Design of optimal Runge-Kutta methods

David I. Ketcheson

King Abdullah University of Science & Technology
(KAUST)

King Abdullah University of Science and Technology KAUST

Acknowledgments

Some parts of this are joint work with:

- Aron Ahmadia
- Matteo Parsani

Outline

1. High order Runge-Kutta methods
2. Linear properties of Runge-Kutta methods
3. Nonlinear properties of Runge-Kutta methods
4. Putting it all together: some optimal methods and applications

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- Strong scaling limits the effectiveness of spatial parallelism alone
- Strategy: keep Δx as large as possible by using high order methods
- But: high order methods cost more and require more memory
- Can we develop high order methods that are as efficient as lower order methods?

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- Reduce storage requirements

Runge-Kutta Methods

To solve the initial value problem:

$$u'(t) = F(u(t)), \quad u(0) = u^0$$

a Runge-Kutta method computes approximations $u^n \approx u(n\Delta t)$:

$$y^i = u^n + \Delta t \sum_{j=1}^{i-1} a_{ij} F(y^j)$$

$$u^{n+1} = u^n + \Delta t \sum_{j=1}^{s-1} b_j F(y^j)$$

The accuracy and stability of the method depend on the coefficient matrix **A** and vector **b**.

Runge-Kutta Methods: a philosophical aside

- An RK method builds up information about the solution derivatives through the computation of intermediate stages
- At the end of a step all of this information is thrown away!
- Use more stages $\implies$ keep information around longer

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The Stability Function

For the linear equation

$$u' = \lambda u,$$

a Runge-Kutta method yields a solution

$$u^{n+1} = \phi(\lambda \Delta t) u^n,$$

where ϕ is called the *stability function* of the method:

$$\phi(z) = \frac{\det(\mathbf{I} - z(\mathbf{A} - \mathbf{e}\mathbf{b}^{\mathrm{T}}))}{\det(\mathbf{I} - z\mathbf{A})}$$

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Example: **Euler's Method**

$$u^{n+1} = u^n + \Delta t F(u); \quad \phi(z) = 1 + z.$$

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For explicit methods of order p:

$$\phi(z) = \sum_{j=0}^{p} \frac{1}{j!} z^j + \sum_{j=p+1}^{s} \alpha_j z^j.$$

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For the linear equation

$$u'(t) = Lu$$

we say the solution is absolutely stable if $|\phi(\lambda \Delta t)| \leq 1$ for all $\lambda \in \sigma(L)$.

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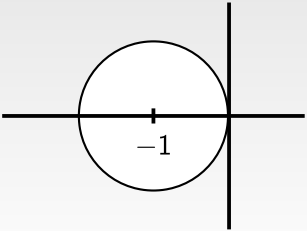


Stability optimization

This leads naturally to the following problem.

Stability optimization

Given L, p, s,

$$\begin{aligned} \text{maximize} \quad & \Delta t \\ \text{subject to} \quad & |\phi(\Delta t \lambda)| - 1 \leq 0, \qquad \lambda \in \sigma(L), \\ \text{where} \quad & \phi(z) = \sum_{j=0}^{p} \frac{1}{j!} z^j + \sum_{j=p+1}^{s} \alpha_j z^j. \end{aligned}$$

Here the decision variables are Δt and the coefficients α_j, $j = p+1, \ldots, s$. This problem is quite difficult; we approximate its solution by solving a sequence of convex problems (DK & A. Ahmadia, arXiv preprint).

Accuracy optimization

We could instead optimize accuracy over some region in $\mathbb{C}$:

Accuracy optimization

Given L, p, s,

$$\begin{aligned} \text{maximize} \quad & \Delta t \\ \text{subject to} \quad & |\phi(\Delta t\lambda) - \exp(\Delta t\lambda| \le \epsilon, \qquad \lambda \in \sigma(L), \\ \text{where} \quad & \phi(z) = \sum_{j=0}^{p} \frac{1}{j!} z^j + \sum_{j=p+1}^{s} \alpha_j z^j. \end{aligned}$$

In the PDE case, we can replace $\exp(\Delta t\lambda)$ with the exact dispersion relation for each Fourier mode.

