# An overview of mixed-precision methods in scientific computing

#### Matteo Croci

Center for Optimization and Statistical Learning Seminar. Northwestern University, 6 October 2022

#### Overview

- 1. Introduction and background
- 2. Optimization
- 3. Numerical linear algebra
- 4. Numerical solution of partial differential equations
- 5. Conclusions

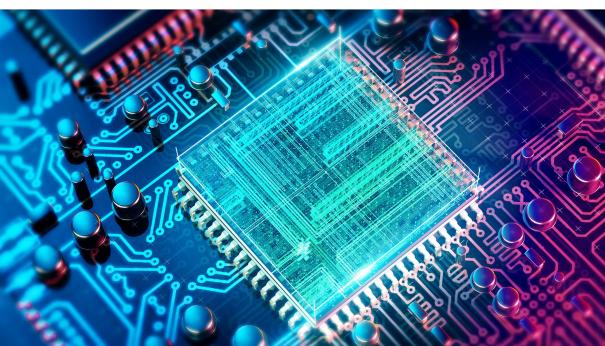
Note: too broad a field to include everything. I will present a few examples per topic.

# 1. Introduction and background

#### Main references:

- A. Abdelfattah, H. Anzt, E. G. Boman, E. Carson, T. Cojean, J. Dongarra, A. Fox, et al. A survey
  of numerical linear algebra methods utilizing mixed-precision arithmetic. The International Journal
  of High Performance Computing Applications, 35(4):344–369, 2021
- N. J. Higham and T. Mary. Mixed precision algorithms in numerical linear algebra. Acta Numerica, 31:347–414, 2022
- M. Croci, M. Fasi, N. J. Higham, T. Mary, and M. Mikaitis. Stochastic rounding: implementation, error analysis and applications. Royal Society Open Science, 9:211631, 2022
- M. P. Connolly, N. J. Higham, and T. Mary. Stochastic rounding and its probabilistic backward error analysis. SIAM Journal on Scientific Computing, 43(1):566–585, 2021
- N. J. Higham. Accuracy and Stability of Numerical Algorithms. SIAM, 2002

Reduced- and mixed-precision algorithms



### Reduced- and mixed-precision algorithms

### Reduced-precision algorithms

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

<sup>&</sup>lt;sup>1</sup>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<sup>1</sup> with many new developments led mainly by the numerical linear algebra and machine learning communities.
- Many new RP/MP algorithms in scientific computing and data science.
- There is still much to discover on the topic.

<sup>&</sup>lt;sup>1</sup>Review articles: [Abdelfattah et al. 2021], [Higham and Mary 2021], [C. et al. 2021].

### Floating point formats

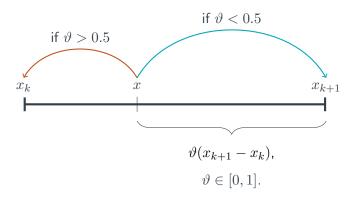
Format	unit roundoff $\boldsymbol{u}$	Range
bfloat16 (half) fp16 (half) fp32 (single) fp64 (double)	$\begin{array}{ll} 2^{-8} & \approx 3.91 \times 10^{-3} \\ 2^{-11} & \approx 4.88 \times 10^{-4} \\ 2^{-24} & \approx 5.96 \times 10^{-8} \\ 2^{-53} & \approx 1.11 \times 10^{-16} \end{array}$	$10^{\pm 38}  10^{\pm 5}  10^{\pm 38}  10^{\pm 308}$

**Important:** don't just focus on u, range is an extremely important factor. Scaling and squeezing techniques are central for a correct reduced-precision implementation.

**Recent trend in scientific computing:** *u* is getting larger: all major chip manufacturers (AMD, ARM, NVIDIA, Intel, ...) have commercialized chips (CPUs, GPUs, TPUs, FPGAs, ...) supporting low-precision computations.

