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BEYOND CLASSICAL STABILITY ANALYSIS ON RUNGE-KUTTA SCHEMES: POSITIVITY AND PHASE PRESERVATION

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INTRODUCTION

In the numerical integration of an ordinary differential equation (ODE), the general concerns are performance, stability, and accuracy. All three are characterized by the method's coefficients as well as the step size. The former is usually not in the hands of the user once a scheme has been established, as coefficients are generally constant, while reducing the step size, which at the same time reduces the performance of the code; it will take longer to cover the desired domain. These generates a trade-off in which the user has to be aware of the pros and cons of using a larger or smaller step size given the requirements of the integration.

One of the different possibilities when integrating ODEs is the Runge-Kutta (RK) method, in which the value of the function that is being integrated, at the next step ϕ^{n+1}, is computed only considering the current step ϕ^n and intermediate approximate values, ϕ_i in the s stages of the scheme, so that

$$\phi_i = \phi^n + h\sum_{j=1}^{s} a_{ij} f(\phi_j), \tag{1a}$$

$$\phi^{n+1} = \phi^n + h\sum_{i=1}^{s} b_i f(\phi_i), \tag{1b}$$

where h is the step size and a_{ij}, b_i are the RK coefficients arranged in the so-called Butcher's tableau.

When the Navier-Stokes equations are semi-discretized,

$$M\mathbf{u} = 0, \tag{2a}$$

$$\Omega\frac{d\mathbf{u}}{dt} + C(\mathbf{u})\mathbf{u} = D\mathbf{u} - \Omega G\mathbf{p}, \tag{2b}$$

a differential algebraic equation (DAE) of order 2 is obtained. The solution of these equations using RK is developed by Sanderse and Koren [1] by means of a projection method.

Originally, the timestep Δt had been selected with the classical CFL condition, which estimates the eigenvalues of the method, and then the expected stable timestep is reduced with the so-called Courant number (or CFL number) to ensure the integration is stable. Later on, Trias and Lehmkuhl [2] used Gershgorin theorem to compute the eigenbounds of the predictor step in the projection method to use the largest possible timestep allowed by the stability region. This same technique can be applied to RK as the stability region is defined by the polynomial

$$R(z) = 1 + \sum_{k=1}^{s} \frac{1}{k!} z^k, \tag{3}$$

for $s \geq p$, being p the order of accuracy of the method. Hence, by the linear stability theory, in a general ODE,

$$\phi^{n+1} = R(h\lambda)\phi^n, \tag{4}$$

where $\lambda \in \mathbb{C}$ is the eigenbound of the system. Hence, stability will be obtained if $|R(h\lambda)| \leq 1$ holds.

Nonetheless, when this method was applied to a simulation with a timestep of 95% of the maximum stable value, some spurious modes appeared in the solution which were evident in the instantaneous fields, as seen in Fig. 1, and generated an overprediction of u_{rms} in the core of the channel. When 85% of the maximum stable timestep was used, then this instability was not present, and instead, the obtained fields were as expected. Trying to understand what generated these instabilities was the main motivation for the development of this work.

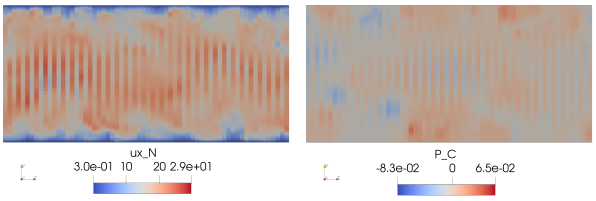

Figure 1: Spurious modes observed in the cross-stream plane at 95% of the maximum stable timestep for a coarse (64^3) $\mathrm{Re}_\tau = 180$ channel flow simulation for velocity (left) and pressure (right).

POSITIVITY-PRESERVING SOLUTIONS

Let us consider the following ODE,

$$\frac{d\phi}{dt} = \lambda\phi, \quad \lambda \in \mathbb{C}, \tag{5}$$

with $\phi(0) = 1$. Since it leads to $\phi(t) = e^{\lambda t}$ as an analytical solution, a monotonic solution is expected. In this first case, consider $\lambda = -1$, hence the stability polynomial $R(z)$ becomes

$$R(h) = 1 + \sum_{k=1}^{s} \frac{(-1)^k}{k!} h^k, \tag{6}$$

where, if $R(h) < 0$, ϕ^{n+1} will change sign and thus the obtained solution will not be monotonic. For instance, by using a third-order scheme, such as the strong-stability preserving third-order Runge-Kutta (SSPRK3) from Shu and Osher [3], $R(h) = 1 - h + \frac{1}{2}h^2 - \frac{1}{6}h^3$, the solution will not be monotonic for $h > 1.6$, as shown in Fig. 2 (left), even though it will be stable for step size values smaller than 2.5.