Stability Optimization: a toy example

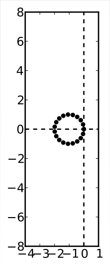
As an example, consider the advection equation

$$u_t + u_x = 0$$

discretized in space by first-order upwind differencing with unit spatial mesh size

$$U_i'(t) = -(U_i(t) - U_{i-1}(t))$$

with periodic boundary condition $U_0(t) = U_N(t)$.



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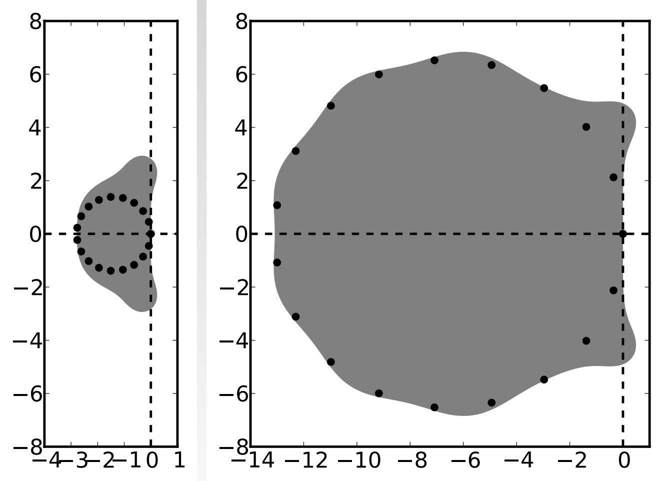


(a) RK(4,4) (b) Optimized 10-stage method

Stability Optimization: a toy example

What is the relative efficiency?

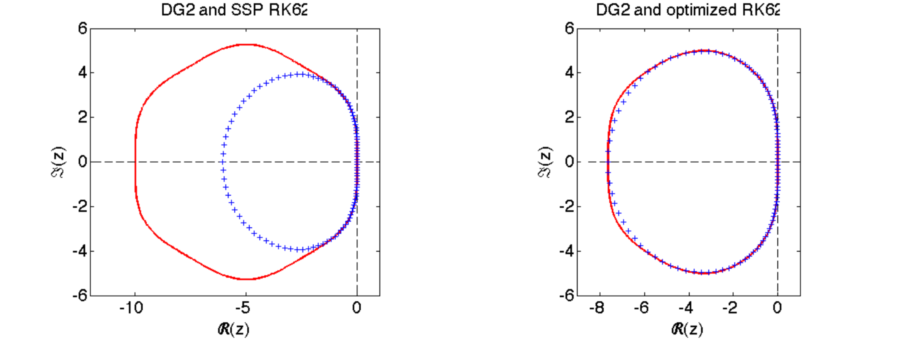
$$\frac{\text{Stable step size}}{\text{Cost per step}}$$

$$\text{RK(4,4):}\ \frac{1.4}{4} \approx 0.35$$

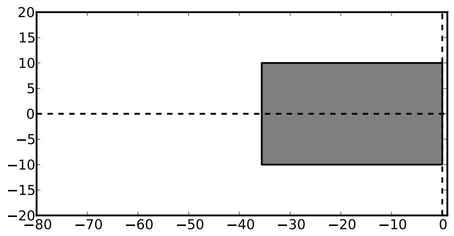
$$\text{RK(10,4):}\ \frac{6}{10} = 0.6$$

By allowing even more stages, can asymptotically approach the efficiency of Euler's method.

