Prehandling and Related Hardware-Oriented Finite Element PDE Solvers Enabling Lower Precision and Tensor Core Computations

Dustin Ruda, Stefan Turek, Dirk Ribbrock

Chair of Applied Mathematics and Numerics (LS3), TU Dortmund University

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technische universität dortmund

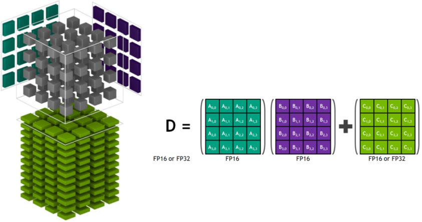
fakultät für mathematik

lehrstuhl für angewandte mathematik und numerik

Motivation – Hardware trends

Tensor Cores (TC)

- Processing units by Nvidia specialized to accelerate AI applications
- Can perform dense matrix multiplications very fast
- Examples of TC GPUs: V100 (2017), A100 (2020), H100 (2023), B200 (2024)



Schematic representation of fused multiply-add ($D = AB + C$) with 4×4 matrices on TC

	FP64	FP64 TC	FP32	FP32 TC / TF32	FP16	FP16 TC
V100	7.8	-	15.7	-	31.4	125
A100	9.7	19.5	19.5	156	78	312
H100	34	67	67	495	n/a	990
B200	n/a	40	n/a	1,100	n/a	2,250

TFlop/s peak rates (realistically achievable)

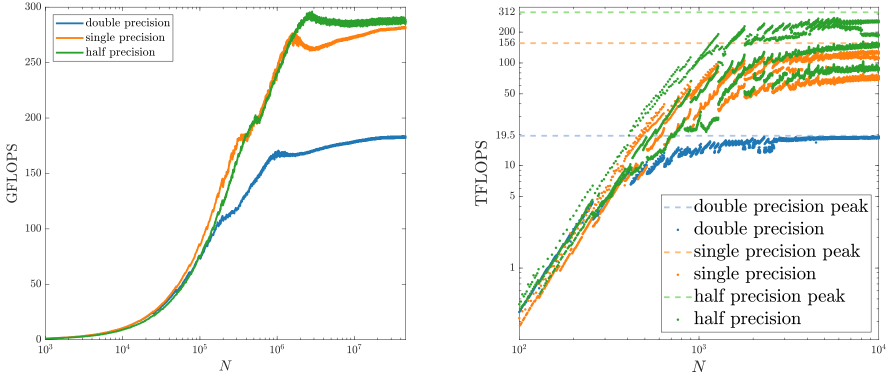
Motivation – Hardware trends

Rank	Name	Accelerator
1	El Capitan	MI300A
2	Frontier	MI250X
3	Aurora	Intel Max GPU
4	JUPITER Booster	GH200
5	Eagle	H100
6	HPC6	MI250X
7	Fugaku	–
8	Alps	GH200
9	LUMI	MI250X
10	Leonardo	A100

Accelerator hardware in supercomputers

- Technology similar to TC by AMD: Matrix Cores (MI250X, MI300A)
- 8 supercomputers in top 10 of TOP500 (June 2025) use Nvidia (4) or AMD (4) accelerator hardware

Motivation – Sparse vs. dense



GFLOPS on A100 for sparse 5-point stencil matrix (CSR) × vector (left) and TFLOPS for dense matrix × dense matrix (right)

Problem statement

- Consider **Poisson's equation**

$$-\Delta u = f \text{ on } \Omega \subset \mathbb{R}^d,\ d \in \{2,3\}$$

  as very a common (sub-)problem and bottleneck in many (e.g. CFD) applications
- TC GPUs have a performance potential of 100+ TFlop/s
- But it is only achievable in **lower precision** (SP or HP) and for **dense** matrix operations

↯ Both contradict basic principles of standard solvers (e.g. multigrid (MG)) for finite element (FE) simulations: Low precision might cause loss of **accuracy** due to high condition numbers ($\mathcal{O}(h^{-2})$) and FE matrices are **sparse**

Aims

- Profitable use of lower precision TC hardware for linear systems in matrix-based FE simulations by constructing suitable hardware oriented solvers

Two-step process:

- **Step 1:** Manipulate linear system to enable SP or HP while preserving sufficient accuracy
- **Step 2:** Adapt solver by densifying operations to leverage TC (large + sparse $\rightarrow$ small + dense)

