell model

$$\partial_t \rho + \partial_x m = 0,$$

$$\partial_t m + \partial_x z = 0,$$

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

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 $\varepsilon \rightarrow 0$ we obtain

$$\partial_t \rho + \partial_x m = 0$$

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

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

Space discretizations

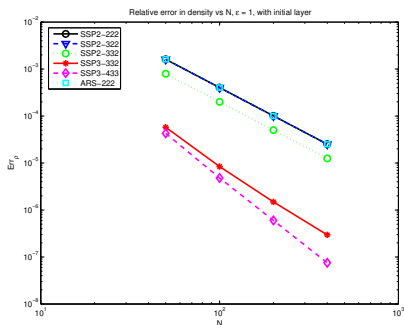
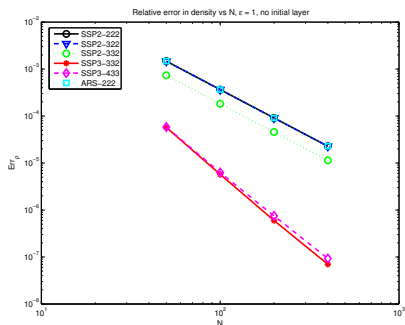
- We can adopt any finite difference/volume or spectral method to approximate the *spatial derivatives*, and use the standard (linear) stability analysis.
- In presence of *shocks and discontinuities* this stability analysis is not sufficient (nonlinear problems can develop discontinuous solutions in 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)* schemes¹⁷.

¹⁷A. Harten '87, T.Chan, X-D.Liu, S.Osher '94, G-S.Jang, C-W.Shu '95

Convergence rates

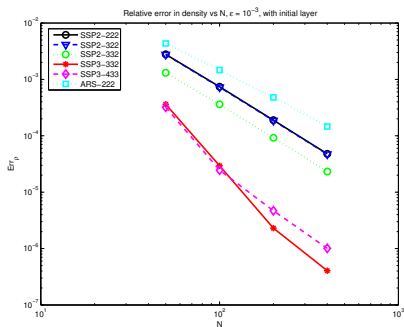
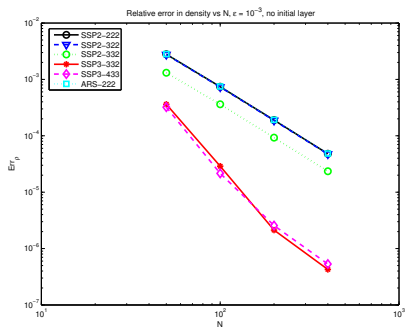
ϵ	1.0	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}
Scheme	Convergence rates for ρ						
IMEX-ARS	2.018	1.513	1.159	1.165	1.165	1.165	1.165
IMEX-SSP2	2.042	2.054	2.051	2.053	2.043	2.042	2.042
IMEX-ARSF	2.044	2.074	2.007	1.982	2.042	2.040	2.040
IMEX-SSP2F	2.050	2.064	2.061	2.065	2.056	2.055	2.055
IMEX-ARS3	2.963	3.013	2.982	2.860	2.482	2.060	2.044
IMEX-BHR	3.119	2.994	2.930	3.117	3.146	3.211	3.187
	Convergence rates for z						
IMEX-ARS	1.950	1.438	1.114	1.121	1.121	1.121	1.121
IMEX-SSP2	2.027	2.045	1.965	1.501	1.309	1.302	1.302
IMEX-ARSF	2.031	2.174	1.762	1.596	2.061	2.040	2.039
IMEX-SSP2F	2.036	2.034	2.038	2.368	2.127	2.052	2.051
IMEX-ARS3	2.982	2.970	2.471	2.386	2.041	2.003	1.999
IMEX-BHR	3.050	2.921	2.780	3.539	3.200	3.019	3.016

Convergence rates



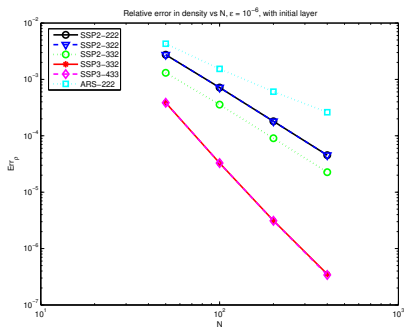
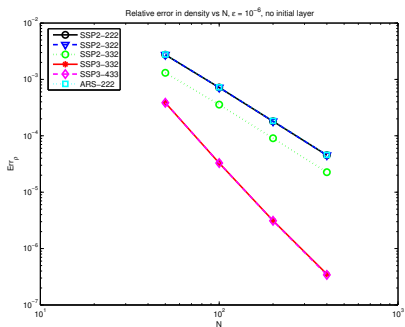
Relative error for different second and third order IMEX-RK schemes for the Broadwell equations with $\epsilon = 1$. Left: no initial layer. Right: initial layer.

