Stability of time discretizations for semi-discrete high order schemes for time-dependent PDEs

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Introduction

We are interested in solving an evolutionary PDE, such as a hyperbolic conservation law

$$u_t + f(u)_x = 0$$

or a convection-diffusion equation

$$u_t + f(u)_x = (a(u)u_x)_x$$

where $a(u) \geq 0$, as well as the multi-dimensional cases.

We will use methods of lines, namely we first discretize the spatial derivatives to obtain an ODE system

$$\frac{d}{dt}u = L(u), \tag{1}$$

where L is the spatial discretization operator (which may be linear or nonlinear). The spatial discretization could be a finite difference method, a finite element method (including discontinuous Galerkin method), a spectral method, etc.

We assume that the spatial discretization is stable. That is, we assume that the solution to the method of lines ODE (1) satisfies

$$\|u(t)\| \leq \|u(0)\| \tag{2}$$

(strong stability) or

$$\|u(t)\| \leq C(t)\|u(0)\| \tag{3}$$

for some constant $C(t)$ depending on t (stability), for some norm, semi-norm, or convex functional $\| \cdot \|$ (e.g. L^2 norm, L^∞ norm, total variation (TV) semi-norm, entropy, ...).

Our objective is to maintain the strong stability (2) or the stability (3) property with a high order accurate time discretization. We will consider both linear and nonlinear problems, with three different types of time disretizations.

SSP time discretization

The strong stability preserving (SSP) high order time discretization, originally called the total variation diminishing (TVD) time discretization (Shu, SISSC 1988; Shu and Osher, JCP 1988), was designed to guarantee strong stability for nonlinear problems.

The SSP framework is as follows. We assume the Euler forward time discretization for the method of lines ODE is strongly stable

$$\|u + \Delta t L(u)\| \leq \|u\|, \tag{4}$$

for a certain norm, semi-norm or convex functional, under a suitable CFL condition

$$\Delta t \leq \Delta t_0. \tag{5}$$

Then the SSP high order Runge-Kutta time discretization satisfies the strong stability property

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

for the same norm, semi-norm or convex functional, under a modified CFL condition

$$\Delta t \leq c\Delta t_0,$$

with the SSP coefficient $c > 0$. Similar definitions can be made for high order multi-step methods or hybrid multi-step Runge-Kutta methods.

The idea is very simple: every stage in the SSP Runge-Kutta method is a convex combination of forward Euler operators.

For example, a second order SSP Runge-Kutta method is:

$$
\begin{aligned}
u^{(1)} &= u^n + \Delta t L(u^n) \\
u^{n+1} &= \frac{1}{2}u^n + \frac{1}{2}u^{(1)} + \frac{1}{2}\Delta t L(u^{(1)}).
\end{aligned}
\tag{6}
$$

Clearly, if the assumption (4) for Euler forward is satisfied under the CFL condition (5), then, under the same CFL condition, we have

$$\|u^{(1)}\| \leq \|u^n\|$$

and

$$\begin{aligned} \|u^{n+1}\| &\leq \frac{1}{2}\|u^n\| + \frac{1}{2}\|u^{(1)} + \Delta t L(u^{(1)})\| \\ &\leq \frac{1}{2}\|u^n\| + \frac{1}{2}\|u^{(1)}\| \\ &\leq \frac{1}{2}\|u^n\| + \frac{1}{2}\|u^n\| \leq \|u^n\| \end{aligned}$$

That is, the second order Runge-Kutta method is SSP with the SSP coefficient $c = 1$ (Shu and Osher, JCP 1988).

Similarly, we can derive a third order SSP Runge-Kutta method as

$$\begin{aligned} u^{(1)} &= u^n + \Delta t L(u^n) \\ u^{(2)} &= \frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}) \\ u^{n+1} &= \frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}). \end{aligned} \tag{7}$$

It is SSP with the SSP coefficient $c = 1$ (Shu and Osher, JCP 1988).

There is no four-stage, fourth order SSP Runge-Kutta method (Kraaijevanger, BIT 1991; Gottlieb and Shu, Math Comp 1998). The following is a five stage, fourth order SSP Runge-Kutta method:

$$
\begin{aligned}
u^{(1)} &= u^n + 0.391752226571890\Delta t L(u^n) \\
u^{(2)} &= 0.444370493651235u^n + 0.555629506348765u^{(1)} \\
&\quad +0.368410593050371\Delta t L(u^{(1)}) \\
u^{(3)} &= 0.620101851488403u^n + 0.379898148511597u^{(2)} \\
&\quad +0.251891774271694\Delta t L(u^{(2)}) \\
u^{(4)} &= 0.178079954393132u^n + 0.821920045606868u^{(3)} \\
&\quad 0.544974750228521\Delta t L(u^{(3)}) \\
u^{n+1} &= 0.517231671970585u^{(2)} \\
&\quad +0.096059710526147u^{(3)} + 0.063692468666290\Delta t L(u^{(3)}) \\
&\quad +0.386708617503269u^{(4)} + 0.226007483236906\Delta t L(u^{(4)})
\end{aligned}
$$

with SSP coefficient $c = 1.508$ (Kraaijevanger, BIT 1991; Spiteri and Ruuth, SINUM 2002).

