Strong Stability Preserving Time Discretizations

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Happy Birthday Antony!

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Motivation

Consider the hyperbolic partial differential equation

$$U_t + f(U)_x = 0.$$

Method of lines approach: we semi-discretize the problem in space, to obtain some ODE of the form

$$\boldsymbol{u}_t = F(\boldsymbol{u})$$

and we evolve this ODE in time using standard methods such as Runge–Kutta or multi-step methods.

- If the solution is discontinuous, then linear L_2 stability analysis is not sufficient for convergence. In that case, we try to build spatial discretizations which satisfy some nonlinear stability properties.
- Sometimes we want our scheme to satisfy non-L_2 properties: positivity, maximum-principle preserving, total variation diminishing, or some non-oscillatory property.

Motivation

Such methods include

- TVD or TVB limiters
- Positivity or maximum principle preserving
- ENO or WENO schemes

These nonlinearly stable spatial discretizations are designed to satisfy a specific property when coupled with forward Euler, under some time-step restriction.

Motivation

Consider ODE system (typically from PDE)

$$\boldsymbol{u}_t = F(\boldsymbol{u}),$$

where spatial discretization $F(\boldsymbol{u})$ is carefully chosen[1] so that the solution from the forward Euler method

$$\boldsymbol{u}^{n+1} = \boldsymbol{u}^n + \Delta t F(\boldsymbol{u}^n),$$

satisfies the monotonicity requirement

$$||\boldsymbol{u}^{n+1}|| \leq ||\boldsymbol{u}^n||,$$

in some norm, semi-norm or convex functional $|| \cdot ||$, for a suitably restricted timestep

$$\Delta t \leq \Delta t_{\mathsf{FE}}.$$

[1] e.g. TVD, TVB, ENO, WENO

Motivation

- We spend a lot of effort to design spatial discretizations which satisfy certain nonlinear, non-inner product stability properties[2] when coupled with forward Euler.
- But then we want the properties to carry over when the spatial discretization is coupled with higher order time-stepping methods (for both accuracy and linear stability reasons)

[2] such as TVD or TVB limiters, positivity or maximum-principle preserving limiters or methods, or ENO or WENO schemes

The Main Idea

The trick is to decompose a higher order method into convex combinations of forward Euler so that if the spatial discretization $F(\boldsymbol{u})$ satisfies the strong stability property

$$||\boldsymbol{u}^n + \Delta t F(\boldsymbol{u}^n)|| \leq ||\boldsymbol{u}^n|| \quad \text{for} \quad \Delta t \leq \Delta t_{\text{FE}}$$

then the Runge–Kutta or multistep method will preserve this property, so that

$$||\boldsymbol{u}^{n+1}|| \leq ||\boldsymbol{u}^n|| \quad \text{for} \quad \Delta t \leq \mathcal{C} \Delta t_{\text{FE}}.$$

Decoupling the analysis

$\mathcal{C}$ is a property only of the time-integrator.
Δt_{FE} is a property of the spatial discretization.

The Main Idea

SSP methods give you a guarantee of provable nonlinear stability

- in arbitrary convex functionals,
- for arbitrary starting values
- for arbitrary nonlinear, non autonomous equations

provided only that forward Euler strong stability is satisfied.

This condition is clearly sufficient. It turns out it is also necessary.

Bounds and Barriers

This is a very strong property, so it should not be surprising that it is associated with time-step bounds and order barriers.

SSP Bounds and Barriers

- Explicit SSP Runge–Kutta methods have order $p \leq 4$ and $\mathcal{C}_{\text{eff}} \leq 1$.
- Explicit SSP multi-step methods do not have an order barrier, but they have the same bound $\mathcal{C}_{\text{eff}} = 1$.
- Any explicit general linear method have $\mathcal{C}_{\text{eff}} \leq 1$.
- Explicit multi-step multi-stage methods have $p > 4$ with better $\mathcal{C}_{\text{eff}}$.
- All implicit SSP Runge–Kutta methods ever found have $\mathcal{C}_{\text{eff}} \leq 2$.
- Implicit SSP Runge–Kutta methods have order $p \leq 6$.
- Implicit SSP multi-step methods do not have an order barrier, but we can prove $\mathcal{C}_{\text{eff}} \leq 2$.
- Implicit SSP multi-step multi-stage methods also have $\mathcal{C}_{\text{eff}} \leq 2$.
- We conjecture that $\mathcal{C}_{\text{eff}} \leq 2$ for any general linear method.