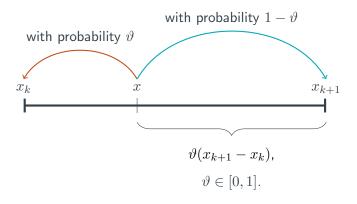
Half vs double max speedups:  $\times 4$  on CPUs,  $\times 32$  on A100 NVIDIA GPUs.

#### Round to nearest



$$\mathrm{fl}(x) = x(1+\delta), \quad \mathrm{with} \quad |\delta| \le \mathbf{\underline{u}}.$$

# Stochastic rounding (review article [C. et al. 2022])



$$\operatorname{sr}(x) = x(1 + \delta(\omega)), \quad |\delta| \le 2u, \quad \text{and} \quad \mathbb{E}[\operatorname{sr}(x)] = x, \quad \mathbb{E}[\delta_i | \delta_1, \dots, \delta_{i-1}] = \mathbb{E}[\delta_i] = 0.$$

Limited (yet growing) hardware support. Many new applications in Sci. Comp. and ML.

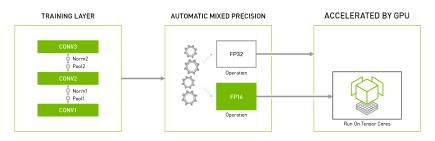
# 2. Optimization

**Note:** Not my field of expertise. Post-seminar discussions are welcome!

#### Main references:

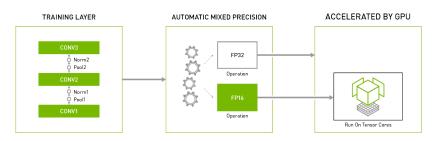
- N. Mellempudi, S. Srinivasan, D. Das, and B. Kaul. Mixed precision training with 8-bit floating point. arXiv preprint arXiv:1905.12334, 2019
- F. Seide, H. Fu, J. Droppo, G. Li, and D. Yu. 1-bit stochastic gradient descent and its application to data-parallel distributed training of speech DNNs. In Fifteenth annual conference of the international speech communication association. Microsoft, 2014
- Y. Xie, R. H. Byrd, and J. Nocedal. Analysis of the BFGS method with errors. SIAM Journal on Optimization, 30(1):182–209, 2020
- F. Tisseur. Newton's method in floating point arithmetic and iterative refinement of generalized eigenvalue problems. SIAM Journal on Matrix Analysis and Applications, 22(4):1038–1057, 2001
- C. Kelley. Newton's method in mixed precision. SIAM Review, 64(1):191–211, 2022

• The machine learning community has been the main driver of experimentation in this field and GPU tensor cores really help making this efficient.



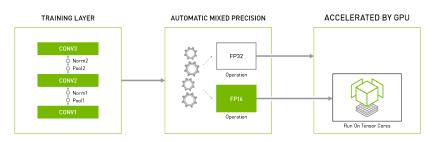
 $\verb|https://developer.nvidia.com/automatic-mixed-precision|.$ 

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- "Easy" to implement: a single line of code allows to switch to single/half mixed-precision in TensorFlow.



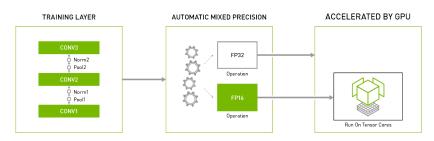
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- Stochastic rounding has been successfully employed to squeeze stochastic gradient descent into quarter precision, see [Mellempudi et al. 2019].



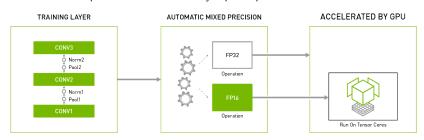
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- From a theoretical point of view: many open questions.



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Limited results in the optimization literature are specific to rounding errors. However, there is work on optimization with noise (see e.g. [Xie, Byrd & Nocedal 2020]).