We could similarly obtain SSP multi-step methods. For example, a second order SSP 3-step method is given by

$$u^{n+1} = \frac{3}{4}u^n + \frac{1}{4}u^{n-2} + \frac{3}{2}\Delta t L(u^n),$$

which is SSP with the SSP coefficient $c = \frac{1}{2}$ (Shu, SISSC 1988). Likewise, a third order 4-step method is given by

$$u^{n+1} = \frac{16}{27}u^n + \frac{16}{9}\Delta t L(u^n) + \frac{11}{27}u^{n-3} + \frac{4}{9}\Delta t L(u^{n-3}),$$

which is SSP with the SSP coefficient $c = \frac{1}{3}$ (Shu, SISSC 1988; Gottlieb, Shu and Tadmor, SIREV 2001).

A very good example of the application of SSP methods is the recent framework (Zhang and Shu, JCP 2010) in obtaining positivity-preserving high order discontinuous Galerkin methods or finite volume schemes for solving Euler equations. A simple scaling limiter with the SSP Runge-Kutta or multistep time discretization can lead to provably high order positivity-preserving (for density and pressure) results. A simulation of Mach 2000 astrophysical jet flow can be computed by this method successfully (which causes blow-ups of many high order codes without this treatment).

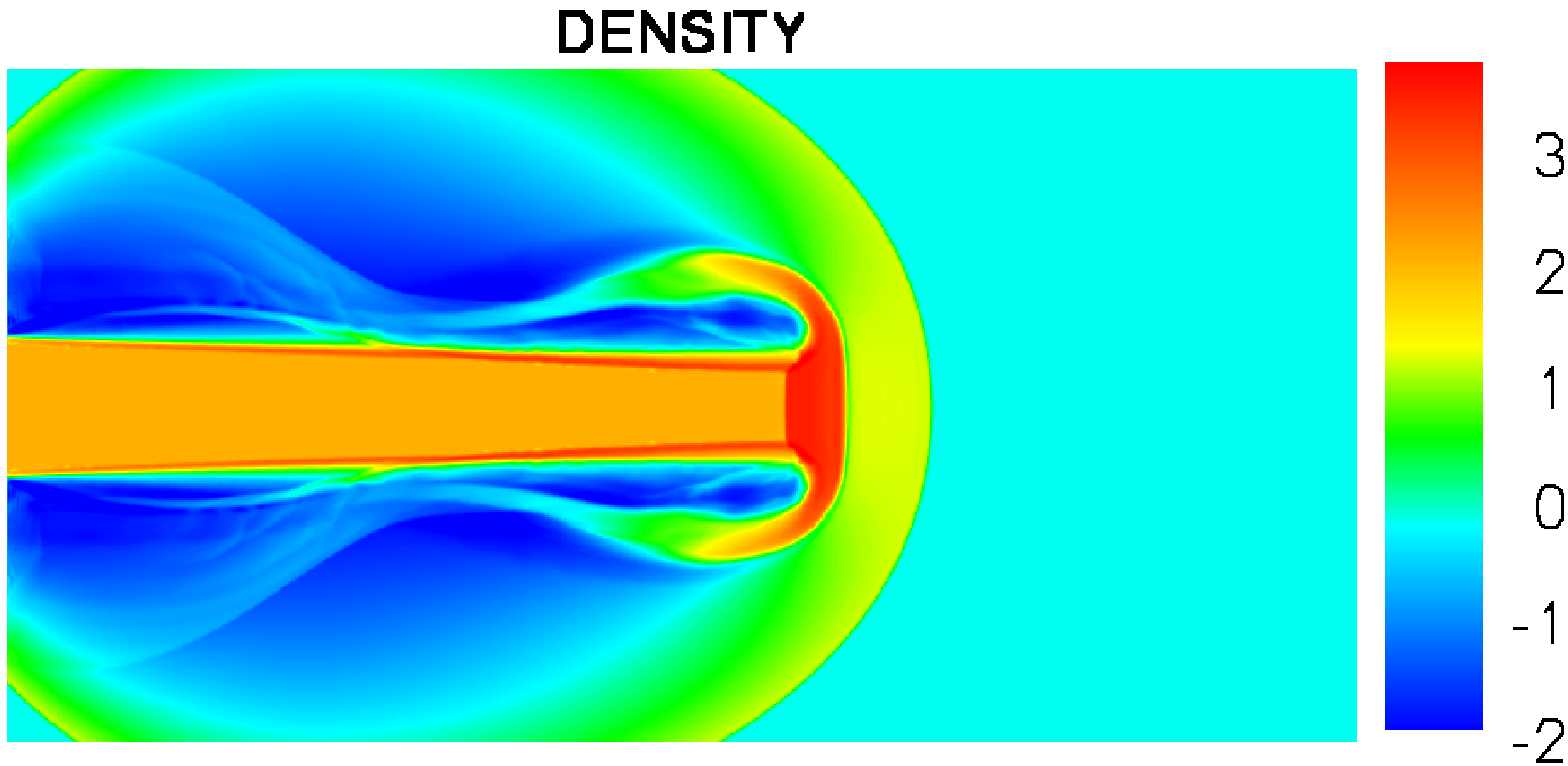

Figure 1: Simulation of Mach 2000 jet without radiative cooling. Scales are logarithmic. Density.

There are issues related to possible negative coefficient in front of $\Delta t L(u)$ (which would require a different spatial discretization operation $\tilde{L}$ to approximate the spatial derivatives in the PDE), and many discussions on obtaining optimal SSP methods with different order barriers in the literature. We would refer to the following papers and books and more recent papers in the literature.

[1] S. Gottlieb, C.-W. Shu and E. Tadmor, *Strong stability-preserving high-order time discretization methods*, SIAM Review, v43 (2001), pp.89-112.

[2] S. Gottlieb, D.I. Ketcheson and C.-W. Shu, *High order strong stability preserving time discretizations*, Journal of Scientific Computing, v38 (2009), pp.251-289.