Second order discontinuous Galerkin discretization of advection:



Stability Optimization: one more example



$s = 20$

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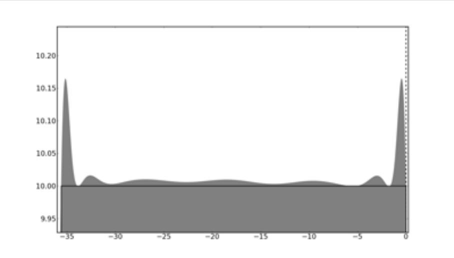

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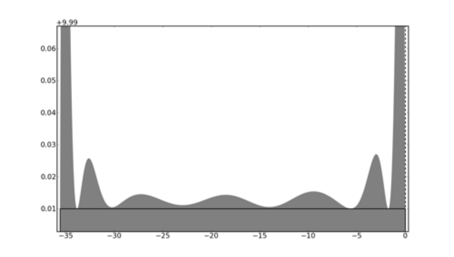

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Nonlinear accuracy

Besides the conditions on the stability polynomial coefficients, high order Runge-Kutta methods must satisfy additional nonlinear order conditions.

- $p = 1$: $\sum_i b_i = 1$
- $p = 2$: $\sum_{i,j} b_i a_{ij} = 1/2$
- $p = 3$: $\sum_{i,j,k} b_i a_{ij} a_{jk} = 1/6$
  $\sum_{i,j,k} b_i a_{ij} a_{ik} = 1/3$

Number of conditions grows factorially (719 conditions for order 10).

Beyond linear stability

Classical stability theory and its extensions focus on

- weak bounds: $\|u^n\| \leq C(t)$
- linear problems
- inner product norms

For hyperbolic PDEs, we are often interested in

- strict bounds $\|u^n\| \leq C$
- nonlinear problems
- L_1, L_∞, TV, or positivity

We refer to bounds of the latter types as strong stability properties. For example:

$$\|u^n\|_{\mathrm{TV}} \leq \|u^{n-1}\|_{\mathrm{TV}}$$

Strong stability preservation

Designing fully-discrete schemes with strong stability properties is notoriously difficult!

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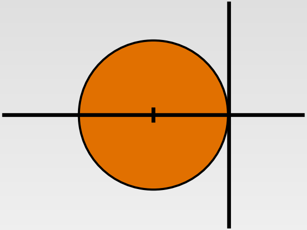

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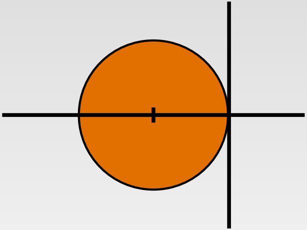

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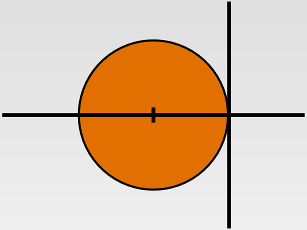

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Strong stability preserving methods provide higher order accuracy while maintaining any convex functional bound satisfied by Euler timestepping.

The Forward Euler condition

Recall our ODE system (typically from a PDE)

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

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

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

satisfies the monotonicity requirement

$$||\mathbf{u}^{n+1}|| \le ||\mathbf{u}^n||,$$

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

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

[1] e.g. TVD, TVB

Runge–Kutta methods as a convex combination of Euler

Consider the two-stage method:

$$\begin{aligned}
\mathbf{y}^1 &= \mathbf{u}^n + \Delta t F(\mathbf{u}^n) \\
\mathbf{u}^{n+1} &= \mathbf{u}^n + \frac{1}{2}\Delta t \left(F(\mathbf{u}^n) + F(\mathbf{y}^1)\right)
\end{aligned}$$

Is $||\mathbf{u}^{n+1}|| \leq ||\mathbf{u}^n||$?

Runge–Kutta methods as a convex combination of Euler

Consider the two-stage method:

$$\begin{aligned}
\mathbf{y}^1 &= \mathbf{u}^n + \Delta t F(\mathbf{u}^n) \\
\mathbf{u}^{n+1} &= \frac{1}{2}\mathbf{u}^n + \frac{1}{2}\left(\mathbf{y}^1 + \Delta t F(\mathbf{y}^1)\right).
\end{aligned}$$

Take $\Delta t \le \Delta t_{\mathsf{FE}}$. Then $||\mathbf{y}^1|| \le ||\mathbf{u}^n||$, so

$$||\mathbf{u}^{n+1}|| \le \frac{1}{2}||\mathbf{u}^n|| + \frac{1}{2}||\mathbf{y}^1 + \Delta t F(\mathbf{y}^1)|| \le ||\mathbf{u}^n||.$$

$$||\mathbf{u}^{n+1}|| \le ||\mathbf{u}^n||$$

Optimized SSP methods

In general, an SSP method preserves strong stability properties satisfied by Euler's method, under a modified step size restriction:

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

A fair metric for comparison is the *effective SSP coefficient*:

$$\mathcal{C}_{\text{eff}} = \frac{\mathcal{C}}{\# \text{ of stages}}$$

By designing high order methods with many stages, we can achieve $\mathcal{C}_{\text{eff}} \to 1$.