Convergence rates



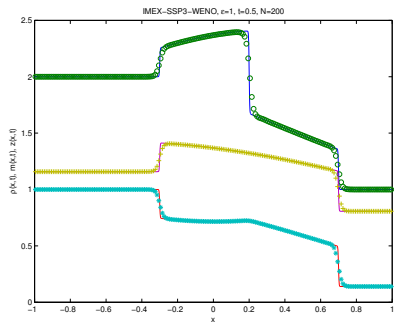
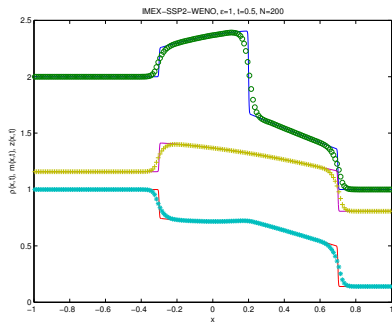
Relative error for different second and third order IMEX-RK schemes for the Broadwell equations with $\epsilon = 10^{-3}$. Left: no initial layer. Right: initial layer.

Convergence rates



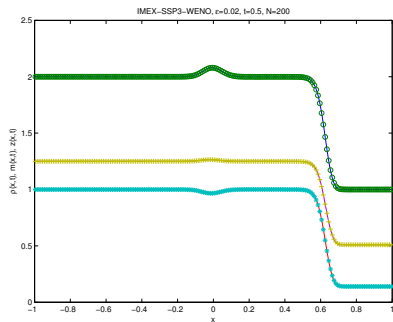
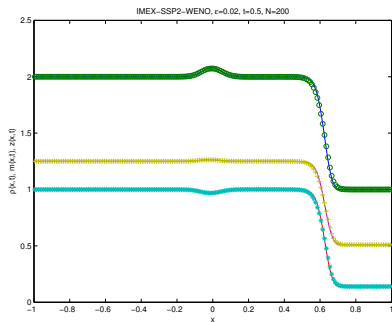
Relative error for different second and third order IMEX-RK schemes for the Broadwell equations with $\epsilon = 10^{-6}$. Left: no initial layer. Right: initial layer.

Shock test



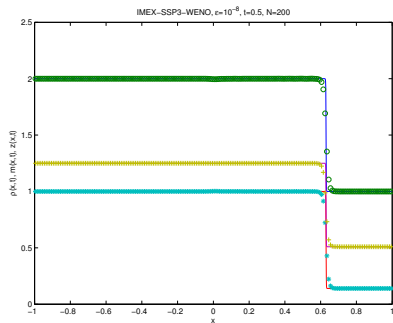
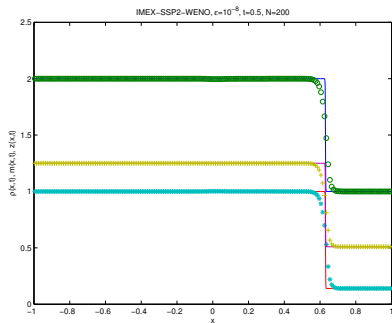
Numerical solution for second and third order SSP IMEX-RK schemes for the Broadwell equations with $\epsilon = 1$

Shock test



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

Shock test



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

Concluding remarks

- *IMEX-schemes* represent a powerful tool for the discretization of multiscale partial differential equations, for example where convection and stiff sources/diffusion are present.
- Other than the AP property, an *efficient implicit solver* is also one of the main ingredients in an IMEX scheme.
- They represent an alternative/complementary approach to domain-decomposition methods. The basic principles can be applied to any PDE where there is the presence of *multiple time/space-scales*.
- **Main problem**
 - ▶ How can we extend the previous approaches to the challenging case of the full Boltzmann equation, where the inversion of the stiff collision operator is computationally prohibitive?