[3] S. Gottlieb, D. Ketcheson and C.-W. Shu, Strong Stability Preserving Runge-Kutta and Multistep Time Discretizations, World Scientific, Singapore, 2011.

IMEX time discretization

If we are solving a convection-diffusion equation

$$u_t + f(u)_x = du_{xx} \tag{8}$$

where $d > 0$, using explicit time discretizations such as the SSP methods discussed before would require a very small time step (if d is not too small). However, a fully implicit method would be costly (since we must solve a nonlinear equation at every time step, or, even if $f(u)$ is linear, we must solve a linear system which is not symmetric positive definite). An implicit-explicit (IMEX) method would be ideal.

Let us write our method of lines ODE as

$$u_t = N(u) + L(u) \tag{9}$$

where $N(u)$ might be the nonlinear term corresponding to convection and $L(u)$ might be the linear term corresponding to diffusion.

If N is the discontinuous Galerkin (DG) discretization of the convection term and L is the local DG (LDG) discretization of the diffusion term, then we have the following stable IMEX schemes developed in (Wang, Shu and Zhang, SINUM 2015 and AMC 2016; Wang, Wang, Shu and Zhang, M^2AN 2016).

The first order IMEX scheme we consider is

$$u^{n+1} = u^n + \Delta t N(u^n) + \Delta t L(u^{n+1}).$$

We have the following stability result:

Proposition 1: There exists a positive constant τ_0 independent of the spatial mesh size h, such that if $\Delta t \leq \tau_0$, then the solution of the first order IMEX LDG scheme satisfies the strong stability property

$$\|u^n\| \leq \|u^0\|, \qquad \forall n. \tag{10}$$

Note: The constant τ_0 is proportional to d/c^2, where c, d are the advection and diffusion coefficients, respectively.

The second order IMEX scheme we consider is (Ascher, Ruuth and Spiteri, Appl. Numer. Math. 1997):

$$\begin{aligned} u^{(1)} &= u^n + \gamma \Delta t N(u^n) + \gamma \Delta t L(u^{(1)}) \\ u^{n+1} &= u^n + \delta \Delta t N(u^n) + (1-\delta)\Delta t N(u^{(1)}) \\ &\quad + (1-\gamma)\Delta t L(u^{(1)}) + \gamma \Delta t L(u^{n+1}) \end{aligned}$$

where $\gamma = 1 - \frac{\sqrt{2}}{2}$, $\delta = 1 - \frac{1}{2\gamma}$.

We can prove the following stability result for the second order IMEX LDG scheme:

Proposition 2: There exists a positive constant τ_0 independent of the spatial mesh size h, such that if $\Delta t \leq \tau_0$, then the solution of the second order IMEX LDG scheme satisfies the strong stability property

$$\|u^n\| \leq \|u^0\|, \qquad \forall n.$$

The third order IMEX scheme we consider is (Calvo, de Frutos and Novo, Appl. Numer. Math. 2001):

$$
\begin{aligned}
u^{(1)} &= u^n + \gamma \Delta t N(u^n) + \gamma \Delta t L(u^{(1)}) \\
u^{(2)} &= u^n + \left(\frac{1+\gamma}{2} - \alpha_1 \right) \Delta t N(u^n) + \alpha_1 \Delta t N(u^{(1)}) \\
&\quad + \frac{1-\gamma}{2} \Delta t L(u^{(1)}) + \gamma \Delta t L(u^{(2)}) \\
u^{(3)} &= u^n + (1-\alpha_2) N(u^{(1)}) + \alpha_2 N(u^{(2)}) \\
&\quad + \beta_1 \Delta t L(u^{(1)}) + \beta_2 \Delta t L(u^{(2)}) + \gamma \Delta t L(u^{(3)}) \\
u^{n+1} &= u^n + \beta_1 \Delta t N(u^{(1)}) + \beta_2 \Delta t N(u^{(2)}) + \gamma \Delta t N(u^{(3)}) \\
&\quad + \beta_1 \Delta t L(u^{(1)}) + \beta_2 \Delta t L(u^{(2)}) + \gamma \Delta t L(u^{(3)})
\end{aligned}
$$

where γ is the middle root of $6x^3 - 18x^2 + 9x - 1 = 0$,
$\gamma \approx 0.435866521508459$, $\beta_1 = -\frac{3}{2}\gamma^2 + 4\gamma - \frac{1}{4}$, $\beta_2 = \frac{3}{2}\gamma^2 - 5\gamma + \frac{5}{4}$.
The parameter α_1 is chosen as -0.35 and $\alpha_2 = \frac{\frac{1}{3} - 2\gamma^2 - 2\beta_2\alpha_1\gamma}{\gamma(1-\gamma)}$.

We can prove the following stability result for the third order IMEX LDG scheme:

Proposition 3: There exists a positive constant τ_0 independent of the spatial mesh size h, such that if $\Delta t \leq \tau_0$, then the solution of the third order IMEX LDG scheme satisfies the strong stability property

$$\|u^n\| \leq \|u^0\|, \qquad \forall n.$$

The same stability results can be obtained for IMEX multi-step LDG methods, with IMEX multi-step schemes in, e.g. (Gottlieb and Wang, JSC 2012).