Example: A highly oscillatory flow field

$$u_t + \left(\cos^2(20x + 45t)u\right)_x = 0 \qquad\qquad u(0,t) = 0$$

Method	c_{eff}	Monotone effective timestep
NSSP(3,2)	0	0.037
SSP(50,2)	0.980	0.980
NSSP(3,3)	0	0.004
NSSP(5,3)	0	0.017
SSP(64,3)	0.875	0.875
RK(4,4)	0	0.287
SSP(5,4)	0.302	0.416
SSP(10,4)	0.600	0.602

Low storage methods

- Straightforward implementation of an s-stage RK method requires $s+1$ memory locations per unknown
- Special low-storage methods are designed so that each stage only depends on one or two most recent previous stages
- Thus older stages can be discarded as the new ones are computed

- It is often desirable to
  - Keep the previous solution around to be able to restart a step
  - Compute an error estimate
- This requires a minimum of three storage locations per unknown

3S Algorithm

$$
\begin{array}{ll}
 & \mathtt{S}_3 := \mathtt{u}^{\mathtt{n}} \\
(y_1) & \mathtt{S}_1 := \mathtt{u}^{\mathtt{n}} \\
 & \mathtt{for\ i} = 2 : \mathtt{m} + 1\ \mathtt{do} \\
 & \quad \mathtt{S}_2 := \mathtt{S}_2 + \delta_{\mathtt{i}-1}\mathtt{S}_1 \\
(y_i) & \quad \mathtt{S}_1 := \gamma_{\mathtt{i}1}\mathtt{S}_1 + \gamma_{\mathtt{i}2}\mathtt{S}_2 + \gamma_{\mathtt{i}3}\mathtt{S}_3 + \beta_{\mathtt{i},\mathtt{i}-1}\Delta\mathtt{tF}(\mathtt{S}_1) \\
 & \mathtt{end} \\
(\hat{u}^{n+1}) & \quad \mathtt{S}_2 := \frac{1}{\sum_{\mathtt{j}=1}^{\mathtt{m}+2}\delta_{\mathtt{j}}}\left(\mathtt{S}_2 + \delta_{\mathtt{m}+1}\mathtt{S}_1 + \delta_{\mathtt{m}+2}\mathtt{S}_3\right) \\
 & u^{n+1} = \mathtt{S}_1
\end{array}
$$

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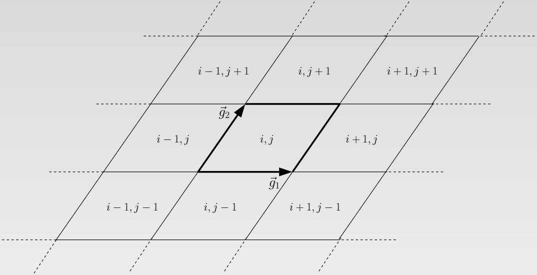
Each of these steps is a complex numerical problem in itself, involving nonconvex optimization in dozens to hundreds of variables, with nonlinear equality and inequality constraints.