Remark

- Also consider many right hand sides (RHS), resp., dense matrix as RHS ($AX = B$)
- Exemplary use case: Global-in-time Navier–Stokes solver $\rightarrow$ solve pressure Poisson problem for all time steps at once

Basic procedure

Starting point: Sparse, ill-conditioned linear system

Prehandling to lower condition number

2D: HFEM

3D: Generating systems

Node **renumbering** exploiting similar cells + **Schur complement(s)**

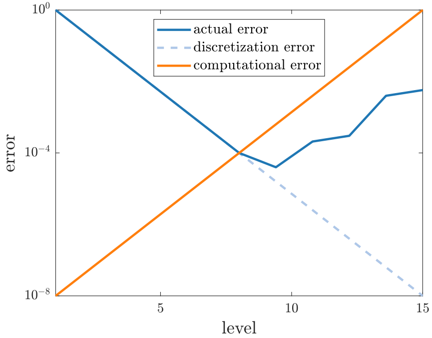
(**Direct method** in 2D)

Semi-iterative method in 2D and 3D

Prehandling – How to handle ill-conditioned Poisson problems

- Error consists of discretization and computational error: $u - \tilde{u}_h = (u - u_h) + (u_h - \tilde{u}_h)$
- **Discr. error:** $\|u - u_h\| = \mathcal{O}(h^{p+1})$
  - Depends on FE space and smoothness
  - Here for simplicity: $p = 1$
- **Comp. error:** $\|u_h - \tilde{u}_h\| \approx \text{cond} \cdot$ "data error"
  - Data error at least TOL of precision
  - Poisson: $\text{cond}(A_h) = \mathcal{O}(h^{-2})$
- Comp. error becomes dominant at h_{crit} at intersection of both errors
- Omit constant factors and equate

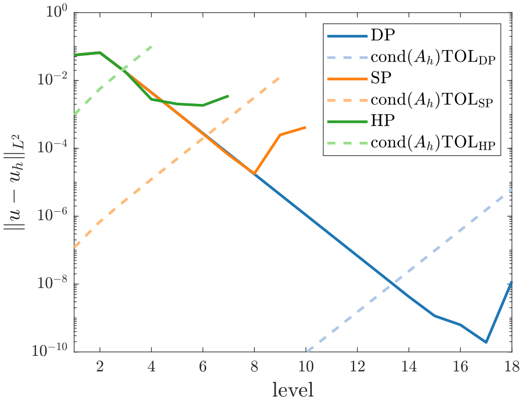
$$\Rightarrow h_{\text{crit}} \approx (\text{cond} \cdot \text{TOL})^{\frac{1}{2}}$$



Illustrative example of actual, discretization and computational error

Prehandling – How to handle ill-conditioned Poisson problems

- Critical mesh size: $h_{\text{crit}} \approx (\text{cond} \cdot \text{TOL})^{\frac{1}{2}}$
- Substitute $\text{cond} \approx h^{-2}$ for Poisson's equation $\Rightarrow h_{\text{crit}} \approx \text{TOL}^{\frac{1}{4}}$
- Example: $(\text{TOL}_{\text{DP}})^{\frac{1}{4}} = 2^{-13} \approx 10^{-3.9}$
  $(\text{TOL}_{\text{SP}})^{\frac{1}{4}} = 2^{-5.75} \approx 10^{-1.7}$
  $(\text{TOL}_{\text{HP}})^{\frac{1}{4}} = 2^{-2.5} \approx 10^{-0.8}$
- Wish: $\text{cond} = \mathcal{O}(1) \Rightarrow h \approx \text{TOL}^{\frac{1}{2}}$
  $\rightarrow$ SP (and even HP?) possible



Computational and actual L^2-error for 1D example

The concept of prehandling of linear systems

Basic idea

- Apply preconditioner **explicitly** to $Ax = b$
- Equivalent system: $\tilde{A}\tilde{x} = \tilde{b}$ where $\tilde{A} = S^{\mathsf{T}}AS$, $\tilde{b} = S^{\mathsf{T}}b$, $x = S\tilde{x}$
- Both yield same solution in exact arithmetic, but accuracy (and iteration numbers) differ in practice because $\mathrm{cond}(A) \neq \mathrm{cond}(\tilde{A})$