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#### Need to consider:

• Noisy function and derivative evaluations:

$$\begin{split} \hat{f}(\boldsymbol{x}) &= f(\boldsymbol{x}) + \varepsilon_f(\boldsymbol{x}), & \text{with} \quad |\varepsilon_0(\boldsymbol{x})| \leq \varepsilon_0, \ \forall \boldsymbol{x}. \\ \widehat{\nabla^i f}(\boldsymbol{x}) &= \nabla^i f(\boldsymbol{x}) + \varepsilon_i(\boldsymbol{x}), & \text{with} \quad \|\varepsilon_i(\boldsymbol{x})\| \leq \varepsilon_i, \ \forall \boldsymbol{x}, \ i = 1, 2. \end{split}$$

• Inexact Newton system solves, linesearch, local models, subproblems, ...

How does the relative size of the errors affect convergence? Which steps can I perform more or less accurately?

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- Designing routines for reduced-/mixed-precision derivative evaluations may be problem-dependent and not straightforward in general.
- Barring underflow/overflow rounding errors are typically linear in u so noise constants are easy to estimate if evaluation routines are type-flexible.
- Mixed-precision NLA methods can be applied and incorporated, e.g. in Newton linear system solves, quasi-Newton updates, trust-region subproblems, ...

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- 1. Std assumptions for Newton local q-quadratic convergence. Lipschitz Hessian.
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#### Newton step:

$$\begin{split} \hat{\boldsymbol{x}}_{k+1} &= \hat{\boldsymbol{x}}_k - (\nabla^2 f(\hat{\boldsymbol{x}}_k) + \varepsilon_2(\hat{\boldsymbol{x}}_k) + \varepsilon_s(\hat{\boldsymbol{x}}_k))^{-1}(\nabla f(\hat{\boldsymbol{x}}_k) + \varepsilon_1(\hat{\boldsymbol{x}}_k)) + \varepsilon_a(\hat{\boldsymbol{x}}_k), \\ \|\varepsilon_1(\boldsymbol{x})\| &\leq \varepsilon_1, \quad \text{(gradient error)}, \quad \|\varepsilon_2(\boldsymbol{x})\| \leq \varepsilon_2, \quad \text{(Hessian error)}, \quad \forall \boldsymbol{x}, \\ \|\varepsilon_a(\boldsymbol{x})\| &\leq \varepsilon_a, \quad \text{(update error)}, \quad \|\varepsilon_s(\boldsymbol{x})\| \leq \varepsilon_s, \quad \text{(linear solve error)}, \quad \forall \boldsymbol{x}. \end{split}$$

### Theorem (Kelley 2022)

Under the above assumptions, the error  $e_k = \hat{x}_k - x^*$  satisfies

$$\|\mathbf{e}_{k+1}\| = O\left(\|\mathbf{e}_k\|^2 + (\varepsilon_2 + \varepsilon_s)\|\mathbf{e}_k\| + \varepsilon_1 + \varepsilon_a\right)$$

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**Note:** Inexact Hessian and linear solves impact convergence rate, but not limiting accuracy. Gradient and update errors do not harm rate, but affect limiting accuracy.

**Warning:** hidden constants proportional to  $\|\nabla^2 f(x^*)^{-1}\|$ ,  $\kappa(\nabla^2 f)$ , and problem size.

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**Typical mixed-precision strategy:** high-precision gradient evaluations and update and low-precision Hessian evaluation/approximation and inversion so that, e.g.

$$\varepsilon_1, \varepsilon_a = O(u^2); \ \varepsilon_2, \varepsilon_s = O(u) \implies \|e_{k+1}\| \approx O(\|e_k\|^2 + u^2).$$

Since the reduction in the rate occurs when  $||e_k|| \le O(u)$  for which  $||e_{k+1}|| = O(u^2)$ .

# 3. Numerical linear algebra

#### Two topics:

- 1. Mixed-precision iterative refinement.
- 2. Mixed-precision Krylov subspace methods.

