High order unconditionally strong stability preserving multi-derivative implicit and IMEX Runge–Kutta methods with asymptotic preserving properties

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Motivation

Given a system of ODEs, generally resulting from a spatial discretization of a PDE, of the form

$$u_t = G(u)$$

that satisfies some forward Euler condition

Forward Euler condition:

$$\|u + \Delta t G(u)\| \leq \|u\| \quad \text{for all} \quad \Delta t \leq \Delta t_{\text{FE}},$$

where $\| \cdot \|$ is some convex functional (e.g. positivity).

Motivation

- In practice, we desire a higher order method that preserves the forward Euler condition, perhaps under a modified time-step restriction $\Delta t \leq \mathcal{C} \Delta t_{\mathsf{FE}}$.
- Higher order methods that can be written as convex combinations of forward Euler steps with $\mathcal{C} > 0$ will preserve the forward Euler condition, and are called *strong stability preserving* (SSP).
- $\mathcal{C}$ is called the SSP coefficient, and we generally want to devise methods that have a large $\mathcal{C}$.

Implicit Methods

- When concerned with linear stability properties, we turn to implicit methods, to alleviate the time-step restriction.
- Considering the SSP property: If G satisfies the forward Euler condition

$$\|u^n + \Delta t G(u^n)\| \leq \|u^n\| \quad \text{for all} \quad \Delta t \leq \Delta t_{\mathrm{FE}},$$

  then the backward Euler method

$$u^{n+1} = u^n + \Delta t G(u^{n+1})$$

  is unconditionally SSP.
- Even implicit methods suffer from an SSP step-size restriction for order $p > 1$!
- The SSP coefficient is usually bounded by twice the number of stages for a Runge–Kutta method.

Unconditionally SSP implicit methods: downwinding

Using (in addition to G) a second operator $\tilde{G}$ that approximates G and satisfies a **Downwind condition:**

$$\|u^n - \Delta t \tilde{G}(u^n)\| \leq \|u^n\| \quad \text{for all} \quad \Delta t \leq \Delta t_{\text{FE}},$$

Ketcheson (2011) found a family of implicit second order ($p = 2$) methods that are unconditionally SSP.

In this talk we will show how to obtain unconditionally SSP implicit methods up to fourth order, *if the operator* $\dot{G} \approx \frac{dG}{dt}$ *satisfies the* **Backward derivative condition:**

$$\|u - \Delta t^2 \dot{G}(u)\| \leq \|u\| \ \ \forall \ \Delta t^2 \leq \dot{k} \, \Delta t_{\text{FE}}^2,$$

for some $\dot{k} > 0$.

Two-derivative methods

- Multi-derivative Runge–Kutta methods have long been used for ODEs
- In 2014 they were considered for PDEs by Tsai et al. and Seal et al.
- For PDEs, the operator $\dot{G}$ is often computed by going back into the PDE, taking the derivative, and then discretizing (i.e. it is the discretization of the derivative, not the derivative of the discretization)
- Two-derivative Runge–Kutta methods make sense for numerical solution of hyperbolic PDEs, because we generally need to compute the Jacobian anyway, and that is the most computationally costly part of the process
- In a GPU computing paradigm, increasing the number of computations while reducing the cost of pulling data in and out of storage is beneficial for efficiency, and two-derivative methods help with this.
- In 2015, Andrew Christlieb asked me if these methods can be SSP ....

SSP Two-derivative methods

We need to understand the contribution of the second derivative term $\dot{G}$ to the strong stability of the method.

In 2016, we considered a "base condition" of the form

Second derivative condition:

$$\|u + \Delta t^2 \dot{G}(u)\| \leq \|u\| \quad \text{for all} \quad \Delta t^2 \leq \tilde{k}\, \Delta t_{\mathrm{FE}}^2,$$

where $\tilde{k} > 0$.

In 2018 we considered as a "base condition" the Taylor series condition

Taylor series condition:

$$\|u + \Delta t G(u) + \frac{1}{2}\Delta t^2 \dot{G}(u)\| \leq \|u\| \quad \text{for all} \quad \Delta t \leq \hat{k}\, \Delta t_{\mathrm{FE}},$$

where $\hat{k} > 0$.

