Solving differential equations in reduced- and mixed-precision

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The University of Texas at Austin
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Overview

1. Introduction and background

2. Solving parabolic PDEs in half precision (joint with M. B. Giles)

3. Mixed-precision explicit stabilised Runge-Kutta methods (with G. Rosilho De Souza)

4. Conclusions

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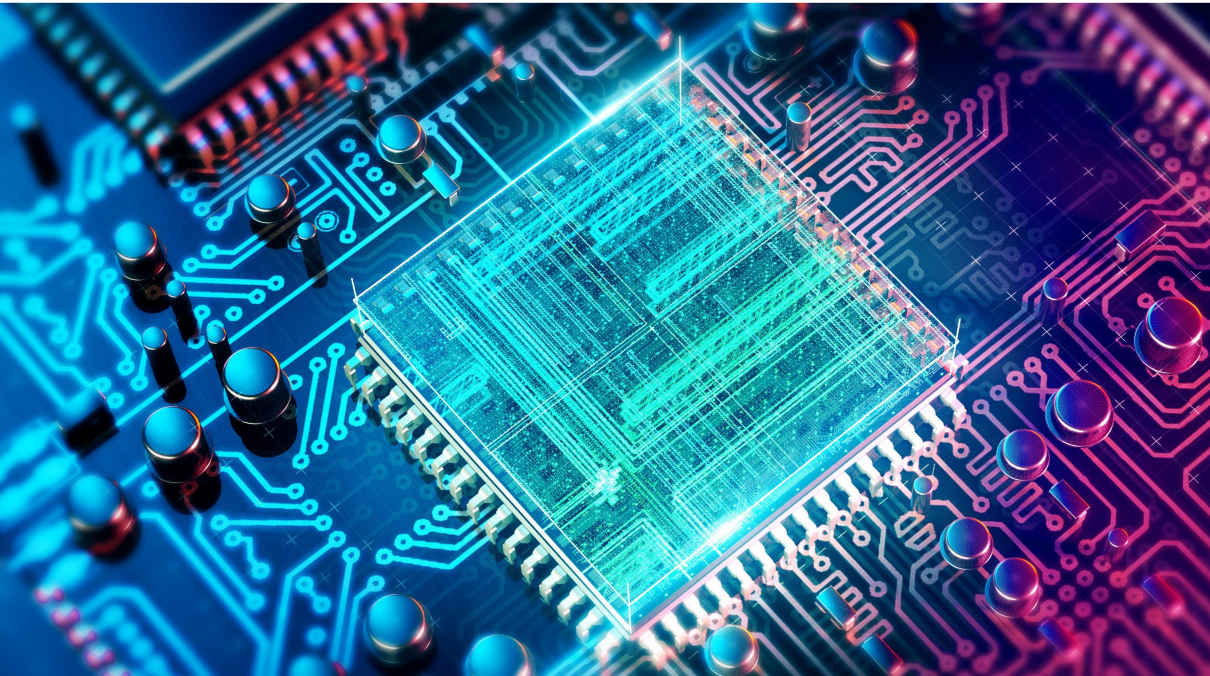
Objective: developing reduced- and mixed-precision DE solvers



Reduced- and mixed-precision algorithms[1]

Reduced-precision algorithms

Reduced-precision algorithms obtain an as accurate solution as possible given the precision while avoiding catastrophic rounding error accumulation.

[1] Review articles: [Abdelfattah et al. 2021], [Higham and Mary 2021], [C. et al. 2021].

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Mixed-precision algorithms combine low- and high-precision computations in order to benefit from the performance gains of reduced-precision while retaining good accuracy.

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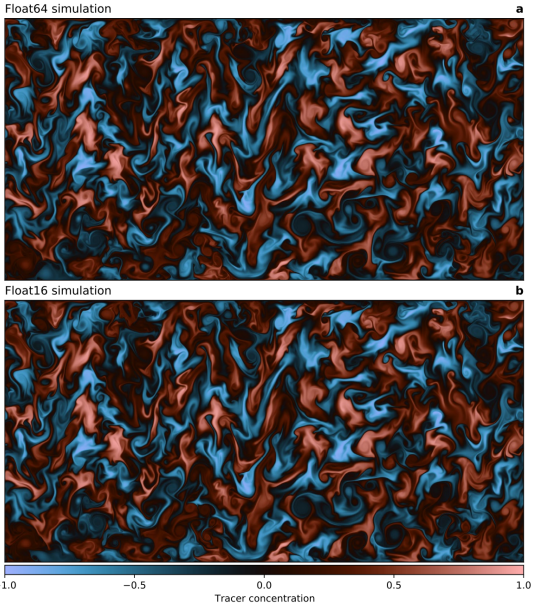
- This is now a very active field of investigation with many new developments led mainly by the numerical linear algebra community.
- Lots of new reduced-/mixed-precision algorithms: matrix factorizations, direct linear solvers, Krylov subspace methods, preconditioning, multigrid, nonlinear solvers.
- There is still much to discover on the topic.

[1] Review articles: [Abdelfattah et al. 2021], [Higham and Mary 2021], [C. et al. 2021].

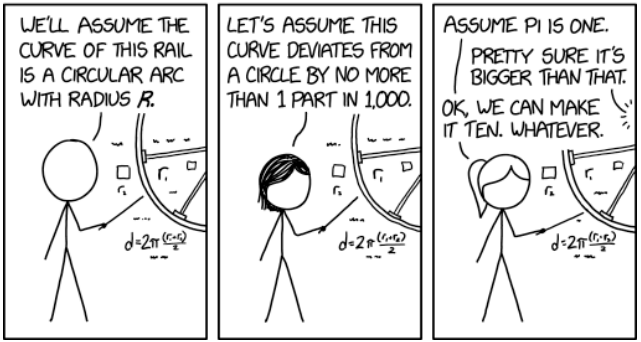
Nonlinear shallow water equations in half precision [Klöwer et al. 2021]



Performed on Fugaku (1st in the TOP500). All other results in this talk are emulated in software.