Multi-derivative methods

If we want to consider multistage multi derivative methods, we need a new condition that includes the derivative.
Once again, the conservation law

$$U_t + f(U)_x = 0$$

is semi-discretized

$$u_t = F(u)$$

and we assume that F satisfies the *forward Euler* condition:

$$\|U^n + \Delta t F(U^n)\| \leq \|U^n\| \quad \text{for} \quad \Delta t \leq \Delta t_{FE} \tag{1}$$

and the second derivative condition:

$$\|U^n + \Delta t^2 \dot{F}(U^n)\| \leq \|U^n\| \quad \text{for} \quad \Delta t \leq K \Delta t_{FE}. \tag{2}$$

Formulating an optimization problem for multi-derivative methods

Given conditions (1) and (4) we can show that if the MDMS method is written in the form

$$y = u^n + \Delta t A F(y) + \Delta t^2 \hat{A} \dot{F}(y) \tag{3}$$

we can add the terms rAy and $\hat{r}\hat{A}y$ to both sides to obtain:

$$\begin{aligned} \left(I + rA + \hat{r}\hat{A}\right) y &= u^n + rA\left(y + \frac{\Delta t}{r} F(y)\right) + \hat{r}\hat{A}\left(y + \frac{\Delta t^2}{\hat{r}} \dot{F}(y)\right) \\ y &= Ru^n + P\left(y + \frac{\Delta t}{r} F(y)\right) + Q\left(y + \frac{\Delta t^2}{\hat{r}} \dot{F}(y)\right) \end{aligned}$$

where

$$R = \left(I + rA + \hat{r}\hat{A}\right)^{-1} \qquad P = rRA \qquad Q = \hat{r}R\hat{A}$$

Formulating an optimization problem for multi-derivative methods

$$y \;=\; Ru^n + P\left(y + \frac{\Delta t}{r}F(y)\right) + Q\left(y + \frac{\Delta t^2}{\hat{r}}\dot{F}(y)\right)$$

Now, we can clearly see that if $r = \sqrt{\hat{r}}K$ then this method preserves the strong stability condition $\|u^{n+1}\| \leq \|u^n\|$ under the time-step restriction $\Delta t \leq r\Delta t_{FE}$ as long as

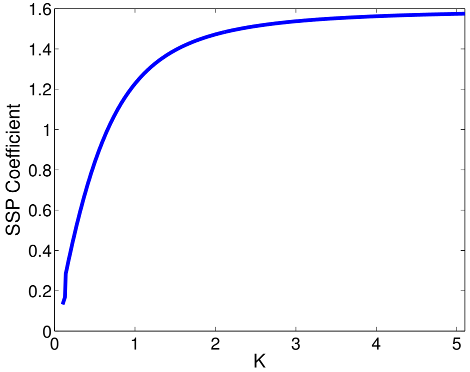
1. $R + P + Q = I$ (which is satisfied because $R + rRA + \hat{r}R\hat{A} = (I + rA + \hat{r}\hat{A})R = I$)
2. $Re \geq 0$, component wise, where e is a vector of ones.
3. $P \geq 0$ component wise
4. $Q \geq 0$ component wise

Optimal third order MSMD methods

Many two-stage two-derivative third order methods exist.