Second order IMEX LDG scheme:

$$\begin{aligned} u^{n+1} &= u^n + \Delta t \left(\frac{3}{2} N(u^n) - \frac{1}{2} N(u^{n-1}) \right) \\ &\quad + \tau \left(\frac{3}{4} L(u^{n+1}) + \frac{1}{4} L(u^{n-1}) \right) \end{aligned}$$

Third order IMEX LDG scheme:

$$\begin{aligned} u^{n+1} &= u^n + \Delta t \left(\frac{23}{12} N(u^n) - \frac{4}{3} N(u^{n-1}) + \frac{5}{12} N(u^{n-2}) \right) \\ &\quad + \Delta t \left(\frac{2}{3} L(u^{n+1}) + \frac{5}{12} L(u^{n-1}) - \frac{1}{12} N(u^{n-3}) \right) \end{aligned}$$

Other extensions:

- The method has been generalized to other types of DG schemes, e.g. to the embedded discontinuous Galerkin method (Fu and Shu, IJNAM 2017).
- The method has been generalized to LDG schemes for solving the drift-diffusion model of semiconductor devices (Liu and Shu, Sci. China Math 2016).
- The method has been generalized to fourth order PDEs (Wang, Zhang and Shu, M^2AN 2017).
- The method has been generalized to incompressible Navier-Stokes equations (Wang, Liu, Zhang and Shu, Math Comp 2019).

- The method has been generalized to solving convection-diffusion equations and convection-dispersion equations using upwind-biased finite difference discretization for the convection terms and central finite difference discretization for the diffusion or dispersion terms (Tan, Cheng and Shu, IJNAM 2021). For the convection-dispersion equations such as the KdV equations, the method is stable under the standard convection CFL condition

$$\Delta t \leq c\Delta x$$

with some constant $c > 0$.

If both the convection and the diffusion terms are nonlinear, then a straight-forward application of the IMEX schemes above may not be the most efficient, as we must solve a nonlinear system per implicit stage. Instead, we could consider writing the PDE as

$$u_t + f(u)_x - (a(u)u_x)_x + a_0 u_{xx} = a_0 u_{xx}$$

and treat all the left-hand side terms explicitly and only the right-hand term implicitly. Here a_0 is a constant, which must be chosen suitably to guarantee stability. This is called the explicit-implicit-null (EIN) method.

In (Wang, Zhang, Wang and Shu, Sci. China Math 2020), we have designed first, second and third order EIN schemes of this type, and performed analysis on the linear problems to guide the choice of a_0 for stability. In the analysis, we assume $a(u) = a$ is a constant (and in numerical experiments, if $a(u)$ is not a constant, we will take a as the the maximum value of $a(u)$).

- For the first and second order IMEX schemes, we can prove unconditional stability if we choose $a_0 \geq \frac{1}{2}a$.
- For the third order IMEX scheme, numerical experiments indicate that it is unconditionally stable if we choose $a_0 \geq 0.54\,a$. However, we are unable to prove it rigorously.

These EIN schemes have been extended in (Tan, Cheng and Shu, JCP 2022; East Asian Journal on Applied Mathematics, to appear) to the following cases:

- For the convection-diffusion equations with nonlinear second order diffusion terms, using finite difference and spectral spatial discretizations;
- For the convection-dispersion equations with nonlinear third order dispersion terms, using finite difference, local discontinuous Galerkin, and spectral spatial discretizations. The condition for stability is the usual CFL condition for convection only;
- For the fourth order convection-biharmonic equations with nonlinear fourth order diffusion terms, using finite difference, local discontinuous Galerkin, and spectral spatial discretizations.

The EIN schemes with variable coefficients:

$$u_t + f(u)_x - (a(u)u_x)_x + (a_0(x)u_x)_x = (a_0(x)u_x)_x$$

with the variable coefficient $a_0(x)$ suitably chosen to reduce the error of the added null terms, have been studied in (Tan, Cheng and Shu, CAMC submitted). For solutions with large spatial variation, the variable coefficient EIN methods achieve smaller errors than those with constant coefficients.

Strongly stable Runge-Kutta methods for linear systems

While SSP time discretization framework is powerful in guaranteeing nonlinear stability, it can only be applied under the assumption that the Euler forward operator is strongly stable under a suitable time step restriction. It thus cannot be applied to the situation that the Euler forward time discretization is unstable, or only stable under very restrictive CFL time step restrictions. In such cases, we must consider high order Runge-Kutta or multi-step methods directly.

We will focus on autonomous linear ordinary differential equation (ODE) systems

$$\frac{d}{dt}u = Lu, \tag{11}$$

e.g. those obtained from method of lines discontinuous Galerkin (DG) schemes for linear hyperbolic problems. Here $u \in \mathbb{R}^N$ and L is an $N \times N$ real constant matrix, where N is the degrees of freedom for the spatial discretization.

If the semidiscrete scheme honors the (weighted) L^2 stability of the original PDE, then for certain symmetric and positive definite matrix H,

$$L^\top H + HL \leq 0 \tag{12}$$

is a semi-negative definite matrix. Here H can be related with both the symmetrizer of the PDE and the mass matrix or quadrature weights of a Galerkin or collocation type spatial discretization.

Examples of spatial discretizations satisfying (12) include the DG method for linear and nonlinear hyperbolic systems (although in this part we are mainly interested in linear hyperbolic systems).

If (12) holds, then we say L is **semi-negative** and (11) satisfies the energy decay law

$$\frac{d}{dt}\|u\|_H^2 = \langle \frac{d}{dt}u, u\rangle_H + \langle u, \frac{d}{dt}u\rangle_H$$
$$= \langle Lu, Hu\rangle + \langle u, HLu\rangle = \langle u, (L^\top H + HL)u\rangle \leq 0. \tag{13}$$

Here $\langle \cdot, \cdot \rangle_H = \langle \cdot, H\cdot \rangle$ with $\langle \cdot, \cdot \rangle$ being the usual l^2 inner product in $\mathbb{R}^N$ and $\|u\|_H = \sqrt{\langle u, u\rangle_H}$.