SSP two-derivative methods

- We can write two-derivative methods as convex combinations of forward Euler and one of the base conditions, and these methods are then SSP, with an appropriate time-step restriction.
- But an implicit multi-derivative Runge–Kutta method will **not** be unconditionally SSP for order $p > 1$
- However, if we use $\dot{G}$ satisfies the **backward derivative condition**

$$\|u - \Delta t^2 \dot{G}(u)\| \leq \|u\| \quad \forall \;\; \Delta t^2 \leq \dot{k} \; \Delta t_{\mathsf{FE}}^2,$$

(for some $\dot{k} > 0$) and G satisfies the **forward Euler condition**

$$\|u + \Delta t G(u)\| \leq \|u\| \quad \forall \;\; \Delta t \leq \Delta t_{\mathsf{FE}},$$

we can obtain implicit multi-derivative Runge–Kutta methods up to order $p = 4$.

Unconditionally SSP two-derivative methods

We can prove that if the operator G satisfies the forward Euler condition, and the operator $\dot{G}$ satisfies the backward derivative condition (both conditionally), then the corresponding implicit methods are SSP *unconditionally*.

If a two-derivative Runge–Kutta method has only implicit evaluations of G and $\dot{G}$:

$$u^{(i)} = r_i u^n + \sum_{j=1}^{i-1} p_{ij} u^{(j)} + \Delta t d_{ii} G(u^{(i)}) + \Delta t^2 \dot{d}_{ii} \dot{G}(u^{(i)}), \qquad i = 1, ..., s,$$
$$u^{n+1} = u^{(s)}.$$

and if all the coefficients $r_i, p_{ij}, and d_{ii}$ are non-negative, and $\dot{d}_{ii}$ are non-positive, **then the method is unconditionally SSP.**

Unconditionally SSP two-derivative methods: second order

The one-stage, second order method is simply the implicit Taylor series method

$$u^{n+1} = u^n + \Delta t G(u^{n+1}) - \frac{1}{2}\Delta t^2 \dot{G}(u^{n+1}).$$

This is not very novel, but it gives us insight into why the negative coefficient is needed for $\dot{G}$.

Unconditionally SSP two-derivative methods: third order

A two-stage, third order unconditionally SSP implicit two-derivative Runge–Kutta method is given by the Shu-Osher coefficients

$$\mathsf{P} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad \mathsf{Re} = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

$$\mathsf{D} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad \dot{\mathsf{D}} = \begin{bmatrix} -\frac{1}{6} & 0 \\ 0 & -\frac{1}{3} \end{bmatrix}.$$

Unconditionally SSP two-derivative methods: fourth order

A five-stage, fourth order unconditionally SSP implicit multi-derivative Runge–Kutta method is given by the Shu-Osher coefficients

$$diag(\mathrm{D}) = \begin{bmatrix} 0.660949255604937 \\ 0.242201390400848 \\ 1.137542996287740 \\ 0.191388711018110 \\ 0.625266691721946 \end{bmatrix}, \quad diag(\dot{\mathrm{D}}) = \begin{bmatrix} -0.177750705279127 \\ -0.354733903778084 \\ -0.403963513682271 \\ -0.161628266349058 \\ -0.218859021269943 \end{bmatrix}$$

$$P = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0.084036809261019 & 0.915963190738981 & 0 & 0 & 0 \\ 0.001511648458457 & 0 & 0.090254853867587 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$

$$\mathrm{Re} = [1, 0, 0, 0.908233497673956, 0]^T .$$

We were unable to find any fifth order methods that satisfy the conditions.

Why is this interesting?

These methods are applicable and unconditionally SSP whenever:

- G satisfies **forward Euler condition**

$$\|u + \Delta t G(u)\| \leq \|u\| \quad \forall \ \Delta t \leq \Delta t_{\mathsf{FE}} > 0,$$

- $\dot{G}$ satisfies the **backward derivative condition**

$$\|u - \Delta t^2 \dot{G}(u)\| \leq \|u\| \quad \forall \ \Delta t^2 \leq \dot{k} \, \Delta t_{\mathsf{FE}}^2,$$

  for some $\dot{k} > 0$.

The forward Euler condition is a natural one and satisfied by most operators G for the convex functionals $\| \cdot \|$ of interest.

The backward derivative condition is actually more natural than it seems at first glance.[1] But first ... let's extend this to implicit-explicit (IMEX) methods.