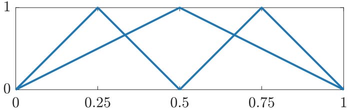
Central requirements for prehandling

- $\mathrm{cond}(\tilde{A}) \ll \mathrm{cond}(A)$
- $\tilde{A}$ is still sparse
- Transformation to $\tilde{A}$, $\tilde{b}$ and x via S is fast (i.e., $\mathcal{O}(N \log N)$)

Candidates for prehandling

- So far two candidates fulfill all requirements: **Hierarchical Finite Element Method** (HFEM, Yserentant et al., 1980s) in 2D and **Generating systems** (GS, Griebel et al., 1990s) in 2D and 3D

Candidates for prehandling – HFEM

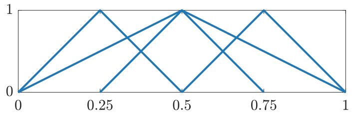


minimum example of hierarchical basis in 1D

- Sequence of refined meshes starting from coarse mesh (h_0) required
- Transformation matrix S is square, $\tilde{A} = S^\mathsf{T} A S$ is symm. positive-definite and sparse
- $\mathrm{cond}(\tilde{A}) = \mathcal{O}\left(\left(\log \frac{1}{h}\right)^2\right)$ (3D: $\mathcal{O}(h^{-1})$)
- Partial Cholesky decomposition on coarse mesh to lower cond:

$$\begin{pmatrix} \widetilde{A}_0 & 0 \\ 0 & \widetilde{D} \end{pmatrix} = L^\mathsf{T} L \to L^{-1} \widetilde{A} L^{-\mathsf{T}}$$

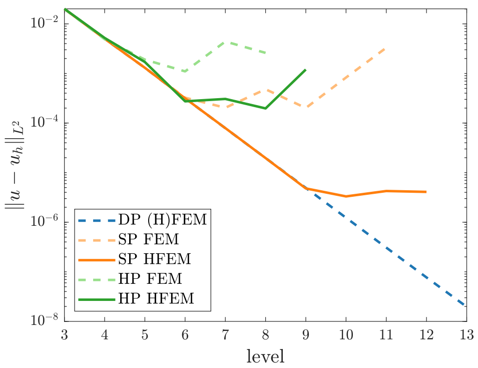
Candidates for prehandling – Generating systems

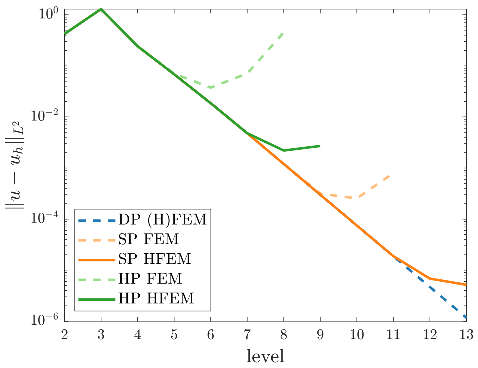


minimum example of generating system in 1D

- Also dependent on sequence of refined meshes
- GS consists of nodal bases on **all** levels and thus, some mesh points are counted repeatedly
- Transformation matrix S is rectangular, $\tilde{A} = S^{\mathsf{T}} A S$ is symm. pos. semi-definite (sufficient for convergence of CG method to non-unique solution) and sparse
- Transforming back by multiplication with S yields unique solution to original system
- Magnification factor of problem size: $^{8}/_{7}$ in 3D
- Jacobi preconditioner corresponds to BPX $\Rightarrow \mathrm{cond}(\tilde{A}) = \frac{\lambda_{\max}}{\lambda_{\min,>0}} = \mathcal{O}(1)$

The effect of prehandling on accuracy in 2D

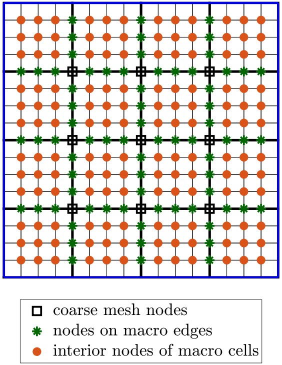


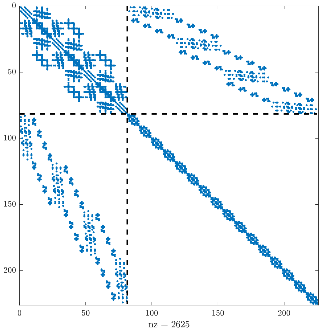


L^2-errors for different levels in 2D in DP, SP, HP without (dashed) and with (solid) **prehandling via HFEM** for **“very smooth”** (left) and **more oscillating** (right) solution