We are concerned with whether this property is preserved at the discrete level, namely, whether

$$\|u^{n+1}\|_H \leq \|u^n\|_H \tag{14}$$

holds after applying an explicit Runge-Kutta (RK) time integrator under a suitably restricted time step.

We would say the explicit RK method is **strongly stable**, if (14) is satisfied when discretizing (11) under the condition (12).

If the problem is coercive, namely

$$L^\top H + HL \leq -\eta L^\top HL$$

for a positive constant $\eta > 0$, then the Euler forward time discretization is strongly stable under a suitable CFL condition. Therefore, all strong stability preserving (SSP) high order Runge-Kutta or multistep time discretizations are strongly stable under similar CFL condition (Levy and Tadmor, SIAM Review 1998; Gottlieb, Shu and Tadmor, SIAM Review 2001). This applies to, e.g. Galerkin type spatial discretizations to parabolic PDEs.

However, semi-discrete schemes for hyperbolic equations are usually not coercive, at least not strongly coercive (that is, $\eta \geq 0$ and it could depend on the mesh size h), so the framework based on coercive properties does not work. Euler forward time discretization is not strongly stable, hence the SSP framework cannot be applied either.

In (Tadmor, Proceedings in Applied Math, SIAM 2002), Tadmor proved that the three-stage, third order Runge-Kutta method is strongly stable for semi-negative ODEs.

Whether the classical fourth order Runge-Kutta method is strongly stable or not remained open until 2017, when (Sun and Shu, Annals of Mathematical Sciences and Applications 2017) provided a counter-example to show that the classical fourth order Runge-Kutta method is not always strongly stable for semi-negative ODEs. Also in (Sun and Shu, Annals of Mathematical Sciences and Applications 2017), it was shown that applying the classical fourth order Runge-Kutta scheme for two consecutive time steps (which can be viewed as an eight-stage, fourth order Runge-Kutta method) is strongly stable for semi-negative ODEs.

A general framework for stability analysis

Consider an explicit RK time discretization for the linear autonomous system (1). The scheme is of the form

$$u^{n+1} = R_s u, \tag{15}$$

where

$$R_s = \sum_{k=0}^{s} \alpha_k (\tau L)^k, \qquad \alpha_0 = 1, \qquad \alpha_s \neq 0. \tag{16}$$

Here τ is the time step and s is the number of stages. For an s-stage method, it is of linear order p if and only if the first $p+1$ terms in the summation (16) coincide with the truncated Taylor series of $e^{\tau L}$. In particular, $p \leq s$.

We would like to examine the strong stability of (15) under the usual CFL condition: if there exists a constant λ, such that

$$\|R_s u\|_H^2 \leq \|u\|_H^2, \tag{17}$$

for all $\tau\|L\|_H \leq \lambda$ and all inputs u. This is equivalent to

$$\|R_s\|_H \leq 1, \tag{18}$$

under the prescribed condition and $\|R_s\|_H$ is the matrix norm of R_s.

A natural attempt is to adopt the following expansion to compare $\|R_s u\|_H^2$ with $\|u\|_H^2$.

$$\begin{aligned} \|R_s u\|_H^2 &= \sum_{i,j=0}^{s} \alpha_i \alpha_j \tau^{i+j} \langle L^i u, L^j u \rangle_H \\ &= \|u\|_H^2 + \sum_{1 \le \max\{i,j\} \le s} \alpha_i \alpha_j \tau^{i+j} \langle L^i u, L^j u \rangle_H. \quad (19) \end{aligned}$$

However, each term $\langle L^i u, L^j u \rangle_H$ may not necessarily have a sign.

The idea for overcoming the difficulty is to convert $\langle L^i u, L^j u\rangle_H$ into linear combinations of terms of the form $\|L^i u\|_H^2$, $[\![L^j u]\!]_H^2$ and $[L^i u, L^j u]_H$. Here

$$[v, w]_H = -\langle v, (L^\top H + HL)w\rangle, \qquad v, w \in \mathbb{R}^N \tag{20}$$

is a semi inner product and

$$[\![v]\!]_H = \sqrt{[v, v]_H} \tag{21}$$

defines the induced semi-norm. Indeed, this can be achieved through the following induction procedure.

Proposition. Suppose $j \geq i$, then

$$\langle L^i u, L^j u\rangle_H = \begin{cases} \|L^i u\|_H^2, & j = i, \\ -\frac{1}{2}[\![L^i u]\!]_H^2, & j = i+1, \\ -\langle L^{i+1}u, L^{j-1}u\rangle_H - [L^i u, L^{j-1}u]_H, & \text{otherwise.} \end{cases}$$

In the context of approximating the spatial derivative ∂_x for periodic functions with L, the proposition is the discrete version of integration by parts. Since L may not preserve the exact anti-symmetry of ∂_x, namely $L^\top H + HL \neq 0$, an extra term $[L^i u, L^{j-1} u]_H$ is produced. Furthermore, $-\frac{1}{2}[\![L^i u]\!]_H^2$ is usually the numerical dissipation from the spatial discretization. In particular, $[\![\cdot]\!]_H$ is the jump semi-norm in the DG method.