[1] If it seemed natural at first glance, we would have considered it in 2016

SSP IMEX multi-derivative methods

Now we are given the problem

$$u_t = F(u) + G(u),$$

where the operators satisfy the following conditions:

$$\textbf{Condition 1:} \quad \|u + \Delta t F(u)\| \leq \|u\| \quad \text{for all} \quad \Delta t \leq \Delta t_{\mathrm{FE}},$$

for some $\Delta t_{\mathrm{FE}} > 0$, and

$$\textbf{Condition 2:} \quad \|u + \Delta t G(u)\| \leq \|u\| \quad \text{for all} \quad \Delta t \leq k \Delta t_{\mathrm{FE}}.$$

(where $k > 0$ can be of any size).

$$\textbf{Condition 3:} \quad \|u - \Delta t^2 \dot{G}(u)\| \leq \|u\| \quad \text{for all} \quad \Delta t^2 \leq \dot{k}\, \Delta t_{\mathrm{FE}}^2,$$

(where $\dot{k} > 0$ can be of any size).

SSP IMEX multi-derivative methods

To evolve in time an equation of the form:

$$u_t = F(u) + G(u),$$

where the SSP time-step restriction coming from F is of a reasonable size, but the SSP time-step restriction coming from G is very small, we extend the implicit methods to an IMEX formulation:

$$\begin{aligned} u^{(i)} &= r_i u^n + \sum_{j=1}^{i-1} p_{ij} u^{(j)} + \sum_{j=1}^{i-1} w_{ij} \left(u^{(j)} + \frac{\Delta t}{r} F(u^{(j)}) \right) \\ &\quad + \Delta t d_{ii} G(u^{(i)}) + \Delta t^2 \dot{d}_{ii} \dot{G}(u^{(i)}), \qquad i = 1, ..., s, \\ u^{n+1} &= u^{(s)}. \end{aligned}$$

SSP IMEX multi-derivative methods

Given operators F and G that satisfy Conditions 1, 2, and 3, with values $\Delta t_{\text{FE}} > 0$, $k > 0$, $\dot{k} > 0$, for some convex functional $\| \cdot \|$, and if the method

$$U = \text{R}\text{e}u^n + \text{P}U + \text{W}\left(U + \frac{\Delta t}{r} F(U) \right) + \Delta t \text{D} G(U) + \Delta t^2 \dot{\text{D}} \dot{G}(U),$$

with $r > 0$ satisfies the conditions

$$\text{Re} \geq 0, \quad \text{P} \geq 0, \quad \text{W} \geq 0, \quad \text{D} \geq 0, \quad \dot{\text{D}} \leq 0,$$

then it preserves the strong stability property $\|u^{n+1}\| \leq \|u^n\|$ under the time-step condition $\Delta t \leq r \Delta t_{\text{FE}}$.

Can we find such SSP IMEX multi-derivative methods?

Yes! Second order:

$$\mathrm{W} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1/2 & 0 \end{bmatrix}, \quad \mathrm{P} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1/2 & 0 & 0 \end{bmatrix}, \quad \mathrm{Re} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix},$$

and

$$diag(\mathrm{D}) = \begin{bmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{bmatrix}, \quad diag(\dot{\mathrm{D}}) = -\begin{bmatrix} 0 \\ \frac{1}{2} \\ 0 \end{bmatrix},$$

with $r = 1$.

Can we find third order SSP IMEX multi-derivative methods?

Yes – but the coefficients are not pretty.

$$W = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0.058453072749259 & 0 & 0 & 0 & 0 & 0 \\ 0.764266518291495 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.292520982667463 & 0 & 0 & 0 \\ 0.173788618990251 & 0 & 0 & 0.281050180194829 & 0 & 0 \\ 0.016811671845949 & 0 & 0 & 0.448630511341543 & 0 & 0 \end{pmatrix},$$

$$P = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0.253395246357353 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.235733481708505 & 0 & 0 & 0 & 0 \\ 0 & 0.123961833526104 & 0 & 0 & 0 & 0 \\ 0.409037644509411 & 0.136123556305509 & 0 & 0 & 0 & 0 \\ 0.203353399602184 & 0 & 0 & 0 & 0.331204417210324 & 0 \end{pmatrix},$$

Third order SSP IMEX multi-derivative methods

$$\text{Re} = \begin{pmatrix} 1 \\ 0.688151680893388 \\ 0 \\ 0.583517183806433 \\ 0 \\ 0 \end{pmatrix}.$$

$$diag(\text{D}) = \begin{pmatrix} 0 \\ 2 \\ 0.388820513661584 \\ 0.083529464436389 \\ 1.793313488277995 \\ 0 \end{pmatrix}, \quad diag(\dot{\text{D}}) = -\begin{pmatrix} 0.871358934880525 \\ 0.856842702601821 \\ 0 \\ 0 \\ 2 \\ 0.205134529930013 \end{pmatrix}.$$

Note that $d_{ii} + \left|\dot{d}_{ii}\right| > 0$ for each stage i.