Solvers taylored for Tensor Core GPUs

- Low condition numbers by prehandling enable low precision but **matrices are still sparse**
- Construct solver consisting as much as possible on multiplications with dense matrices
- Same principle in 2D (HFEM) and 3D (GS): Subdivide nodes into:
  - nodes in the interior of the coarse mesh cells (cell by cell in same order)
  - "all remaining nodes" containing those on coarse mesh edges (+ repeated nodes of GS)





- Matrix form:

$$\begin{pmatrix} A_1 & B \\ B^\top & C \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

- C decomposes into independent blocks C_i
- Blocks are equal if corresponding to similar cells
- Only C grows like N $(= \#\text{Dof})$

Solvers taylored for Tensor Core GPUs

- Applying Schur Complement to $\begin{pmatrix} A_1 & B \\ B^\mathsf{T} & C \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$ yields

Semi-iterative Method

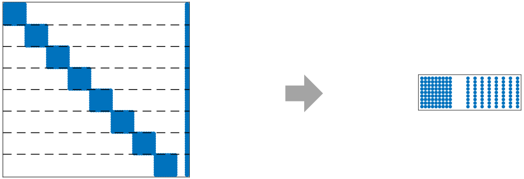
$$\underbrace{\left(A_1 - BC^{-1}B^\mathsf{T}\right)}_{\hat{A}} u = b_1 - BC^{-1}b_2 \qquad \text{(with CG)}$$

$$v = C^{-1}\left(b_2 - B^\mathsf{T}u\right)$$

- $\hat{A}$ can be computed explicitly (2D) or used implicitly (better option in 3D)
- Robust with respect to anisotropic meshes with high aspect ratios (moderate increase of iteration numbers)
- In special cases: Structure of $\hat{A}$ allows further Schur complement yielding the **direct method** with high memory usage, but highly performant (up to 60 TFlop/s)
  (Ruda, D. et al., Very fast finite element Poisson solvers on lower precision accelerator hardware: A proof of concept study for Nvidia Tesla V100, IJHPCA, 2022)

How to treat multiplications with C^{-1}

- Only C_i need to be inverted (once for each group of similar macro cells)
  $\longrightarrow C^{-1}$ block diagonal matrix with dense blocks C_i^{-1}
- C_i are small, well-conditioned HFEM matrices, $\mathcal{O}(N)$ storage for C_i^{-1}
- Efficient implementation by simultaneous computation



- Complexity $\mathcal{O}\left(N^{3/2}\right)$ but very fast calculation by TC almost at peak performance

Storage requirement of the semi-iterative method

- Exemplary toy problem: Poisson's equation on unit square/cube, equidistant Q1 mesh, variable coarse mesh size h_0
- Relevant for **storage**: C_i^{-1}, B and $\hat{A}$ in 2D / A_1 in 3D

2D: HFEM

$\frac{1}{h}$	$\frac{N}{10^6}$	$\frac{1}{h_0}$	$\hat{A}$	C_i^{-1}	B	total
1024	1.05	16	15	15.1	1.0	**31**
		32	25	0.9	1.6	**27**
2048	4.19	32	19	3.8	1.0	**24**
		64	40	0.2	1.6	**42**
4096	16.77	32	16	15.5	0.7	**32**
		64	27	0.9	1.0	**29**

3D: Generating Systems

$\frac{1}{h}$	$\frac{N}{10^6}$	$\frac{1}{h_0}$	A_1	C_i^{-1}	B	total
128	2.05	4	11.3	433.3	15.4	**460**
		8	22,1	5.6	16.6	**44**
		16	37.1	0.1	15.3	**52**
256	16.58	8	14.2	53.5	16.5	**84**
		16	24.9	0.7	17.7	**43**
		32	39.5	0.01	16.4	**56**

Number of nonzero entries relative to N

- Moderate storage requirement for appropriate choice of h_0 compared to $9N$ in 2D / $27N$ in 3D with standard FEM (in DP)
- Explicit $\hat{A}$ in 3D: $400N - 1,400N \longrightarrow$ implicit variant preferred