We then have

Lemma. (Energy equality) Given H and $R_s = \sum_{k=0}^{s} \alpha_k (\tau L)^k$ with $\alpha_0 = 1$. There exists a unique set of coefficients $\{\beta_k\}_{k=0}^{s} \cup \{\gamma_{i,j}\}_{i,j=0}^{s-1}$, such that for all u and L satisfying $L^\top H + HL \leq 0$,

$$\|R_s u\|_H^2 = \sum_{k=0}^{s} \beta_k \tau^{2k} \|L^k u\|_H^2 + \sum_{i,j=0}^{s-1} \gamma_{i,j} \tau^{i+j+1} [L^i u, L^j u]_H, \qquad \gamma_{i,j} = \gamma_{j,i}. \tag{22}$$

To facilitate our discussion, we introduce the following definitions.

Definition. The leading index of R_s, denoted as k^*, is the positive integer such that $\beta_{k^*} \neq 0$ and $\beta_k = 0$ for all $1 \leq k < k^*$. The coefficient β_{k^*} is called the leading coefficient. The k^*-th order principal submatrix $\Gamma^* = (\gamma_{i,j})_{0 \leq i,j \leq k^*-1}$ is called the leading submatrix.

Note that k^* is well-defined since $\beta_s = \alpha_s^2 \neq 0$, which implies $k^* \leq s$.

Theorem. (Necessary condition) The method is not strongly stable if $\beta_{k^*} > 0$. More specifically, if $\beta_{k^*} > 0$, then there exists a constant λ, such that $\|R_s\|_H > 1$ if $0 < \tau\|L\|_H \leq \lambda$ and $L^\top H + HL = 0$.

Theorem. (Sufficient condition) If $\beta_{k^*} < 0$ and Γ^* is negative definite, then there exists a constant λ such that $\|R_s\|_H \leq 1$ if $\tau\|L\|_H \leq \lambda$.

Stability of Runge-Kutta methods

Linear RK methods: For general nonlinear systems, to admit accuracy order higher than four, RK methods must have more stages than its order. However, for autonomous linear systems, the desired order of accuracy can be achieved with the same number of stages. All such methods would be equivalent to the Taylor series method

$$R_p = P_p = \sum_{k=0}^{p} \frac{(\tau L)^k}{k!}. \tag{23}$$

We use the general framework to obtain the strong stability (SS) properties of linear RK methods from first to twelfth order.

p	k^*	β_{k^*}	Γ^*	$\lambda(\Gamma^*)$	SS
1	1	1	$-\begin{pmatrix} 1 \end{pmatrix}$	-1.00000	no
2	2	$\frac{1}{4}$	$-\begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$	-1.30902 -1.90983×10^{-1}	no
3	2	$-\frac{1}{12}$	$-\begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} \end{pmatrix}$	-1.26759 -6.57415×10^{-2}	yes
4	3	$-\frac{1}{72}$	$-\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{8} \\ \frac{1}{6} & \frac{1}{8} & \frac{1}{24} \end{pmatrix}$	-1.30128 -7.93266×10^{-2} $+5.60618 \times 10^{-3}$	no*
5	3	$\frac{1}{360}$	$-\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{8} \\ \frac{1}{6} & \frac{1}{8} & \frac{1}{20} \end{pmatrix}$	-1.30150 -8.07336×10^{-2} -1.10151×10^{-3}	no
6	4	$\frac{1}{2880}$	$-\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{6} & \frac{1}{24} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{8} & \frac{1}{30} \\ \frac{1}{6} & \frac{1}{8} & \frac{1}{20} & \frac{1}{72} \\ \frac{1}{24} & \frac{1}{30} & \frac{1}{72} & \frac{1}{240} \end{pmatrix}$	-1.30375 -8.21871×10^{-2} -1.40529×10^{-3} -1.60133×10^{-4}	no
7	4	$-\frac{1}{20160}$	$-\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{6} & \frac{1}{24} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{8} & \frac{1}{30} \\ \frac{1}{6} & \frac{1}{8} & \frac{1}{20} & \frac{1}{72} \\ \frac{1}{24} & \frac{1}{30} & \frac{1}{72} & \frac{1}{252} \end{pmatrix}$	-1.30375 -8.21836×10^{-2} -1.36301×10^{-3} -7.86229×10^{-6}	yes

Table 1: Linear RK methods: from first order to seventh order.

p	k^*	β_{k^*}	$\lambda(\Gamma^*)$	SS
8	5	$-\frac{1}{201600}$	-1.30384 -8.22588×10^{-2} -1.38580×10^{-3} -9.32706×10^{-6} $+2.24989 \times 10^{-6}$	?
9	5	$\frac{1}{1814400}$	-1.30384 -8.22588×10^{-2} -1.38585×10^{-3} -9.75366×10^{-6} -3.11800×10^{-8}	no
10	6	$\frac{1}{221772800}$	-1.30384 -8.22613×10^{-2} -1.38688×10^{-3} -9.91006×10^{-6} -4.70638×10^{-8} -1.63872×10^{-8}	no

Table 2: Linear RK methods: from eighth order to tenth order.

p	k^*	β_{k^*}	$\lambda(\Gamma^*)$	SS
11	6	$-\frac{1}{239500800}$	-1.30384 -8.22613×10^{-2} -1.38688×10^{-3} -9.90966×10^{-6} -3.87351×10^{-8} -7.87018×10^{-11}	yes
12	7	$-\frac{1}{3353011200}$	-1.30384 -8.22614×10^{-2} -1.38691×10^{-3} -9.91617×10^{-6} -3.93334×10^{-8} $+1.45458 \times 10^{-10}$ -8.54170×10^{-11}	?

Table 3: Linear RK methods: from eleventh order to twelfth order.