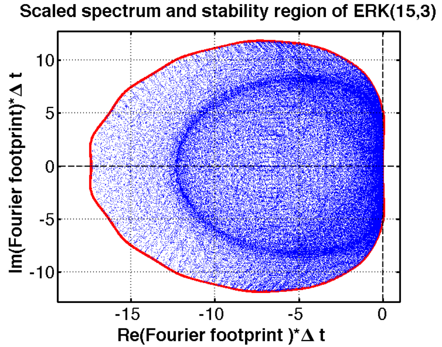
Optimizing for the SD spectrum

- On regular grids, SD leads to a block-Toeplitz operator
- We perform a von Neumann-like analysis using a "generating pattern"



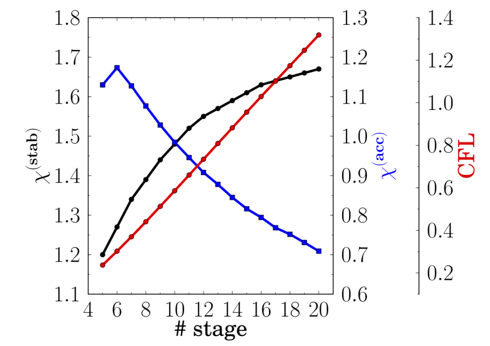
$$\frac{d\mathbf{W}_{i,j}}{dt} + \frac{a}{\Delta g}\left(\mathbf{T}^{0,0}\,\mathbf{W}_{i,j} + \mathbf{T}^{-1,0}\,\mathbf{W}_{i-1,j} + \mathbf{T}^{0,-1}\,\mathbf{W}_{i,j-1}\right.$$
$$\left. + \mathbf{T}^{+1,0}\,\mathbf{W}_{i+1,j} + \mathbf{T}^{0,+1}\,\mathbf{W}_{i,j+1}\right) = 0$$

Optimizing for the SD spectrum



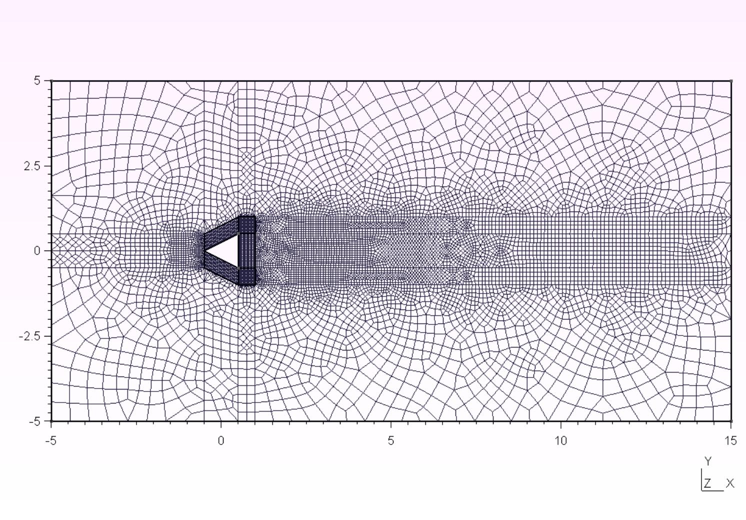
- Blue: eigenvalues; Red: RK stability boundary
- The convex hull of the generated spectrum is used as a proxy to accelerate the optimization process

Optimizing for the SD spectrum



- Primarily optimized for stable step size
- Secondary optimization for nonlinear accuracy and low-storage (3 memory locations per unknown)

Application: flow past a wedge



fully unstructured mesh

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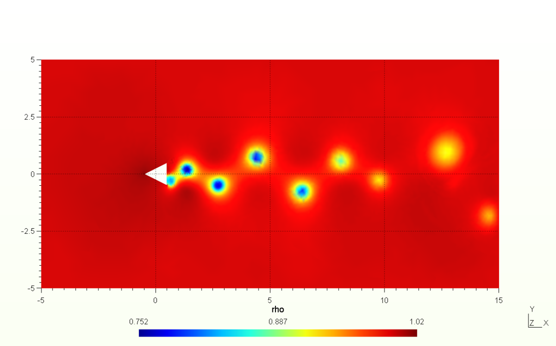

Density at $t = 100$

- 62% speedup using optimized method

Conclusions

- Numerical optimization allows for flexible, targeted design of time integrators
- Stability optimization based on spectra from a model (linear) problem on a uniform grid seems to work well even for nonlinear problems on fully unstructured grids
- Significant speedup can be achieved in practice (greater for higher order methods)