Floating point formats

Format	"Precision" u	$x_{\min}$	$x_{\max}$
bfloat16 (half)	$2^{-8} \approx 3.91 \times 10^{-3}$	1.18×10^{-38}	3.39×10^{38}
fp16 (half)	$2^{-11} \approx 4.88 \times 10^{-4}$	6.10×10^{-5}	6.55×10^{4}
fp32 (single)	$2^{-24} \approx 5.96 \times 10^{-8}$	1.18×10^{-38}	3.40×10^{38}
fp64 (double)	$2^{-53} \approx 1.11 \times 10^{-16}$	2.22×10^{-308}	1.80×10^{308}



exact arithmetic | half precision | no precision

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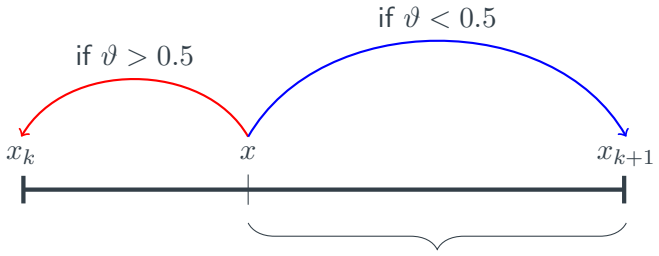
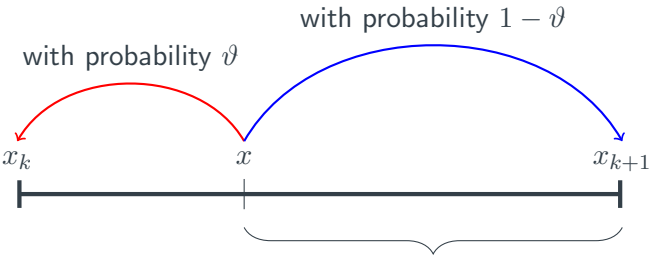
Round to nearest



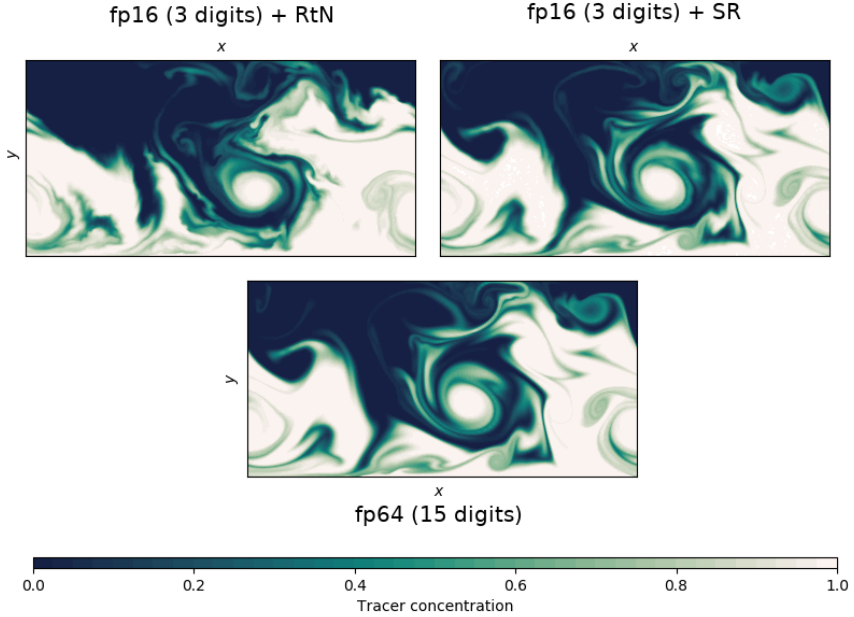
$$\mathsf{fl}(x) = x(1+\delta), \quad \text{with} \quad |\delta| \leq u.$$

Stochastic rounding



$\mathsf{sr}(x) = x(1+\delta(\omega)), \quad \text{with} \quad |\delta(\omega)| \leq 2u, \quad \text{and} \quad \mathbb{E}[sr(x)] = x.$

Interesting results (thanks to Milan Klöwer)



RtN might cause stagnation

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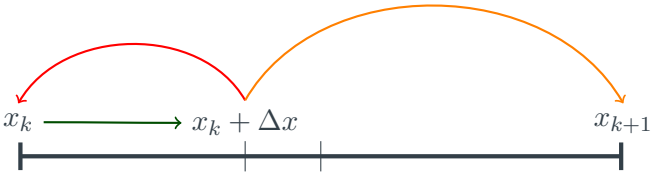
SR is resilient to stagnation



Other properties of SR [C. et al. 2022]

The good:

- SR roundoffs are zero mean and mean-independent: $\mathbb{E}[\delta_i|\delta_1, \ldots, \delta_{i-1}] = \mathbb{E}[\delta_i] = 0$.
- Rounding errors accumulate like $O(\sqrt{n}u)$ rather than $O(nu)$.
- Evaluation of linear functions is exact in expectation. $O(u^2)$ bias for C^2 functions.

The less good:

- Limited (yet growing) hardware support.

Heat equation as a test problem

$$\begin{cases} \dot{\mathrm{u}}(t,\boldsymbol{x}) = \nabla^2 \mathrm{u}(t,\boldsymbol{x}) + f(t,\boldsymbol{x}), & \boldsymbol{x} \in D = [0,1]^d, \quad t > 0, \\ \mathrm{u}(0,\boldsymbol{x}) = \mathrm{u}_0(x), & \boldsymbol{x} \in D, \\ \mathrm{u}(t,\boldsymbol{x}) = g(\boldsymbol{x}), & \boldsymbol{x} \in \partial D, \qquad t > 0. \end{cases}$$

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We use **finite differences** in space: let $\boldsymbol{U}(t) \in \mathbb{R}^K$ with $\boldsymbol{U}_i(t) \approx \mathfrak{u}(t,\boldsymbol{x}_i)$, then

$$\text{(e.g. in 1D)} \quad \dot{\boldsymbol{U}}_i = \frac{1}{h^2}\left(\boldsymbol{U}_{i+1} - 2\boldsymbol{U}_i + \boldsymbol{U}_{i-1}\right) + f(t,\boldsymbol{x}_i) \quad \rightsquigarrow \quad \dot{\boldsymbol{U}}(t) = -A\boldsymbol{U}(t) + \boldsymbol{F}(t).$$

In 1D, $A = \text{tridiag}(-1,2,-1)/h^2 \in \mathbb{R}^{K\times K}$. A is the (spd) **stiffness matrix** or discrete laplacian.