Is this useful?

Can we justify the backward derivative condition?[2]

$$\|u - \Delta t^2 \dot{G}(u)\| \leq \|u\| \quad \text{for all} \quad \Delta t^2 \leq \dot{k}\, \Delta t_{\mathsf{FE}}^2,$$

Yes! Kinetic equations with hyperbolic limit:

$$u_t = T(u) + \frac{1}{\varepsilon} Q(u)$$

may have this property.

[2]in fact, I just need an unconditional implicit condition, not a conditional explicit condition.

Some examples

An ODE model:

$$\begin{cases} u_1' = u_2, \\ u_2' = \dfrac{1}{\varepsilon} f(u_1)\left(g(u_1) - u_2\right), \end{cases}$$

where f and g are some functions of u_1, and $f(u_1) > 0$. We have

$$\dot{Q}(u) = -f(u_1)Q(u).$$

A hyperbolic relaxation PDE

$$\begin{cases} \partial_t u_1 + \partial_x u_2 = 0, \\ \partial_t u_2 + \partial_x u_1 = \dfrac{1}{\varepsilon}\left(F(u_1) - u_2\right), \end{cases}$$

where F is some function of u_1. It can be verified that

$$\dot{Q}(u) = -Q(u).$$

The Broadwell model

he Broadwell model is a simple discrete velocity kinetic model:

$$\begin{cases} \partial_t f_+ + \partial_x f_+ = \frac{1}{\varepsilon}(f_0^2 - f_+ f_-), \\ \partial_t f_0 = -\frac{1}{\varepsilon}(f_0^2 - f_+ f_-), \\ \partial_t f_- - \partial_x f_- = \frac{1}{\varepsilon}(f_0^2 - f_+ f_-), \end{cases} \tag{1}$$

where $f_+ = f_+(t,x)$, $f_0 = f_0(t,x)$, and $f_- = f_-(t,x)$ denote the densities of particles with speed 1, 0, and -1, respectively.
Define $f = (f_+, f_0, f_-)^T$, $T(f) = (-\partial_x f_+, 0, \partial_x f_-)^T$, and
$Q(f) = (f_0^2 - f_+ f_-, -(f_0^2 - f_+ f_-), f_0^2 - f_+ f_-)^T$
We see that

$$\dot{Q}(f) = -\rho Q(f).$$

The Bhatnagar-Gross-Krook (BGK) model

The BGK model is a widely used kinetic model introduced to mimic the full Boltzmann equation:

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon}(M - f), \quad x, v \in \mathbb{R}^d,$$

where $f = f(t, x, v)$ is the probability density function and M is the Maxwellian:

$$M(t, x, v) = \frac{\rho(t, x)}{(2\pi T(t, x))^{d/2}} \exp\left(-\frac{|v - u(t, x)|^2}{2T(t, x)}\right),$$

the density ρ, bulk velocity u and temperature T are given by the moments of f. Here we have

$$\dot{Q}(f) = -Q(f).$$

SSP multi-derivative IMEX for kinetic equations with hyperbolic limit

- **"Unconditional" positivity:** These multi-derivative IMEX methods of 2nd and 3rd order preserve positivity of the solution under a step-size condition that depends only on T, not on Q or (more importantly) ε.
- **Asymptotic preserving:** These methods are asymptotic preserving as long as $\mathrm{D} + \left|\dot{\mathrm{D}}\right| > 0$.
- **Discrete entropy decay:** In the case of the Broadwell model and BGK equation, the SSP property can also be used to prove the discrete entropy decay property of the numerical method.