Complexity and performance estimate

Semi-iterative Method

$$\underbrace{\left(A_1 - BC^{-1}B^\mathsf{T}\right)}_{\hat{A}} u = b_1 - BC^{-1}b_2$$

$$v = C^{-1}\left(b_2 - B^\mathsf{T}u\right)$$

- **Composition of the method:**
  - $1 \times B$, $1 \times C^{-1}$ to compute RHS
  - **Iterative step:** $1 \times \hat{A}$ (explicit or implicit) + 2 dot products + 3 axpy per iteration
  - Intermediate step: $1 \times B^\mathsf{T}$
  - **Direct Step:** $1 \times C^{-1}$

- Entire method in SP/TF32 on TC GPU
- Majority of the work: Dense matrix operations; Small part: sparse $\times$ dense and BLAS1
- Matrix properties, iteration numbers and benchmark results on A100 (H100) in SP for all occuring operations (given many RHS) $\longrightarrow$ **performance model**
- Metric beyond Flop/s for comparability: millions of unknowns solved per second (MDof/s)

Performance estimate

2D:

$\frac{1}{h}$	$\frac{1}{h_0}$	#iter	cond(C_i)	total $\frac{\text{Flop}}{N}$	share dense	GFlop/s	MDof/s
1024	16	30	24	16,400	94.4%	27,400	**1,670**
	32	24	17	4,900	75.4%	6,700	1,360
2048	32	28	24	16,600	93.5%	21,600	**1,300**
	64	23	17	5,600	66.4%	4,100	730
4096	32	31	32	64,700	98.4%	58,700	910
	64	25	24	16,900	91.9%	15,600	**920**

3D:

$\frac{1}{h}$	$\frac{1}{h_0}$	#iter	cond(C_i)	total $\frac{\text{Flop}}{N}$	share dense	GFlop/s	MDof/s
128	4	8	54	555,300	99.9%	110,400	200
	8	11	23	75,400	98.3%	50,800	**670**
	16	18	9	12,500	79.3%	6,500	520
256	8	11	54	713,700	99.8%	107,500	150
	16	18	23	114,900	98.0%	47,400	**410**
	32	35	9	23,400	77.3%	6,100	260

- Comparative result with **optimized MG** in C++-based FE software package (FEAT3) on AMD CPU in DP: $\leq$ **15 MDof/s**

Results on H100

- Results on **H100** GPU[1] ($\approx 3\times$peak rates of A100 in SP with TC)
- Speedup 1.3–1.9 for sparse×dense and 1.5–3.5 for dense×dense compared to A100
- **Comparison of MDof/s:**

2D

$\frac{1}{h}$	$\frac{1}{h_0}$	A100	H100
1024	16	1,670	2,860
	32	1,360	2,430
2048	32	1,300	2,220
	64	730	1,180
4096	32	910	2,020
	64	920	1,540

3D

$\frac{1}{h}$	$\frac{1}{h_0}$	A100	H100
128	4	200	480
	8	670	1,160
	16	520	840
256	8	150	440
	16	410	680
	32	260	400

- **Typical hardware oriented approach: "optimal" configuration depends on problem(size) and hardware**

[1]Kindly provided for use on JURECA by Forschungszentrum Jülich
`https://www.fz-juelich.de/en/ias/jsc/systems/supercomputers/jureca`

Prehandling for convection-diffusion

- So far: Poisson's equation; in general similar results for self-adjoint, positive definite, elliptic, linear, second order PDEs (proven)
- Study generating systems for stationary **convection-diffusion** problem numerically (in spite of lack of proof for $\mathrm{cond}(\tilde{A}) \ll \mathrm{cond}(A)$)

$$-\varepsilon \Delta u + b \cdot \nabla u = f \text{ on } \Omega \subset \mathbb{R}^2, \text{ diffusion coefficient } \varepsilon > 0, \text{ convection field } b : \mathbb{R}^2 \to \mathbb{R}^2$$