#### **Review articles** (citing all mentioned references):

- A. Abdelfattah, H. Anzt, E. G. Boman, E. Carson, T. Cojean, J. Dongarra, A. Fox, et al. A survey
  of numerical linear algebra methods utilizing mixed-precision arithmetic. The International Journal
  of High Performance Computing Applications, 35(4):344–369, 2021
- N. J. Higham and T. Mary. Mixed precision algorithms in numerical linear algebra. Acta Numerica, 31:347–414, 2022

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### Mixed-precision iterative refinement

Solve  $Ax_0 = b$  using LU factorization in precision u and store the LU factors.

For k = 1, 2, ...

- 1. Compute residual  $r_k = b Ax_k$  at precision  $u^2$ .
- 2. Solve  $Ad_k = r_k$  at precision u by re-using the LU factors.
- 3.  $x_{k+1} = x_k + d_k$  at precision  $u^2$ .

Since  $\|e_0\| = O(u)$  the previous theorem gives that

$$\|\mathbf{e}_1\| = O(\|\mathbf{e}_0\|^2 + u\|\mathbf{e}_0\| + u^2) = O(u^2).$$

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**Advantages:** LU factorization performed only once in low precision. Limiting accuracy dictated by  $u^2$  provided  $\kappa_{\infty}(A)$  is small enough.

### GMRES-IR [Carson & Higham 2017-18, Amestoy et al. 2021]

Now use three precisions:  $u_l \ge u \ge u^2$ . In [Amestoy et al. 2021] they use five.

#### **GMRES-IR**

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- 3.  $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \boldsymbol{d}_k$  at precision u.

#### Result:

- Provided that  $\kappa_{\infty}(A) \ll u^{-1}$  we obtain a limiting accuracy of O(u) where the hidden constant is independent from  $\kappa_{\infty}(A)$ .
- This approach is efficient since again the LU factorization is performed only once and in low precision, and GMRES typically converges in a handful of iterations.
- GMRES-IR is more robust to ill-conditioning than LU-based iterative refinement.

# Mixed-precision iterative refinement in the literature

Mixed-precision iterative refinement is at the heart of many recent mixed-precision developments in numerical linear algebra, including:

- Sparse approximate factorizations (e.g. replace LU with a sparse approximation), cf. [Amestoy et al. 2022].
- Least square problems (see e.g. [Carson et al. 2020]).
- Eigenvalue problems (see e.g. [Tisseur 2001]).
- Multigrid (see e.g. [Tamstorf et al. 2021] and [McCormick et al. 2021]).
- Krylov subspace methods, cf. [Anzt et al. 2010, Lindquist et al. 2021].

**Complex theory:** the theory describing the finite precision behavior of iterative methods is extensive and complex. Review on Lanczos-CG: [Meurant & Strakoš 2006].

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1. **Iterative refinement.** Use lower precision in inner solver.

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Three approaches: (see review articles for more details and info):

- 1. **Iterative refinement.** Use lower precision in inner solver.
- 2. **MP preconditioning.** Apply/implement preconditioner in low precision.
- 3. MP iterative methods. Adaptively change precision of inner products/matvecs.

# 4. Numerical solution of partial differential equations

#### Main references:

- M. Croci, M. Fasi, N. J. Higham, T. Mary, and M. Mikaitis. Stochastic rounding: implementation, error analysis and applications. Royal Society Open Science, 9:211631, 2022
- M. Klöwer, S. Hatfield, M. Croci, P. D. Düben, and T. N. Palmer. Fluid simulations accelerated with 16 bits: Approaching 4x speedup on A64FX by squeezing ShallowWaters.jl into Float16.
   Journal of Advances in Modeling Earth Systems, 2021
- M. Croci and M. B. Giles. Effects of round-to-nearest and stochastic rounding in the numerical solution of the heat equation in low precision. *IMA Journal of Numerical Analysis*, 2022. URL https://doi.org/10.1093/imanum/drac012
- M. Croci and G. R. de Souza. Mixed-precision explicit stabilized Runge-Kutta methods for single-and multi-scale differential equations. Journal of Computational Physics, 2022

# 4a. Towards climate simulations in half precision

**Joint with:** M. Klöwer and T. N. Palmer (University of Oxford), S. Hatfield and P. D. Düben (European Centre for Medium-Range Weather Forecasts).