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In 1D, $A = \text{tridiag}(-1,2,-1)/h^2 \in \mathbb{R}^{K\times K}$. A is the (spd) **stiffness matrix** or discrete laplacian. Discretising in time with a **Runge-Kutta** method yields the numerical scheme:

$$\boldsymbol{U}^{n+1} = S\boldsymbol{U}^n + \Delta t \boldsymbol{F}^n$$

for some matrix S dependent on $\Delta t A$, hence on $\lambda = \Delta t/h^2$. For instance,

$$\boldsymbol{U}^{n+1} = (I - \Delta t A)\boldsymbol{U}^n + \Delta t \boldsymbol{F}^n_{\text{FE}}, \quad \text{(FE)}, \qquad \boldsymbol{U}^{n+1} = (I + \Delta t A)^{-1}\boldsymbol{U}^n + \Delta t \boldsymbol{F}^n_{\text{BE}}, \quad \text{(BE)}.$$

In this part of the talk we work in **bfloat16 half precision**, $u = 2^{-8} \approx 4 \times 10^{-3}$.

Use the delta form

How to best implement the Runge-Kutta scheme? Use the **delta form**!

$$\textbf{Standard form:} \quad \boldsymbol{U}^{n+1} = S\boldsymbol{U}^n + \Delta t \boldsymbol{F}^n.$$

$$\textbf{Delta form:} \quad \boldsymbol{U}^{n+1} = \boldsymbol{U}^n + \Delta t \left(-\tilde{S} A \boldsymbol{U}^n + \tilde{\boldsymbol{F}}^n \right) = \boldsymbol{U}^n + \Delta \boldsymbol{U}^n.$$

e.g. $S_{\mathsf{FE}} = (I - \Delta t A)$, $\tilde{S}_{FE} = 1$, and $S_{\mathsf{BE}} = \tilde{S}_{\mathsf{BE}} = (I + \Delta t A)^{-1}$.

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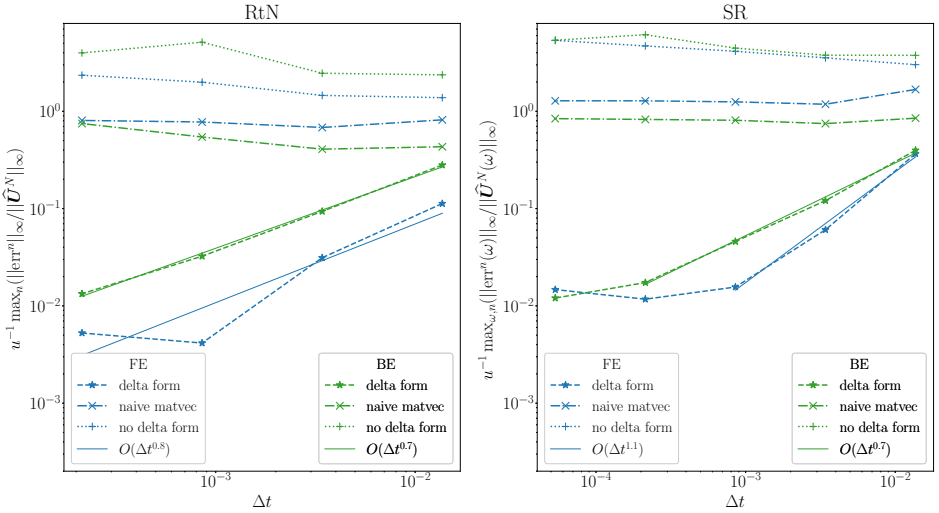
e.g. $S_{\mathsf{FE}} = (I - \Delta t A)$, $\tilde{S}_{FE} = 1$, and $S_{\mathsf{BE}} = \tilde{S}_{\mathsf{BE}} = (I + \Delta t A)^{-1}$.

- Errors in the computation of $S\boldsymbol{U}^n$ are of order u (machine precision).
- Errors in the computation of $\Delta \boldsymbol{U}^n$ are of order $\Delta t^p u$, $p > 0$.

We prove that:

- The delta form produces much smaller rounding errors at each time step.
- Most of the rounding errors in the delta form are introduced into the final addition.

Worst-case local rounding errors in 2D



Note: from now on we use the delta form.

RtN vs SR

Why is RtN in low precision bad for the heat equation?

a) Stagnation:

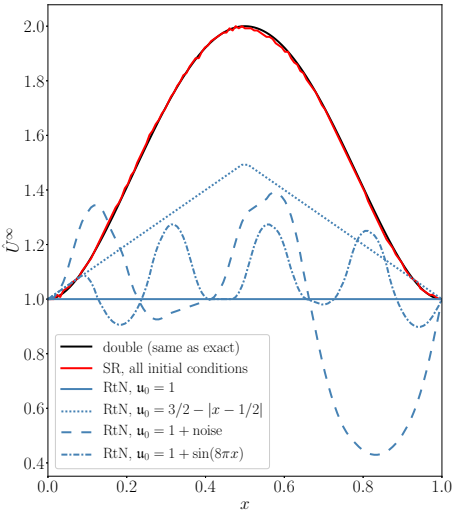
- RtN always stagnates for sufficiently small Δt (recall $\Delta \boldsymbol{U}^n = O(u\Delta t^p)$).
- The RtN solution is initial condition, discretization and precision dependent.

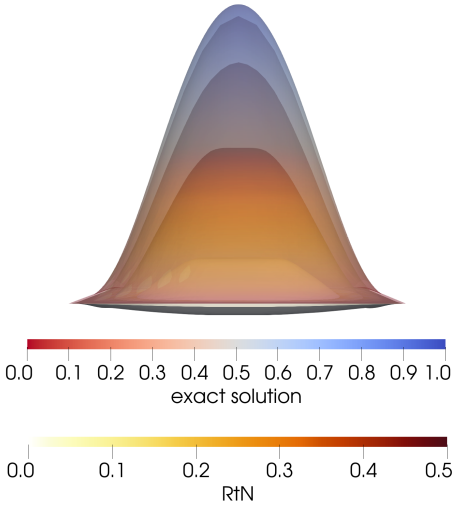
b) Global error:

- RtN rounding errors are strongly correlated and "amplify each other".
- RtN global errors grow like $O(u\Delta t^{-1})$ until stagnation.

SR fixes all these issues!

a) Stagnation (left 1D, right 2D)





RtN computations are discretization and initial condition dependent. SR works!

b) Global rounding errors [C. and Giles 2020]

Let $\varepsilon^n \in \mathbb{R}^K$ be the vector containing all rounding errors introduced at time step n.
Define the global rounding error $\boldsymbol{E}^n = \hat{\boldsymbol{U}}^n - \boldsymbol{U}^n$. It can be shown that

$$\boldsymbol{E}^{n+1} = S\boldsymbol{E}^n + \varepsilon^n.$$

Traditional results for ODEs [Henrici 1962-1963, Arató 1983]: ε^n is $O(\Delta t^2)$.