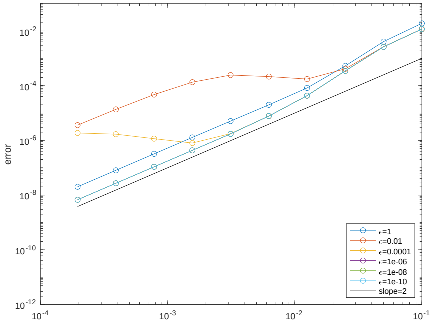
Numerical Examples: The Broadwell model

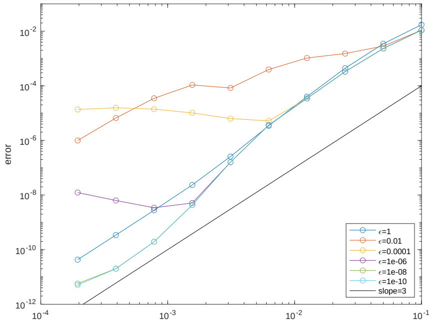
Consider the Broadwell model (1) on the domain $x \in [0, 2]$ with periodic boundary condition, with inconsistent initial data

$$
\begin{aligned}
f_+(0,\cdot) &= 1 + 0.2\exp(0.3\sin(\pi x)), \quad f_-(0,\cdot) = \exp(0.2\cos(2\pi x)),\\
f_0(0,\cdot) &= \frac{1}{1+0.3\sin(\pi x)}.
\end{aligned}
$$

We discretize in space by the fifth order finite volume positivity preserving WENO scheme (Shu & Zhang).
The collision operator Q is evaluated pointwise on the Gauss quadrature points in each cell.
CFL number as $\Delta t = \frac{1}{2}\Delta x$, evolve the solution up to final time $T = 0.1$.
The error is computed by the L^2 norm of the difference between the numerical solution and one with a refined mesh.

Numerical Examples: The Broadwell model





Second order (left) and third order (right). We see the design order of accuracy in the kinetic regime ($\varepsilon = O(1)$ and Δt is relatively small) and the fluid regime ($\varepsilon \ll 1$ and Δt is not very small), while in the intermediate regime (when ε and Δt are comparable) one can see some order reduction.

Numerical Examples: The BGK equations

We consider the 1D BGK model on the physical domain $x \in [0, 2]$ with periodic boundary condition, and inconsistent initial data given by

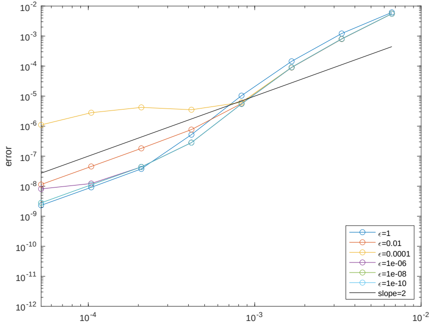
$$f(0, x, v) = 0.7M[\tilde{\rho}(x), \tilde{u}(x), \tilde{T}(x)](v) + 0.3M[\tilde{\rho}(x), -0.5\tilde{u}(x), \tilde{T}(x)](v),$$

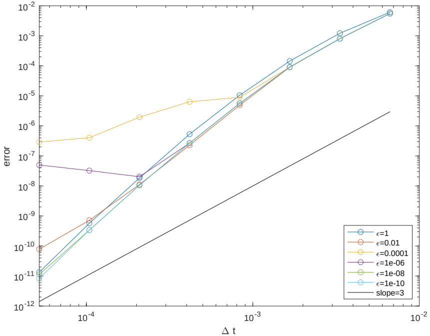
with

$$\tilde{\rho}(x) = 1 + 0.2\sin(2\pi x), \quad \tilde{u}(x) = 1, \quad \tilde{T}(x) = \frac{1}{1 + 0.2\sin(\pi x)}.$$

The velocity domain is truncated into $[-v_{max}, v_{max}]$ with $v_{max} = 15$ and discretized with $N_v = 150$ grid points.

Numerical Examples: The BGK equations





Left: Clear 2nd order accuracy when Δt is small enough (so that the time error dominates) for both $\varepsilon = O(1)$ and $\varepsilon \ll 1$. Order reduction in the intermediate regime.

For the 3rd order scheme, when $\varepsilon = O(1)$ or $\varepsilon \ll 1$, the error converges at a **higher** than expected rate even for the smallest Δt in the simulation, which suggests that the spatial error is still dominating.

Conclusions

- Using the backward derivative condition gives us unconditional SSP implicit methods.
- We can extend these to IMEX methods where the SSP condition depends only on the explicit part.
- The backward derivative arises naturally from a class of equations that are of interest (kinetic equations with hyperbolic limit).
- We can obtain 3rd order IMEX methods that are asymptotic preserving and positivity preserving, and have a decaying discrete entropy property, under a time-step that is independent of the term that is handled implicitly.

Happy Birthday!