Algorithm type: reduced-precision (half).

#### Main references:

 M. Klöwer, S. Hatfield, M. Croci, P. D. Düben, and T. N. Palmer. Fluid simulations accelerated with 16 bits: Approaching 4x speedup on A64FX by squeezing ShallowWaters.jl into Float16.
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# Towards climate simulations in half precision [Klöwer et al. 2021]

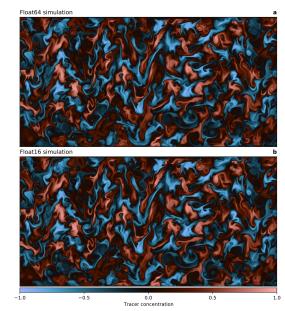
### Shallow-water eqs for 2D oceanic flow:

$$\begin{cases} \dot{\boldsymbol{v}} + \boldsymbol{v} \cdot \nabla \boldsymbol{v} + \hat{\boldsymbol{z}} \times \boldsymbol{v} = -\nabla \eta + \Delta^2 \boldsymbol{v} - \boldsymbol{v} + \boldsymbol{F}, \\ \dot{\eta} + \nabla \cdot (\boldsymbol{v}h) = 0, \\ \dot{q} + \boldsymbol{v} \cdot \nabla q = -\tau (q - q_0). \end{cases}$$

**Numerical scheme:** explicit 4th-order timestepping on a staggered grid.

#### Techniques used for fp16 simulations:

- Scaling and squeezing.
- Kahan compensated summation.
- Performed using A64FX chips on Fugaku (1st in TOP500).



**Note:** all other results in this part of the talk use *precision emulation* in software.

# 4b. Solving parabolic PDEs in half precision

Joint with: M. B. Giles (University of Oxford)

Algorithm type: reduced-precision (half), using stochastic rounding.

#### Main references:

- M. Croci and M. B. Giles. Effects of round-to-nearest and stochastic rounding in the numerical solution of the heat equation in low precision. *IMA Journal of Numerical Analysis*, 2022. URL https://doi.org/10.1093/imanum/drac012
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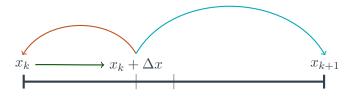
# RtN might cause stagnation



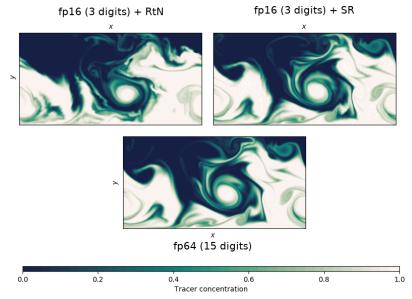
# RtN might cause stagnation



# SR is resilient to stagnation



# Interesting results by Milan Klöwer (University of Oxford)



**Note:** not just due to stagnation, SR decorrelates errors and causes error cancellation!

### RtN vs SR

Why is RtN in low precision bad for parabolic PDEs?

#### a) Stagnation:

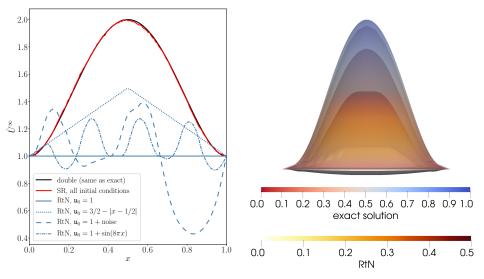
• RtN always stagnates for sufficiently small  $\Delta t$ .

### b) Global error:

RtN rounding errors are strongly correlated and grow rapidly until stagnation.