We can distinguish two cases:

RtN: we can only assume the worst-case scenario, $|\varepsilon_i^n| = O(u)$ for all n, i.

SR: the ε_i^n are zero-mean, independent in space and mean-independent in time.

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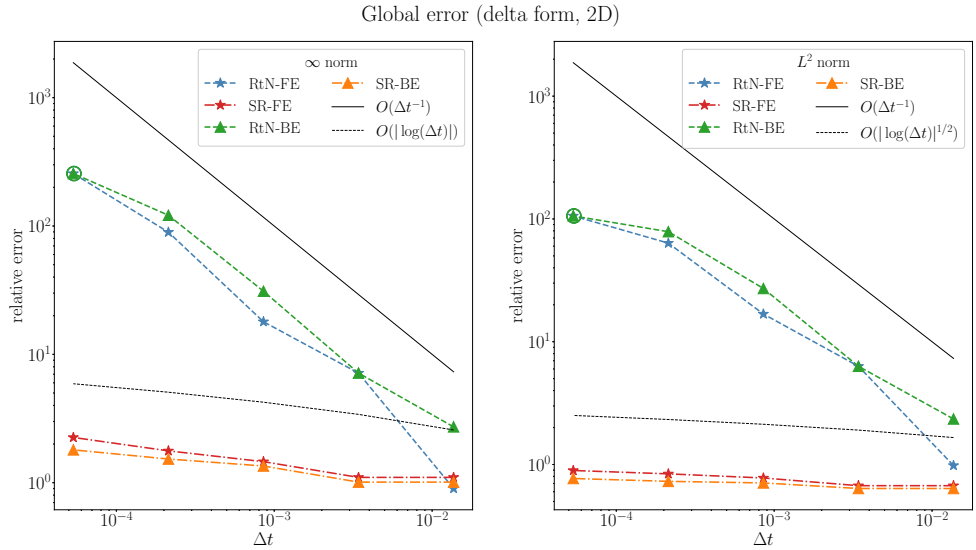
Mode	Norm	1D	2D	3D
RtN	L^2, ∞	$O(u\Delta t^{-1})$	$O(u\Delta t^{-1})$	$O(u\Delta t^{-1})$
SR	$\mathbb{E}[\|\|\cdot\|\|_\infty^2]^{1/2}$	$O(u\Delta t^{-1/4}\ell(\Delta t)^{1/2})$	$O(u\ell(\Delta t))$	$O(u\ell(\Delta t)^{1/2})$
SR	$\mathbb{E}[\|\|\cdot\|\|_{L^2}^2]^{1/2}$	$O(u\Delta t^{-1/4})$	$O(u\ell(\Delta t)^{1/2})$	$O(u)$

Asymptotic global rounding error blow-up rates; $\ell(\Delta t) = |\log(\lambda^{-1}\Delta t)|$.

b) Global rounding errors (here at steady-state)



Note: relative error = error $\times$ $(u||\boldsymbol{U}^N||)^{-1}$

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Framework and objective

We consider mixed-precision explicit RK schemes for the solution of ODEs in the form

$$\boldsymbol{y}'(t) = \boldsymbol{f}(t, \boldsymbol{y}(t)), \quad \boldsymbol{y}(0) = \boldsymbol{y}_0,$$

where $\boldsymbol{f}(t, \boldsymbol{y})$ is of sufficiently smooth, and from now on set $\boldsymbol{f} = \boldsymbol{f}(\boldsymbol{y}(t))$ for simplicity. In our experiments: the ODE is a result of a method-of-lines discretisation of a PDE.

Objective

Evaluate $\boldsymbol{f}$ in low-precision as much as possible without affecting accuracy or stability.

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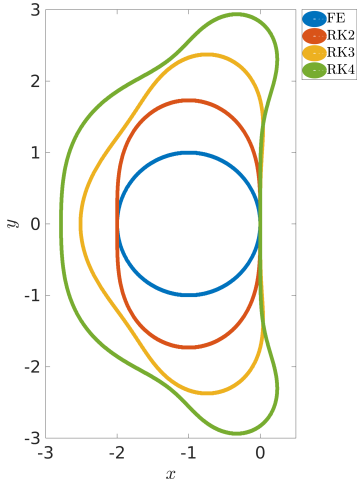
Why do we focus on explicit methods?

- The development of mixed-/reduced-precision linear/nonlinear iterative solvers is a very active field of research. Lots of exciting new work: [Abdelfattah et al. 2020].
- Avoiding nonlinear/linear solves is in general a big advantage. We use stabilised RK methods to minimise timestep restrictions.

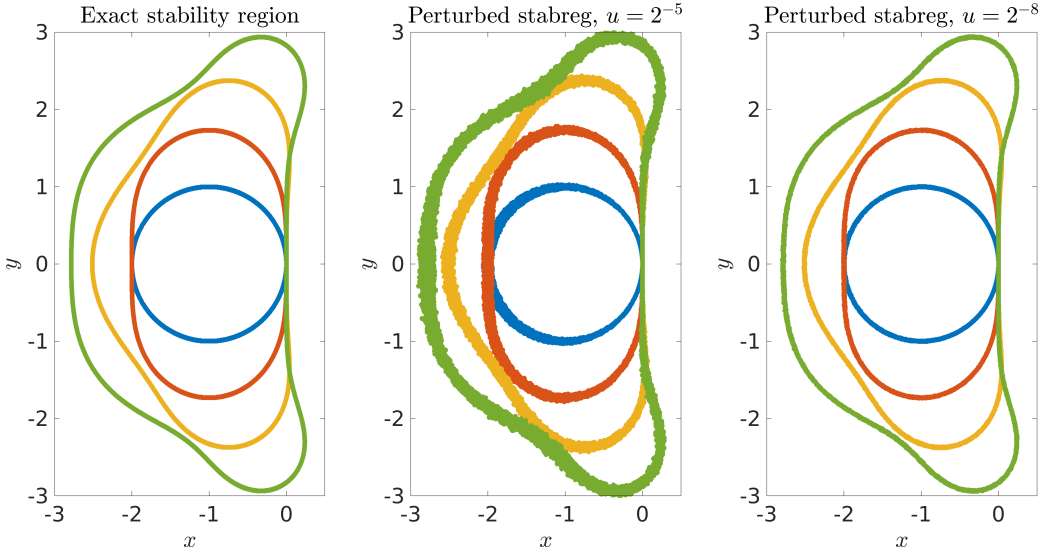
Note: in this part of the talk we only use RtN.