Nonetheless, in the case of having a complex eigenvalue, using this approach is not so straightforward. Hence, let $\lambda = -||\lambda||e^{-i\phi}$. Introducing it in the stability polynomial,

$$\begin{aligned} R(h\lambda) = 1 + \sum_{k=1}^{s} \frac{(-1)^k}{k!} (h||\lambda||)^k \cos(k\phi) \\ + i \sum_{k=1}^{s} \frac{(-1)^{k+1}}{k!} (h||\lambda||)^k \sin(k\phi), \end{aligned} \tag{7}$$

the polynomial can be split into a real and imaginary part, $R = R_r + iR_i$. By introducing it into the linear stability analysis equation, ϕ^n should be treated as complex so that $\phi^n = \phi_r^n + i\phi_i^n$. Expressed as a matrix equation,

$$\begin{pmatrix} \phi_r^{n+1} \\ \phi_i^{n+1} \end{pmatrix} = \underbrace{\begin{pmatrix} R_r & -R_i \\ R_i & R_r \end{pmatrix}}_{A} \begin{pmatrix} \phi_r^{n} \\ \phi_i^{n} \end{pmatrix}, \tag{8}$$

in which the oscillations will appear if and only if the matrix A fulfills $x^T Ax > 0$, $\forall x \in \mathbb{R}^2$. This will only hold if $R_r > 0$, being the same condition as for a purely diffusive case.

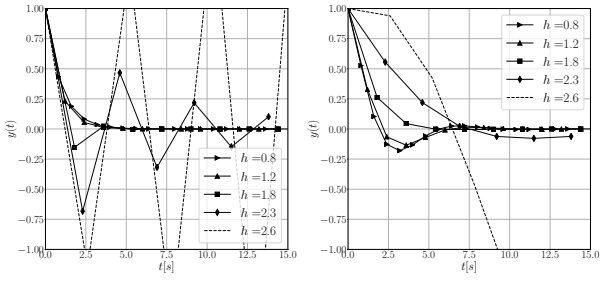

Figure 2: Numerical solutions for different h values for $d_t\phi = (-\cos(\alpha) + i\sin(\alpha))\phi$ with a SSPRK3 scheme, for $\alpha = 0$ (left) and $\alpha = 60^o$ (right)

PHASE-PRESERVING SOLUTIONS

In the previous section, the conditions for badly suited real contributions in the stability polynomial are presented. However, what happens when the imaginary contribution becomes negative? A sudden change of sign for the imaginary term will imply that the phase of this stability coefficient varies in π, which at the same time will transport the solution for half a period. Hence, having a negative imaginary contribution from the stability polynomial should also be avoided.

As shown in Fig. 2 (right), for $h > 2.5$, the phase of the solution has changed. In addition, an increase in magnitude can be observed as the solution is closer to the stability limit, which is surpassed for $h = 2.75$.

LIMITING THE STABILITY REGION FOR RUNGE-KUTTA SCHEMES

The observation of these phenomena generates the need to consider adding these conditions when setting the timestep of the numerical simulation. Hence, the "go-to" zone will be determined as follows,

$$\begin{cases} |R(h\lambda)| \leq 1, \\ R_r(h\lambda) > 0, \\ R_i(h\lambda) > 0, \end{cases} \tag{9}$$

so that both the sign and the phase of the solution are preserved, considering a stable integration in the first place. This will thus define two additional regions on top of the classical stability region: first of all, the positivity-preserving region will consist of all those combinations of $h\lambda$ such that $R_r > 0$ and thus, no synthetic change in the monotonicity of the solution should be observed. On the other hand, the phase-preserving region will be determined by the combinations of $h\lambda$ such that $R_i > 0$, and thus the phase is preserved throughout the integration.

By applying these conditions to the stability polynomial to limit the stability region of the scheme, the results from Fig. 3 are obtained for a third-order RK scheme. It can be observed that in integrations with eigenvalues with angles of approximately between 30 and 50 degrees, for a third-order scheme, the whole stability region can be exploited, as both the sign and as the phase will be preserved as long as the integration is stable. The applicability of these results to CFD in deeper detail is expected to be presented in the workshop.

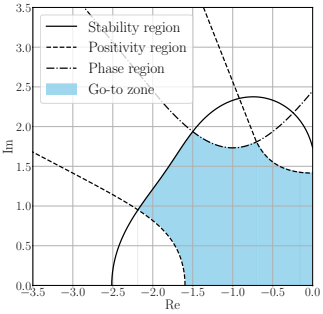

Figure 3: Stability region of a third-order Runge-Kutta scheme (black), with the positivity region (red) as well as the phase region (blue).

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