#### SR fixes all these issues!

# a) Stagnation (heat equation, 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]:  $\varepsilon^n$  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  $\varepsilon_i^n$  are zero-mean, independent in space and mean-independent in time.

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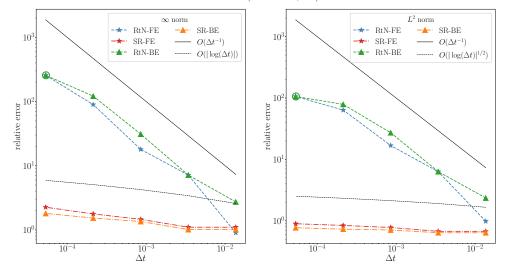
**SR:** the  $\varepsilon_i^n$  are zero-mean, independent in space and mean-independent in time.

Mode	Norm	1D	2D	3D
RtN	$L^2, \infty$	$O(u\Delta t^{-1})$	$O(u\Delta t^{-1})$	$O(u\Delta t^{-1})$
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;  $\ell(\Delta t) = |\log(\Delta t)|$ .

# b) Global rounding errors (2D heat equation)

Global error (delta form, 2D)



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

# 4c. Mixed-precision explicit Runge-Kutta methods Joint with: G. Rosilho De Souza (USI Lugano).

**Algorithm type:** mixed-precision (double/bfloat16) using round-to-nearest.

#### Main reference:

 M. Croci and G. R. de Souza. Mixed-precision explicit stabilized Runge–Kutta methods for single-and multi-scale differential equations. Journal of Computational Physics, 2022

### Framework and objective

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

$$y'(t) = f(t, y(t)), \quad y(0) = y_0,$$

where f(t, y) is sufficiently smooth, and from now on set f = f(y(t)) for simplicity.

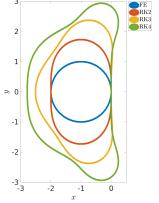
### Objective

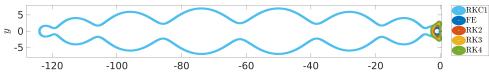
Evaluate f in low-precision as much as possible without affecting accuracy or stability.

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

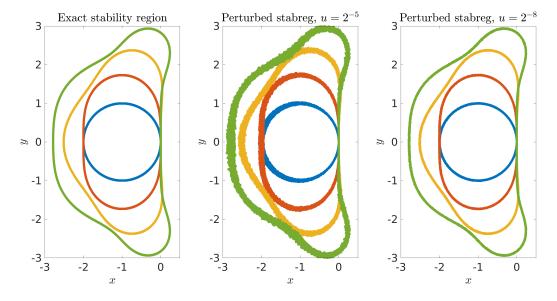
### Absolute stability

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  $|R_s(z)| < 1$ .

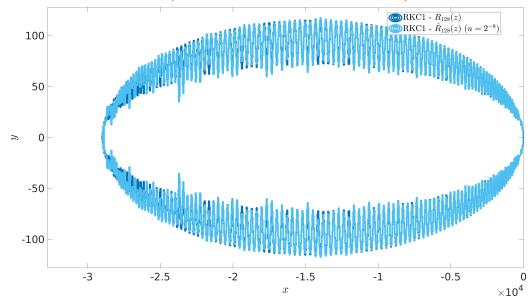




# Linear stability for RK methods (in practice)



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



# Order-preserving mixed-precision RK methods

### Assumption

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.

We saw that RP methods do not converge, hence they are not order-preserving.

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**Our idea:** store solution in high precision and use only q high-precision function evaluations to obtain a q-order-preserving mixed-precision RK method.

We can construct q-order preserving RK methods for any q for linear problems, and for q=1,2 for nonlinear problems. We can prove both stability and convergence.

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**Note:** We mainly focused on stabilized methods since they are low-order, but use a lot of function evaluations to maximize stability.