For each K the optimal method depends on resulting optimal $\mathcal{C}$ depends on the value of K. We found optimal methods for the range $0.1 \leq K \leq 5$. The interesting thing is that these optimal methods all have a Taylor series method as the first stage, with Δt replaced by $a\Delta t$, where

$$a = \frac{1}{r}\left(K\sqrt{K^2+2} - K^2\right).$$

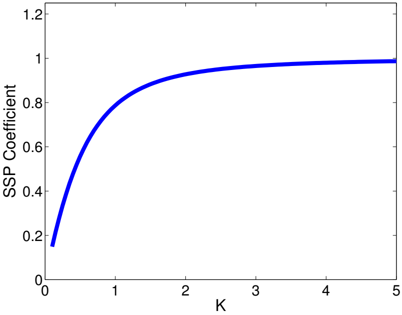


Optimal fourth order MSMD methods

The two-stage two-derivative fourth order method is unique:

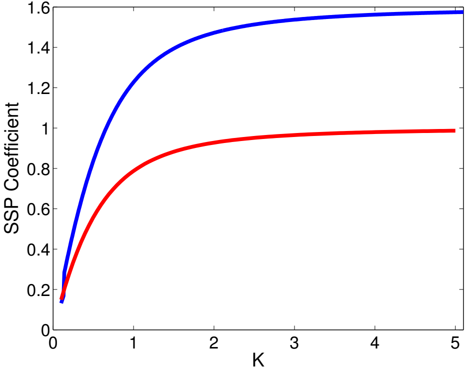
$$
\begin{aligned}
U^* &= U^n + \frac{\Delta t}{2} F(U^n) + \frac{\Delta t^2}{8} \dot{F}(U^n) \\
U^{n+1} &= U^n + \Delta t F(U^n) + \frac{\Delta t^2}{6} (\dot{F}(U^n) + 2\dot{F}(U^*)).
\end{aligned}
$$

The first stage of the method is a Taylor series method with $\frac{\Delta t}{2}$, while the second stage can be written as a linear combination of a forward Euler and a vanishing energy term (but not a Taylor series term). The SSP coefficient of this method is larger as K increases.



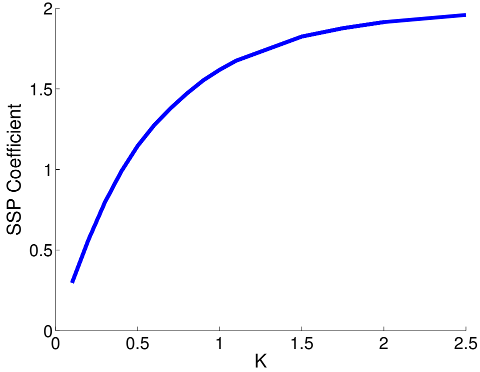
Comparison of optimal SSP two stage two derivative methods

For 2-stage, 2-derivative methods, the SSP coefficients of the third and fourth order methods have similar looking curves, but the SSP coefficient of the third order methods (blue) is much larger than that of the fourth order method (red).



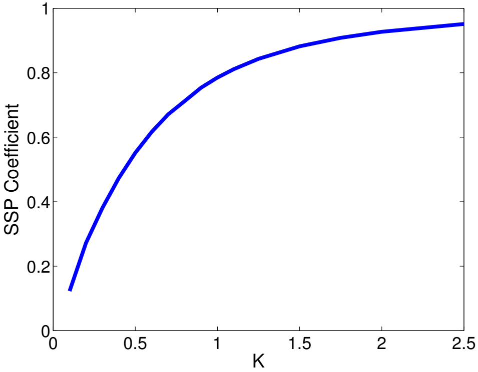
Optimal fourth order MSMD methods

If we increase the number of stages to three, we can construct whole families of methods that obtain fourth-order accuracy, and are SSP with a larger allowable time step.