The classical fourth order method: The classical fourth order method with four stages, which is widely used in practice due to its stage and order optimality, is unfortunately not covered under the framework. In (Sun and Shu, Annals of Mathematical Sciences and Applications 2017), we found a counter example to show that the method is not strongly stable, but successively applying the method for two steps yields a strongly stable method with eight stages.

Proposition. (Sun and Shu, 2017) The fourth order RK method with four stages is not strongly stable. More specifically, for $H = I$ and $L = -\begin{pmatrix} 1 & 2 & 2 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{pmatrix}$, we have $\|P_4\| > 1$, if $\tau\|L\|_H > 0$ is sufficiently small.

Theorem. (Sun and Shu, 2017) The fourth order RK method with four stages is strongly stable in two steps. In other words, there exists a constant λ, such that $\|(P_4)^2\|_H \leq 1$ if $\tau\|L\|_H \leq \lambda$.

Here we examine multi-step strong stability of the fourth order method using our framework. Note the derivation using this framework is slightly different from that in (Sun and Shu, Annals of Mathematical Sciences and Applications 2017). Note that the method is both two-step and three-step strongly stable (with the same time step size), which means the norm of the solution after the first step is always bounded by the initial data, if sufficiently small uniform time steps are used.

$(P_4)^m$	k^*	β_{k^*}	Γ^*	$\lambda(\Gamma^*)$	SS
$(P_4)^2$	3	$-\frac{1}{36}$	$-\begin{pmatrix} 2 & 2 & \frac{4}{3} \\ 2 & \frac{8}{3} & 2 \\ \frac{4}{3} & 2 & \frac{19}{12} \end{pmatrix}$	-5.73797 -4.99093×10^{-1} -1.29329×10^{-2}	yes
$(P_4)^3$	3	$-\frac{1}{24}$	$-\begin{pmatrix} 3 & \frac{9}{2} & \frac{9}{2} \\ \frac{9}{2} & 9 & \frac{81}{8} \\ \frac{9}{2} & \frac{81}{8} & \frac{97}{8} \end{pmatrix}$	-2.28380×10^{1} -1.21069 -7.62892×10^{-2}	yes

Table 4: The classic fourth order method: multi-step strong stability.

Theorem. The four-stage fourth order RK method has the following property. With uniform time steps such that $\tau\|L\|_H \leq \lambda$ for sufficiently small λ, $\|u^n\|_H \leq \|u^0\|_H$ for all $n > 1$.

SSP Runge-Kutta methods: The five stage, fourth order SSP RK method in (Kraaijevanger, BIT 1991; Spiteri and Ruuth, SINUM 2002) takes the form

$$\text{SSPRK(5,4)} = P_4 + 4.477718303076007 \times 10^{-3}(\tau L)^5. \qquad (24)$$

Besides SSPRK(5,4), we will also consider two commonly used low storage SSPRK methods, a third order method with four stages SSPRK(4,3) and a fourth order method with ten stages SSPRK(10,4) (Kraaijevanger, BIT 1991; Spiteri and Ruuth, SINUM 2002).

The two methods are

$$\text{SSPRK(4,3)} = P_3 + \frac{1}{48}(\tau L)^4, \tag{25}$$

and

$$\begin{aligned}\text{SSPRK(10,4)} =& P_4 + \frac{17}{2160}(\tau L)^5 + \frac{7}{6480}(\tau L)^6 + \frac{1}{9720}(\tau L)^7 \\ &+ \frac{1}{155520}(\tau L)^8 + \frac{1}{4199040}(\tau L)^9 + \frac{1}{251942400}(\tau L)^{10},\end{aligned} \tag{26}$$

We remark that the strong stability of SSPRK(10,4) has been proved in Ranocha and Öffner, JSC 18. We are simply reexamine it using our framework.

SSPRK	k^*	β_{k^*}	Γ^*	$\lambda(\Gamma^*)$	SS
(4,3)	2	$-\frac{1}{24}$	$-\begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{3} \end{pmatrix}$	-1.26759 -6.57415×10^{-2}	yes
(10,4)	3	$-\frac{1}{3240}$	$-\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{8} \\ \frac{1}{6} & \frac{1}{8} & \frac{107}{2160} \end{pmatrix}$	-1.30149 -8.06493×10^{-2} -7.35115×10^{-4}	yes
(5,4)	3	-4.93345×10^{-3}	$-\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{8} \\ \frac{1}{6} & \frac{1}{8} & \frac{1}{24} \end{pmatrix}$	-1.30140 -8.00541×10^{-2} $+1.97309 \times 10^{-3}$	no*
$(5,4)^2$	3	-9.86690×10^{-3}	$-\begin{pmatrix} 2 & 2 & \frac{4}{3} \\ 2 & \frac{8}{3} & 2 \\ \frac{4}{3} & 2 & 1.5923 \end{pmatrix}$	-5.74021 -5.01739×10^{-1} -1.70056×10^{-2}	yes
$(5,4)^3$	3	-1.48004×10^{-2}	$-\begin{pmatrix} 3 & \frac{9}{2} & \frac{9}{2} \\ \frac{9}{2} & 9 & \frac{81}{8} \\ \frac{9}{2} & \frac{81}{8} & 12.138 \end{pmatrix}$	-2.28450×10^{1} -1.21415 -7.93174×10^{-2}	yes

Table 5: SSPRK methods: strong stability and multi-step strong stability.

Theorem. The property stated for the classical four stage, fourth order Runge-Kutta method also holds for SSPRK(5,4).