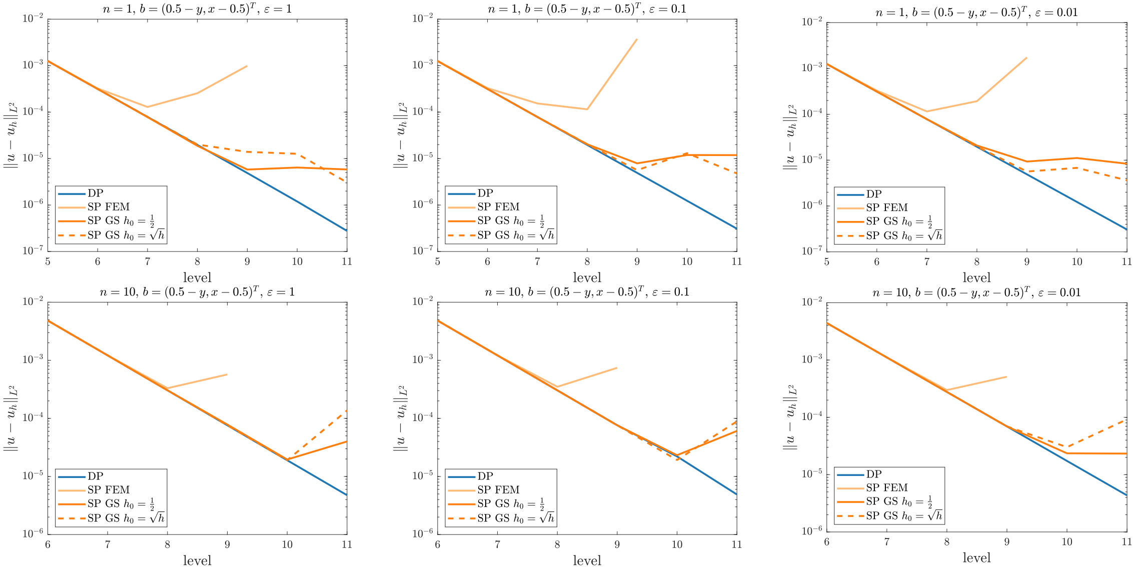
- Vortical convection $b(x, y) = (1/2 - y, x - 1/2)^{\mathsf{T}}$ moderate ($\varepsilon \geq 10^{-2}$) so that standard FE discetization is stable
- Consider GMRES preconditioned by Jacobi, Gauss–Seidel (GS), symmetric GS (SGS) and compare matrix density, iteration numbers and accuracy for standard FEM vs. generating systems

Prehandling for convection-diffusion: iteration numbers

$\frac{1}{h}$	$\frac{1}{h_0}$	$\frac{NNZ}{N}$	plain/Jacobi $\varepsilon = 1$	plain/Jacobi 10^{-1}	plain/Jacobi 10^{-2}	GS 1	GS 10^{-1}	GS 10^{-2}	SGS 1	SGS 10^{-1}	SGS 10^{-2}
512	FEM	9	629	678	1,010	728	850	1,797	260	279	527
	2	87	19	19	31	11	11	19	6	6	9
	4	84	20	21	32	11	11	19	6	6	10
	8	78	22	23	36	14	14	20	8	8	10
1024	FEM	9	1,259	1,356	2,018	1,462	1,657	3,694	516	556	1,031
	2	98	20	20	32	11	11	19	6	6	9
	4	95	21	22	34	11	11	19	6	6	10
	8	89	24	24	37	14	14	20	8	8	10
2048	FEM	9	2,517	2,712	4,034	2,861	3,182	7,397	1,031	1,111	2,050
	2	109	21	21	34	11	11	19	6	6	10
	4	106	23	23	36	11	11	20	6	6	10
	8	100	25	26	38	14	15	20	8	9	10

- Bottom line: Prehandling via generating systems works for moderate convection (**Step 1** ✓)
- Perfomance gain by low precision and sparse × dense (**Step 2** more challenging)

Prehandling for convection-diffusion: accuracy



Conclusion and outlook

Conclusion

- It is possible to exploit Lower-Precision and also Accelerator Hardware for PDE computing by prehandling and a related semi-iterative approach

Outlook

- Deeper analysis of suitable preconditioners for the iterative step and initial guesses for the solution vector to reduce number of iterations
- Investigate the feasibility of transforming different matrices C_i into one

References

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Figures

- p.1: `https://developer.nvidia.com/blog/tensor-core-ai-performance-milestones/`
- pp. 6, 12: Ruda et al. (2022), IJHPCA 36(4) (see above)