Absolute stability

Dahlquist's test problem: $y' = \lambda y$, $y(0) = 1$.
s-stage RK method $y^n = R_s(z)^n$, where $z = \Delta t \lambda = x + iy$. Stable if $|R_s(z)| < 1$.



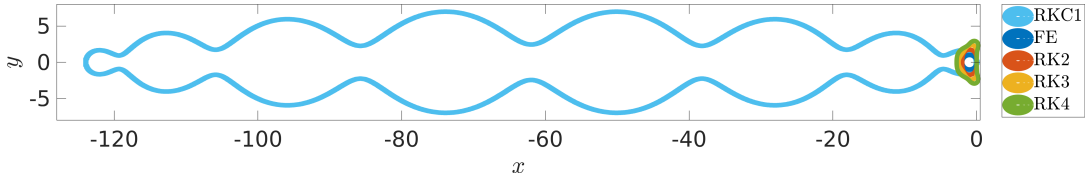
Linear stability for RK methods (in practice)



Explicit stabilized Runge-Kutta methods[2]

Idea: pick the poly $R_s(z)$ so as to maximise the stability region. For parabolic problems: use orthogonal polys, e.g. Runge-Kutta-Chebyshev (RKC). $\rightsquigarrow O(s^2)$ region.

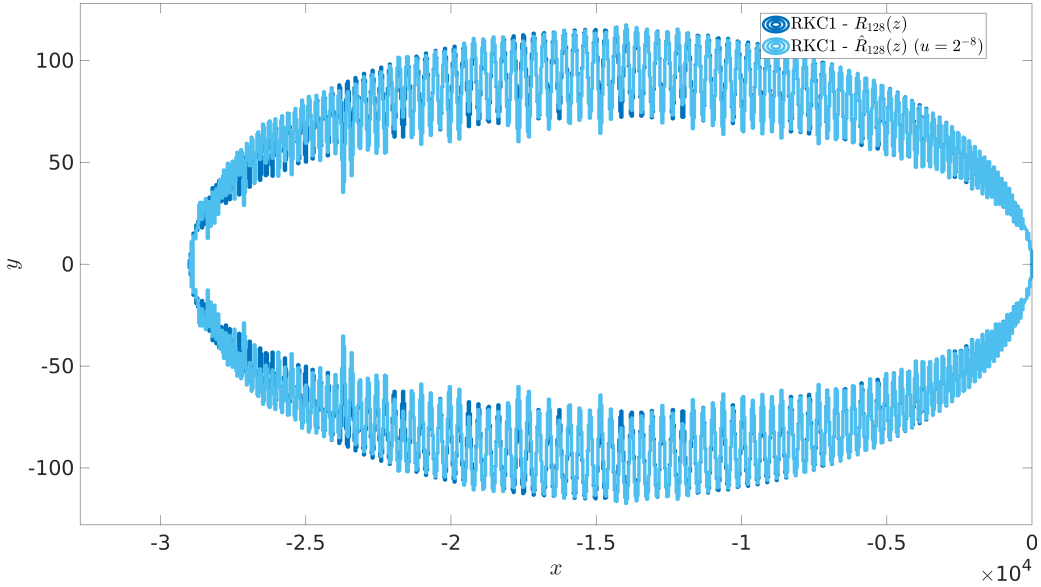
ESRK methods are of low-order ($p \leq 4$), but they use a lot of stages to maximise stability (i.e. not for accuracy purposes) $\rightarrow$ can do most of these in low precision!



Absolute stability region of RKC1 with $s = 8$ vs those of other explicit methods.

[2]Refs: [van der Houwen and Sommeijer 1980], many papers by Abdulle and collaborators.

Linear stability for RKC (in practice, $s = 128$, $u = 2^{-8}$)



Linear problems, i.e. $\boldsymbol{f}(\boldsymbol{y}) = A\boldsymbol{y}$

Consider the exact solution at $t = \Delta t$ and its corresponding p-th order RK approximation:

$$\boldsymbol{y}(\Delta t) = \exp(\Delta t A)\boldsymbol{y}_0 = \sum_{j=0}^{\infty} \frac{(\Delta t A)^j}{j!}\boldsymbol{y}_0,$$

$$\boldsymbol{y}_1 = \sum_{j=0}^{p} \frac{(\Delta t A)^j}{j!}\boldsymbol{y}_0 + O(\Delta t^{p+1}).$$

Giving a local error of $\tau = \Delta t^{-1}||\boldsymbol{y}(\Delta t) - \boldsymbol{y}_1|| = O(\Delta t^p)$.

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Evaluating the scheme in finite precision yields:

$$\hat{\boldsymbol{y}}_1 = \varepsilon + \boldsymbol{y}_0 + \sum_{j=1}^{p} \frac{\Delta t^j}{j!} \left(\prod_{k=1}^{j} (A + \Delta A_k) \right) \boldsymbol{y}_0 + O(\Delta t^{p+1}).$$

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Let us consider the following scenarios:

1. We have $\varepsilon = O(u)$ and we get $\tau = O(u\Delta t^{-1} + \Delta t^p)$. Rapid error growth!

Linear problems

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1. We have $\varepsilon = O(u)$ and we get $\tau = O(u\Delta t^{-1} + \Delta t^p)$. Rapid error growth!
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Linear problems

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1. We have $\varepsilon = O(u)$ and we get $\tau = O(u\Delta t^{-1} + \Delta t^p)$. Rapid error growth!
2. Exact vector operations: $\varepsilon = 0$ so $\tau = O(u + \Delta t^p)$. $O(u)$ limiting accuracy and loss of convergence.
3. First $q \geq 1$ matvecs exact. Now $\varepsilon = 0$ and $\Delta A_k = 0$ for $k = 1, \ldots, q$, so $\tau = O(u\Delta t^q + \Delta t^p)$. Recover q-th order convergence!

Order-preserving mixed-precision RK methods

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Operations performed in high-precision are exact.

Definition (Order-preserving mixed-precision RK method)

A p-th order mixed-precision RK method is q-order-preserving ($q \in \{1, \dots, p\}$), if it converges with order q under the above assumption.

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Existing methods: Standard mixed-precision RK schemes perform all function evaluations in low-precision and they are therefore not order-preserving.

Our objective: Use q function evaluations in high precision to obtain a q-order-preserving mixed-precision RK method.

Result: We can construct q-order preserving RK methods for any q for linear problems, and for $q = 1, 2$ for nonlinear problems. Today we focus on RKC methods.