# Linear problems, i.e. f(y) = Ay

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

$$egin{aligned} oldsymbol{y}(\Delta t) &= \exp(\Delta t A) oldsymbol{y}_0 = \sum_{j=0}^{\infty} rac{(\Delta t A)^j}{j!} oldsymbol{y}_0, \ oldsymbol{y}_1 &= \sum_{j=0}^{p} rac{(\Delta t A)^j}{j!} oldsymbol{y}_0 + O(\Delta t^{p+1}). \end{aligned}$$

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:

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

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

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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!

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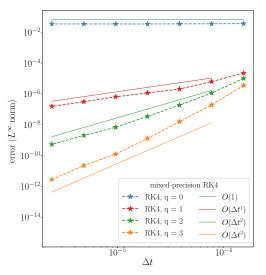
- 1. We have  $\varepsilon = O(u)$  and we get  $\tau = O(u\Delta t^{-1} + \Delta t^p)$ . Rapid error growth!
- 2. Exact vector operations:  $\varepsilon = 0$  so  $\tau = O(u + \Delta t^p)$ . O(u) limiting accuracy and loss of convergence.

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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!
- 2. Exact vector operations:  $\varepsilon = 0$  so  $\tau = O(u + \Delta t^p)$ . O(u) limiting accuracy and loss of convergence.
- 3. First  $q \ge 1$  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!

# Numerical results - convergence (3D heat eqn)

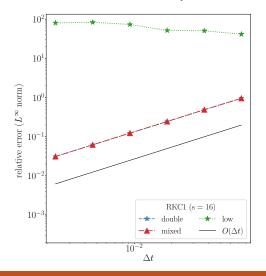


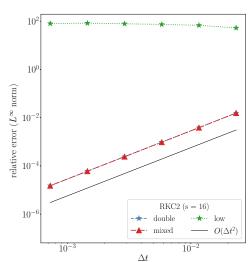
The transition from order p to order q happens roughly when  $\Delta t = O(||A||^{-1}u^{\frac{1}{p-q}})$ 

### Numerical results - convergence

1D Brussellator model for chemical autocatalytic reactions (with Dirichlet BCs):

$$\left\{ \begin{array}{l} \dot{\mathfrak{u}} = \alpha \Delta \, \mathfrak{u} + \mathfrak{u}^2 \, \mathbf{v} - (b+1) \, \mathfrak{u} + a \\ \dot{\mathbf{v}} = \alpha \Delta \, \mathbf{v} - \mathfrak{u}^2 \, \mathbf{v} + b \, \mathfrak{u} \end{array} \right.$$

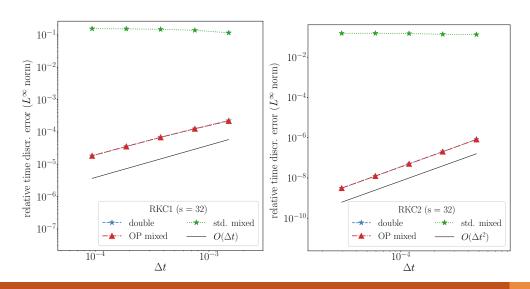




### Numerical results - convergence

Nonlinear diffusion model, 1D 4-Laplace diffusion operator (with Dirichlet BCs):

$$\dot{\mathfrak{u}} = \nabla \cdot (\|\nabla \mathfrak{u}\|_2^2 \nabla \mathfrak{u}) + f$$



# 4. Conclusions

#### Outlook

### To sum up

- Reduced-/mixed-precision algorithms require a careful implementation, but can bring significant memory, cost, and energy savings.
- Many new reduced and mixed-precision algorithms for scientific computing and data science were developed in recent years. Hardware support is growing.
- Advice for new developers: find which operations are more costly or more sensitive to rounding errors before designing a mixed-precision method.
- Advice for new practitioners: keep GPU and FPGA applications in mind as that's
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# Thank you for listening!

Papers, slides, and more info at: https://croci.github.io Email: matteo.croci@austin.utexas.edu

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