The behavior of SSPRK(5,4) is very similar to that of the classic fourth order method, since it is almost the four-stage method except for a small fifth order perturbation. Although the method can not be judged within this framework, one can indeed use the same counter example for the classical fourth order RK to disprove its strong stability.

Embedded RK methods in NDSolve: We consider embedded RK pairs that are used in NDSolve, a function for numerically solving differentiable equations in the commercial software Mathematica. Embedded RK methods are pairs of RK methods sharing the same stages. The notation $p(\hat{p})$ is commonly used, if two methods in the pair are of order p and order $\hat{p}$ respectively. The difference $u^{n+1} - \hat{u}^{n+1}$ can be used for local error estimates for time step adaption.

We examine strong stability of all such pairs used in Mathematica from order $2(1)$ to order $9(8)$. These methods are chosen with several desired properties being considered, including the FSAL (First Same As Last) strategy and stiffness detection capability.

Methods	s	$p/\hat{p}$	k^*	β_{k^*}	$\lambda(\Gamma^*)$	SS
2(1)	3	2	2	$\frac{1}{4}$	-1.30902 -1.90983×10^{-1}	no
		1	1	1	-1.00000	no
3(2)	4	3	2	$-\frac{1}{12}$	-1.26759 -6.57415×10^{-2}	yes
		2	2	$\frac{1}{12}$	-1.28130 -1.11257×10^{-1}	no
4(3)	5	4	3	$-\frac{1}{72}$	-1.30128 -7.93266×10^{-2} $+5.60618 \times 10^{-3}$	no*
		3	2	$-\frac{119041}{4485456}$	-1.26759 -6.57415×10^{-2}	yes
5(4)	8	5	3	$-\frac{43}{6209280}$	-1.3015 -8.07336×10^{-2} -1.10151×10^{-3}	yes
		4	3	$\frac{51767}{367590960}$	-1.30150 -8.07430×10^{-2} -1.14174×10^{-3}	no

*The fourth order method in the 4(3) pair is exactly the classic four-stage fourth order method for autonomous linear systems.

Table 6: Embedded RK pairs: from $2(1)$ to $5(4)$ pairs.

Methods	s	$p/\hat{p}$	k^*	β_{k^*}	$\lambda(\Gamma^*)$	SS
6(5)	9	6	4	$\frac{79007}{2560896000}$	-1.30375 -8.21839×10^{-2} -1.36689×10^{-3} -2.38718×10^{-5}	no
		5	3	$\frac{1233467}{9027158400}$	-1.30150 -8.07336×10^{-2} -1.10151×10^{-3}	no
7(6)	10	7	4	$\frac{29615605063}{3896766536040000}$	-1.30375 -8.21836×10^{-2} -1.36301×10^{-3} -7.86229×10^{-6}	no
		6	4	$-\frac{20202919901}{1855603112400000}$	-1.30375 -8.21833×10^{-2} -1.35985×10^{-3} $+5.49402 \times 10^{-6}$	?

Table 7: Embedded RK pairs: from $6(5)$ to $7(6)$ pairs.

Methods	s	p	k^*	β_{k^*}	$\lambda(\Gamma^*)$	SS
8(7)	13	8	5	-3.21308×10^{-7}	-1.30384 -8.22588×10^{-2} -1.38584×10^{-3} -9.71236×10^{-6} $+1.43671 \times 10^{-7}$	?
		7	4	-2.39706×10^{-6}	-1.30375 -8.21836×10^{-2} -1.36301×10^{-3} -7.86229×10^{-6}	yes
9(8)	16	9	5	-8.95352×10^{-9}	-1.30384 -8.22588×10^{-2} -1.38585×10^{-3} -9.75366×10^{-6} -3.11800×10^{-8}	yes
		8	5	-5.46447×10^{-7}	-1.30384 -8.22588×10^{-2} -1.38585×10^{-3} -9.78641×10^{-6} -1.64476×10^{-7}	yes

Table 8: Embedded RK pairs: $8(7)$ pair and $9(8)$ pair.

Characterization of strongly stable methods:

Theorem. Consider a linear RK method of order p with p stages.

(i) The method is not strongly stable if $p \equiv 1 \pmod 4$ or $p \equiv 2 \pmod 4$.

(ii) The method is strongly stable if $p \equiv 3 \pmod 4$.

Theorem. An RK method of odd linear order p is strongly stable if and only if

$$(-1)^{\frac{p+1}{2}} \left(\alpha_{p+1} - \frac{1}{(p+1)!} \right) < 0. \tag{27}$$

Theorem. An RK method of even linear order p is strongly stable if

$$(-1)^{\frac{p}{2}+1}\left(\alpha_{p+2}-\alpha_{p+1}+\frac{1}{p!(p+2)}\right)<0, \tag{28}$$

and

$$(-1)^{\frac{p}{2}+1}\left(\frac{p}{2}!\right)^2\left(\alpha_{p+1}-\frac{1}{(p+1)!}\right)<\varepsilon. \tag{29}$$

Here ε is the smallest eigenvalue of the Hilbert matrix of order $\frac{p}{2}+1$.

References:

[1] Z. Sun and C.-W. Shu, *Strong stability of explicit Runge-Kutta time discretizations*, SIAM Journal on Numerical Analysis, v57 (2019), pp.1158-1182.

[2] Y. Xu, Q. Zhang, C.-W. Shu and H. Wang, *The* L^2*-norm stability analysis of Runge-Kutta discontinuous Galerkin methods for linear hyperbolic equations*, SIAM Journal on Numerical Analysis, v57 (2019), pp.1574-1601.

The End

THANK YOU!