Mixed-precision RKC methods

One step of an s-stage RKC scheme in exact arithmetic is given by:

$$\begin{cases} \boldsymbol{d}_0 = \boldsymbol{0}, \quad \boldsymbol{d}_1 = \mu_1 \Delta t \boldsymbol{f}(\boldsymbol{y}^n), \\ \boldsymbol{d}_j = \nu_j \boldsymbol{d}_{j-1} + \kappa_j \boldsymbol{d}_{j-2} + \mu_j \Delta t \boldsymbol{f}(\boldsymbol{y}^n + \boldsymbol{d}_{j-1}) + \gamma_j \Delta t \boldsymbol{f}(\boldsymbol{y}^n), \quad j = 2, \ldots, s, \\ \boldsymbol{y}^{n+1} = \boldsymbol{y}^n + \boldsymbol{d}_s. \end{cases}$$

For a q-order preserving method we need to make sure all rounding errors are $O(\Delta t^{q+1})$.

Mixed-precision RKC methods

One step of a tentative mixed-precision scheme is given by:

$$\begin{cases} \hat{\boldsymbol{d}}_0 = \boldsymbol{0}, \quad \hat{\boldsymbol{d}}_1 = \mu_1 \Delta t \boldsymbol{f}(\hat{\boldsymbol{y}}^n), \\ \hat{\boldsymbol{d}}_j = \nu_j \hat{\boldsymbol{d}}_{j-1} + \kappa_j \hat{\boldsymbol{d}}_{j-2} + \mu_j \Delta t \hat{\boldsymbol{f}}(\hat{\boldsymbol{y}}^n + \hat{\boldsymbol{d}}_{j-1}) + \gamma_j \Delta t \boldsymbol{f}(\hat{\boldsymbol{y}}^n), \quad j = 2, \ldots, s, \\ \hat{\boldsymbol{y}}^{n+1} = \hat{\boldsymbol{y}}^n + \hat{\boldsymbol{d}}_s. \end{cases}$$

For a q-order preserving method we need to make sure all rounding errors are $O(\Delta t^{q+1})$.

The red term leads to an $O(u\Delta t)$ error! $\Rightarrow$ Must rewrite.

Mixed-precision RKC methods

We can rewrite:

$$\begin{cases} \hat{\boldsymbol{d}}_0 = \boldsymbol{0}, \quad \hat{\boldsymbol{d}}_1 = \mu_1 \Delta t \boldsymbol{f}(\hat{\boldsymbol{y}}^n), \\ \hat{\boldsymbol{d}}_j = \nu_j \hat{\boldsymbol{d}}_{j-1} + \kappa_j \hat{\boldsymbol{d}}_{j-2} + \mu_j \Delta t \hat{\Delta} \boldsymbol{f}_{j-1} + (\mu_j + \gamma_j) \Delta t \boldsymbol{f}(\hat{\boldsymbol{y}}^n), \quad j = 2, \dots, s, \\ \hat{\boldsymbol{y}}^{n+1} = \hat{\boldsymbol{y}}^n + \hat{\boldsymbol{d}}_s. \end{cases}$$

For a q-order preserving method we need to make sure all rounding errors are $O(\Delta t^{q+1})$.

The above is now a q-order preserving method as long as

$$\hat{\Delta} \boldsymbol{f}_j = \left(\boldsymbol{f}(\hat{\boldsymbol{y}}^n + \hat{\boldsymbol{d}}_{j-1}) - \boldsymbol{f}(\hat{\boldsymbol{y}}^n) \right) + O(\Delta t^q) = \Delta \boldsymbol{f}_j + O(\Delta t^q), \quad \forall j.$$

Note: if $\hat{\Delta} \boldsymbol{f}_j = \Delta \boldsymbol{f}_j$ we recover the exact RKC scheme.

Computing the $\hat{\Delta}\boldsymbol{f}_j$ terms - RKC1

For RKC1 we want

$$\hat{\Delta}\boldsymbol{f}_j = \Delta\boldsymbol{f}_j + O(\Delta t) = \Big(\boldsymbol{f}(\hat{\boldsymbol{y}}^n + \hat{\boldsymbol{d}}_{j-1}) - \boldsymbol{f}(\hat{\boldsymbol{y}}^n)\Big) + O(\Delta t), \quad \forall j.$$

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It is sufficient that $\hat{\Delta}\boldsymbol{f}_j = \boldsymbol{f}'_j(\hat{\boldsymbol{y}}^n)\hat{\boldsymbol{d}}_j + O(\Delta t)$ since $\Delta\boldsymbol{f}_j = \boldsymbol{f}'_j(\hat{\boldsymbol{y}}^n)\hat{\boldsymbol{d}}_j + O(\Delta t)$.

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Lots of options available to approximate/evaluate $\boldsymbol{f}'(\hat{\boldsymbol{y}}^n)$ (can use low precision).

Computing the $\hat{\Delta}\boldsymbol{f}_j$ terms - RKC2

For RKC2 we want

$$\hat{\Delta}\boldsymbol{f}_j = \Delta\boldsymbol{f}_j + O(\Delta t^2) = \Big(\boldsymbol{f}(\hat{\boldsymbol{y}}^n + \hat{\boldsymbol{d}}_{j-1}) - \boldsymbol{f}(\hat{\boldsymbol{y}}^n)\Big) + O(\Delta t^2), \quad \forall j.$$

Computing the $\hat{\Delta}\boldsymbol{f}_j$ terms - RKC2

For RKC2 we want

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Let $\hat{\boldsymbol{v}}_j = \hat{\boldsymbol{d}}_j - c_j\Delta t\boldsymbol{f}(\boldsymbol{y}^n)$, which is $O(\Delta t^2)$. We split $\Delta\boldsymbol{f}_j = \Delta_1\boldsymbol{f}_j + \Delta_2\boldsymbol{f}_j$, where

$$\begin{aligned}
\Delta_1\boldsymbol{f}_j &= \boldsymbol{f}(\hat{\boldsymbol{y}}^n + c_{j-1}\Delta t\boldsymbol{f}(\hat{\boldsymbol{y}}^n) + \hat{\boldsymbol{v}}_{j-1}) - \boldsymbol{f}(\hat{\boldsymbol{y}}^n + c_{j-1}\Delta t\boldsymbol{f}(\hat{\boldsymbol{y}}^n)),\\
\Delta_2\boldsymbol{f}_j &= \boldsymbol{f}(\hat{\boldsymbol{y}}^n + c_{j-1}\Delta t\boldsymbol{f}(\hat{\boldsymbol{y}}^n)) - \boldsymbol{f}(\hat{\boldsymbol{y}}^n).
\end{aligned}$$