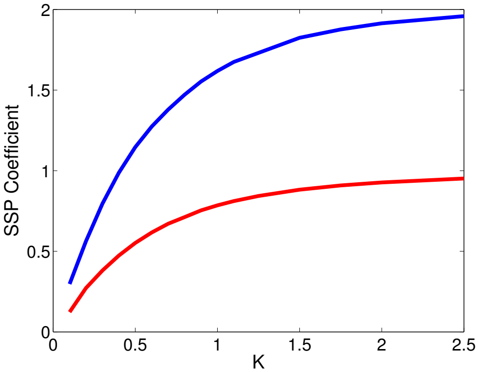
Optimal fifth order MSMD methods

Three stage fifth order methods can be found, with SSP coefficients that grow with K.
These methods break the explicit SSP Runge–Kutta order barrier.



Comparison of optimal SSP three stage two derivative methods

For 3-stage, 2-derivative methods, the SSP coefficients of the fourth and fifth order methods have similar looking curves, but the SSP coefficient of the fourth order methods (blue) is much larger than that of the fifth order method (red).



How SSP MSMD methods perform in practice

We look at a linear advection equation $u_t = u_x$ with a weighted essentially non oscillatory (WENO) method in space and the time-stepping method

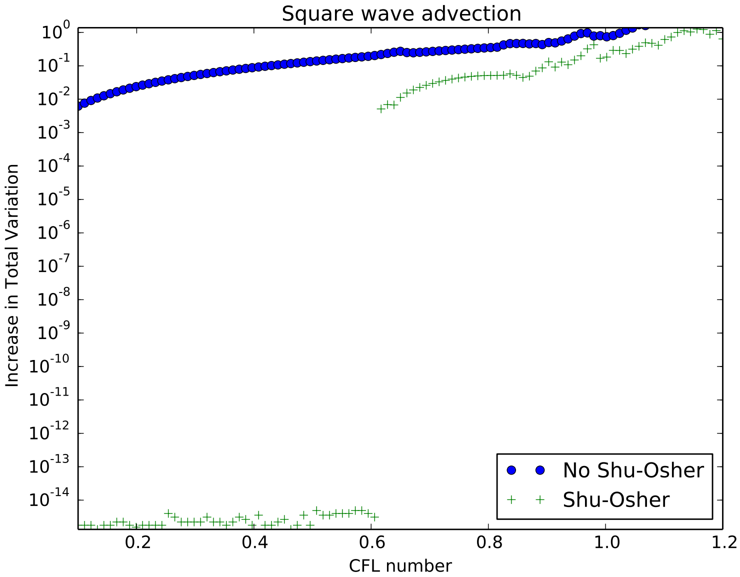
$$\begin{aligned} y^* &= y^n + \frac{2}{3}\Delta t W\left(F^n + \frac{1}{3}\Delta t \dot{F}^n\right) \\ u^{n+1} &= u^n + \Delta t W\left(\frac{5}{8}F^n + \frac{3}{8}F^* + \frac{1}{8}\Delta t(\dot{F}^n + \dot{F}^*)\right) \end{aligned}$$

which can also be written as:

$$\begin{aligned} y^* &= y^n + \frac{2}{3}\Delta t W\left(F^n + \frac{1}{3}\Delta t \dot{F}^n\right) \\ u^{n+1} &= \frac{7}{16}u^n + \frac{9}{16}y^* + \Delta t W\left(\frac{1}{4}F^n + \frac{3}{8}F^* + \frac{1}{8}\Delta t \dot{F}^*\right) \end{aligned}$$

These recent results due to David Seal.

How SSP MSMD methods perform in practice



Conclusions

SSP Runge–Kutta methods give you a guarantee of provable nonlinear stability in arbitrary convex functionals, for arbitrary starting values for arbitrary nonlinear, non autonomous equations provided only that forward Euler strong stability is satisfied.
SSP multistage multi derivative methods give you this same guarantee, provided that the second derivative condition:

$$\|U^n + \Delta t^2 \dot{F}(U^n)\| \leq \|U^n\| \quad \text{for} \quad \Delta t \leq K \Delta t_{FE}.$$

is satisfied as well.
Future work:

- Methods with a forward Euler and Taylor series condition (already in progress).
- Sixth order methods.
- More testing in practice.

Thank You!