Computing the $\hat{\Delta}\boldsymbol{f}_j$ terms - RKC2

For RKC2 we want

$$\hat{\Delta}\boldsymbol{f}_j = \Delta\boldsymbol{f}_j + O(\Delta t^2) = \Big(\boldsymbol{f}(\hat{\boldsymbol{y}}^n + \hat{\boldsymbol{d}}_{j-1}) - \boldsymbol{f}(\hat{\boldsymbol{y}}^n)\Big) + O(\Delta t^2), \quad \forall j.$$

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It is sufficient to approximate both terms with $O(\Delta t^2)$ error. Again we use derivatives:

$$\begin{aligned}\hat{\Delta}_1\boldsymbol{f}_j &= \hat{\boldsymbol{f}}'(\hat{\boldsymbol{y}}^n + c_j\Delta t\boldsymbol{f}(\hat{\boldsymbol{y}}^n))\hat{\boldsymbol{v}}_j = \Delta_1\boldsymbol{f}_j + O(\Delta t^2),\\ \hat{\Delta}_2\boldsymbol{f}_j &= c_j\Delta t\boldsymbol{f}'(\hat{\boldsymbol{y}}^n)\boldsymbol{f}(\hat{\boldsymbol{y}}^n) = \Delta_2\boldsymbol{f}_j + O(\Delta t^2),\end{aligned}$$

Linear stability

Theorem

Let $\boldsymbol{f}(\boldsymbol{y}) = A\boldsymbol{y}$ with A being a symmetric npd matrix. Our order-p schemes satisfy

$$\hat{\boldsymbol{y}}^{n+1} = R_s^p(\Delta t A)\hat{\boldsymbol{y}}^n + \boldsymbol{r}_s^p(\hat{\boldsymbol{y}}^n),$$

where $\boldsymbol{r}_s^p$ contains the rounding errors introduced at time step n,

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where $\boldsymbol{r}_s^p$ contains the rounding errors introduced at time step n, and is bounded by

$$\|\boldsymbol{r}_s^p\|_2 \leq \Psi_p(\Delta t, A)\left((1 + C_p(s,\varepsilon)\Delta t u)^{s-1} - 1\right)\|\hat{\boldsymbol{y}}^n\|_2.$$

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$\Psi_p(\Delta t, A)$ is method-dependent and given by

$$\Psi_1(\Delta t, A) = \max_{k=1,\ldots,s-1} \|R_k^p(\Delta t A) - I\|_2 = O(\Delta t), \qquad \text{for RKC1},$$

$$\Psi_2(\Delta t, A) = \max_{k=1,\ldots,s-1} \|R_k^p(\Delta t A) - I - c_k \Delta t A\|_2 = O(\Delta t^2), \qquad \text{for RKC2}.$$

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Note: For large Δt and s we have $\Psi_1(\Delta t A) \leq 2$, $\Psi_2(\Delta t A) \leq 2 + \Delta t\|A\|_2 \leq cs^2$.
$\Rightarrow$ Mixed-precision RKC2 is unstable for large Δt and s.

Stabilising RKC2

Recall: we computed $\hat{\Delta}\boldsymbol{f}_j = \hat{\Delta}_1\boldsymbol{f}_j + \hat{\Delta}_2\boldsymbol{f}_j$, where $\hat{\Delta}_1\boldsymbol{f}_j = \boldsymbol{f}'(\dots)\hat{\boldsymbol{v}}_j = O(\Delta t^2)$.

The culprit is the $\hat{\boldsymbol{v}}_j$ term: for small Δt this is small and ensures 2nd order convergence, but for large Δt it becomes huge and leads to instability!

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To fix this, consider the 1-order preserving evaluation of $\hat{\Delta}\boldsymbol{f}_j$ (same as for RKC1):

$$\tilde{\Delta}\boldsymbol{f}_j = \boldsymbol{f}'_j(\hat{\boldsymbol{y}}_j)\hat{\boldsymbol{d}}_j + O(\Delta t).$$

This leads to a stable scheme for large Δt, but is only first-order accurate for small Δt.

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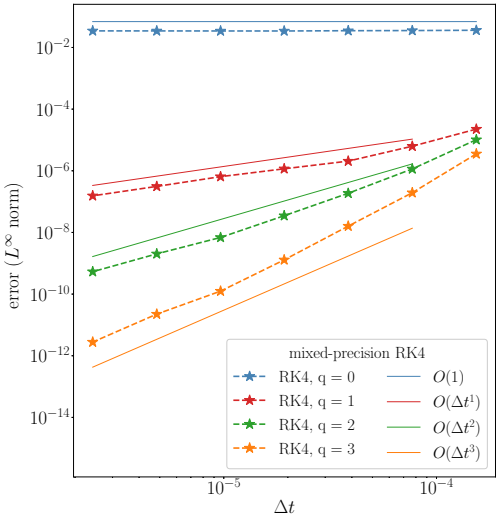
Solution: set $\hat{\Delta}\boldsymbol{f}_j = \begin{cases} \hat{\Delta}_1\boldsymbol{f}_j + \hat{\Delta}_2\boldsymbol{f}_j, & \text{if } \|\hat{\boldsymbol{v}}_j\|_2 \le \|\hat{\boldsymbol{d}}_j\|_2, \\ \tilde{\Delta}\boldsymbol{f}_j, & \text{if } \|\hat{\boldsymbol{v}}_j\|_2 > \|\hat{\boldsymbol{d}}_j\|_2. \end{cases}$

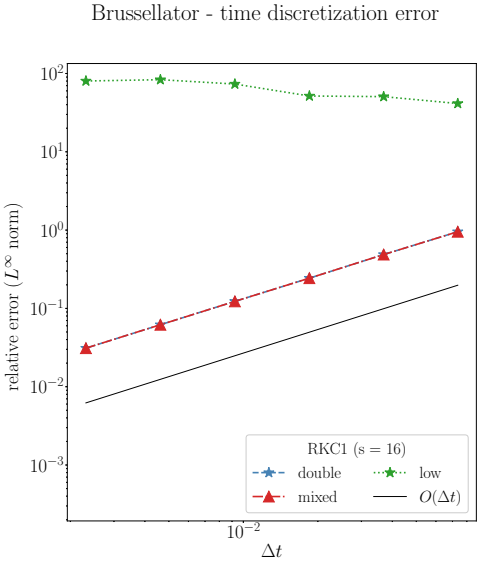
This leads to a 2nd-order *and* stable method. Can prove $\Psi_{2,\text{new}} = \min(\Psi_1, \Psi_2) \le 2$.

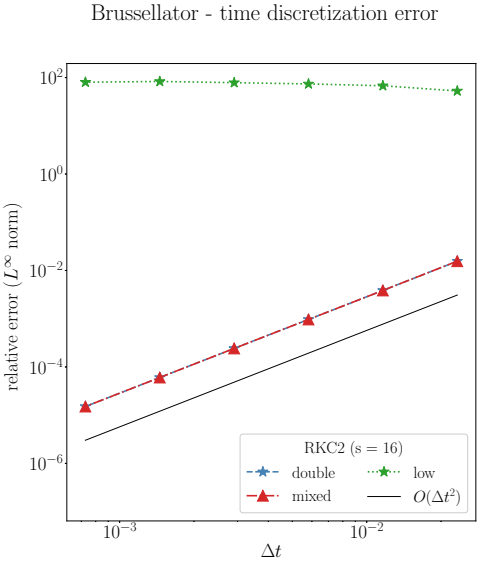
Numerical results - convergence (3D heat eqn, half precision)



The transition from order p to order q happens roughly when $\Delta t = O(||A||^{-1} u^{\frac{1}{p-q}})$

Numerical results - convergence (Brussellator, half precision)





Overview

1. Introduction and background

2. Solving parabolic PDEs in half precision (joint with M. B. Giles)

3. Mixed-precision explicit stabilised Runge-Kutta methods (with G. Rosilho De Souza)

4. Conclusions

Outlook

To sum up

- Reduced-/mixed-precision algorithms require a careful implementation, but can bring significant memory, cost, and energy savings.
- SR makes computations very resilient to stagnation and error accumulation. If used correctly it can make reduced-precision computations very robust.
- We can make ESRK methods as accurate as their high precision equivalent and as cheap as their fully low-precision counterpart.
- Our work extends to multirate ESRK and to RK methods in general for $q = 1, 2$.
- We used a custom-built C++ low-precision emulator for most results.

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- We used a custom-built C++ low-precision emulator for most results.

Thank you for listening!

Thank you for listening! If you want to know more...

Papers and more info at: `https://croci.github.io`

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APPENDIX

Exploit exact subtraction

How to best implement the matrix-vector product $-A\boldsymbol{U}^n$?

$$\frac{\boldsymbol{U}_{i+1}^n - 2\boldsymbol{U}_i^n + \boldsymbol{U}_{i-1}^n}{h^2}, \qquad \frac{(\boldsymbol{U}_{i+1}^n - \boldsymbol{U}_i^n) - (\boldsymbol{U}_i^n - \boldsymbol{U}_{i-1}^n)}{h^2}.$$

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Leads to $O(h^{-2})$ error! **Leads to near-exact matvecs.**

A similar trick works for FEM as well. Only requires small modification of CSR matvecs.

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A similar trick works for FEM as well. Only requires small modification of CSR matvecs.

Parts of a Theorem [C. and Giles 2020]

If $a, b \in \mathbb{R}$ are exactly represented in floating point arithmetic, and

$$|a - b| \leq \min(|a|, |b|)$$

then $(a - b)$ is computed exactly.

See also Section 2.5 in "Accuracy and Stability of Numerical Algorithms" by Nick Higham.

Computational savings

The mixed-precision scheme is cheaper by roughly a factor

$$\varrho = \frac{(s-q)(r-1)}{sr}, \quad \text{where} \quad r = \frac{\text{Cost of RHS evals in high}}{\text{Cost of RHS evals in low}}.$$

A scheme in double/half yields $r = 4^\ell$ for $O(N^\ell)$-cost RHS evaluations.

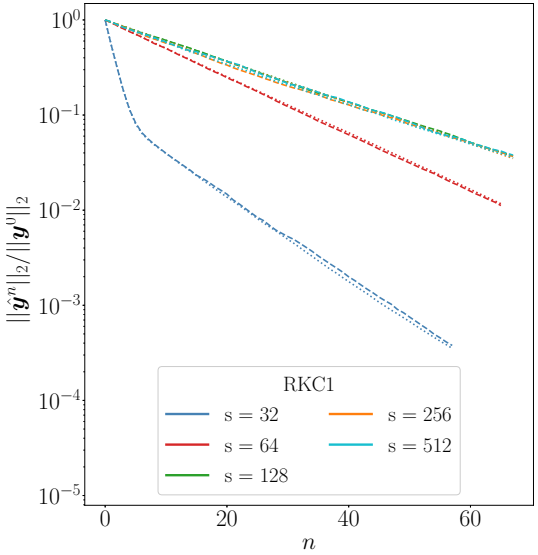
- For RK4 and $\ell = 1$ this leads to 56% $(q = 1)$ and 40% $(q = 2)$ savings.
- Stabilised methods have lots of stages and low order: can essentially take $s \to \infty$, giving $\varrho \to 1 - 1/r$. E.g. this leads to 75% savings if $\ell = 1$.

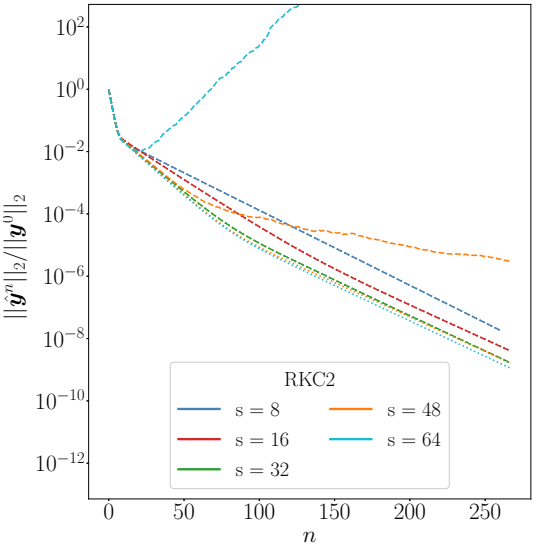
Note: We have ignored additional savings related to memory/caching effects.

Linear stability result - some comments

- The bounds account for rounding errors propagating from previous stages, an overlooked phenomenon in standard RKC theory [Verwer et al. 1990].
- No stability in the classical sense: local errors are amplified for large Δt.
- Rounding errors act on all frequencies and destroy any spectral relation between the iterates forbidding any stability analysis based on eigenvalues.
- We can only prove actual stability under stringent conditions on $\mathrm{cond}(A)$.
- The previous result is a very pessimistic worst-case bound that does not seem to affect computations in practice.

Numerical results - stability (2D nonlinear heat eqn, half precision)





Numerical results - error vs number of stages