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Very Fast FEM Poisson Solvers on Lower Precision Accelerator Hardware

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Motivation

Prec.	double	double + TC	single	single + TC	half	half + TC
V100	7.8	-	15.7	-	31.4	**125**
A100	9.7	19.5	19.5	**156**	-	**312**
H100	30	60	60	500	120	1,000

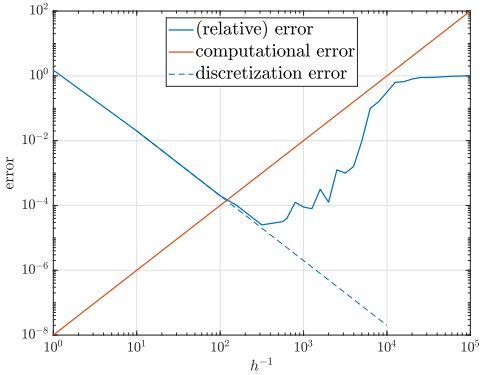
TFlop/s peak rates for **NVIDIA V100** (2017), **A100** (2020) and **H100** (Q3 2022)
(similar: AMD Matrix Core)

- 100+ TFlop/s only achievable in **lower precision** by **Tensor Cores** (TC)
- Peak rates only achievable with **dense** matrix operations
- **Aim**: Profitable use of this hardware for linear systems in FE simulations (CFD)
- Consider **Poisson's equation**: Global-in-time Navier–Stokes solver allows for solving Pressure Poisson problems for all time steps at once → many right hand sides (RHS)

↯ Standard FEM solvers (MG) require double precision (DP) and include large, sparse matrices → *Prehandling* and new *Schur complement-based methods*

How to handle ill-conditioned Poisson-like Problems

- **Split the error:**
  $u - \widetilde{u}_h = (u - u_h) + (u_h - \widetilde{u}_h)$
- **Discr. Error:**
  $$\|u - u_h\| = \mathcal{O}\left(h^{p+1}\right)$$
  - depending on **FEM space** and **smoothness**
  - Here for simplicity: $p = 1$
- **Comp. Error:**
  $\|u_h - \widetilde{u}_h\| \approx \mathrm{cond} \cdot$ "data error"
  - Data error at least TOL of respective precision
  - Poisson: $\mathrm{cond}\left(A_h\right) = \mathcal{O}\left(h^{-2}\right)$

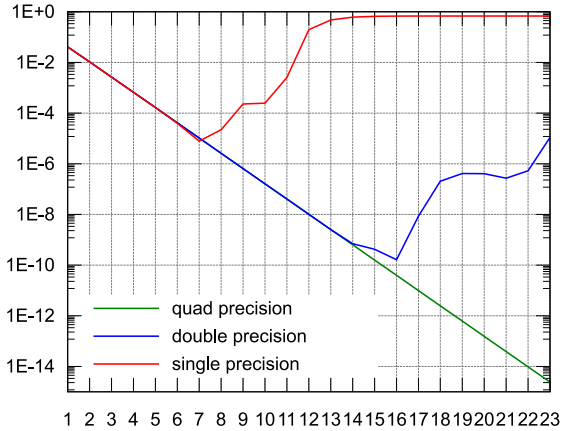


Source: Ruda et al, 2022

- Critical h at intersection of both errors: Discr. Error $\approx$ Comp. Error $\Rightarrow h \approx (\mathrm{cond} \cdot \mathrm{TOL})^{\frac{1}{2}}$

How to handle ill-conditioned Poisson-like Problems

- Critical grid width: $h \approx (\mathrm{cond} \cdot \mathrm{TOL})^{\frac{1}{2}}$
- Poisson $-\Delta u = f$: Substitute $\mathrm{cond} = \mathcal{O}\left(h^{-2}\right) \Rightarrow h \approx \mathrm{TOL}^{\frac{1}{4}}$
- 1D example: $(\mathrm{TOL}_{\mathrm{SP}})^{\frac{1}{4}} = 2^{-5.75}$
  $(\mathrm{TOL}_{\mathrm{DP}})^{\frac{1}{4}} = 2^{-13}$
- Wish: $\mathrm{cond} = \mathcal{O}(1) \Rightarrow h \approx \mathrm{TOL}^{\frac{1}{2}}$
  $\rightarrow$ SP (and even HP?) possible



L^2-error with standard FEM in 1D, $h = 2^{-\mathrm{level}}$
Source: Ruda et al., 2022

Concept of Prehandling of Linear Systems

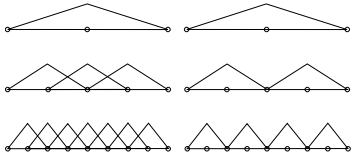
Preconditioning: $x^{k+1} = x^k - C^{-1}\left(Ax^k - b\right)$

Prehandling: $x^{k+1} = x^k - \left(C^{-1}Ax^k - C^{-1}b\right) = x^k - \left(\widetilde{A}x^k - \widetilde{b}\right)$

- Yields same solution (if converged and with "infinite precision") and same iteration numbers, but $\mathrm{cond}(A) \lesseqgtr \mathrm{cond}\left(\widetilde{A}\right)$ since different linear systems
- **Central idea:** Explicitly transforming $Ax = b$ into equivalent $\widetilde{A}\widetilde{x} = \widetilde{b}$, $B\widetilde{x} = x$ with:
  1) $\mathrm{cond}\left(\widetilde{A}\right) \ll \mathrm{cond}(A)$
  2) $\widetilde{A}$ only moderately less sparse than A
  3) Tranformation to $\widetilde{A}$, $\widetilde{b}$ (resp. x via B) fast (i.e. $\mathcal{O}(N \log N)$)

HFEM: Ideas, Realization & Properties

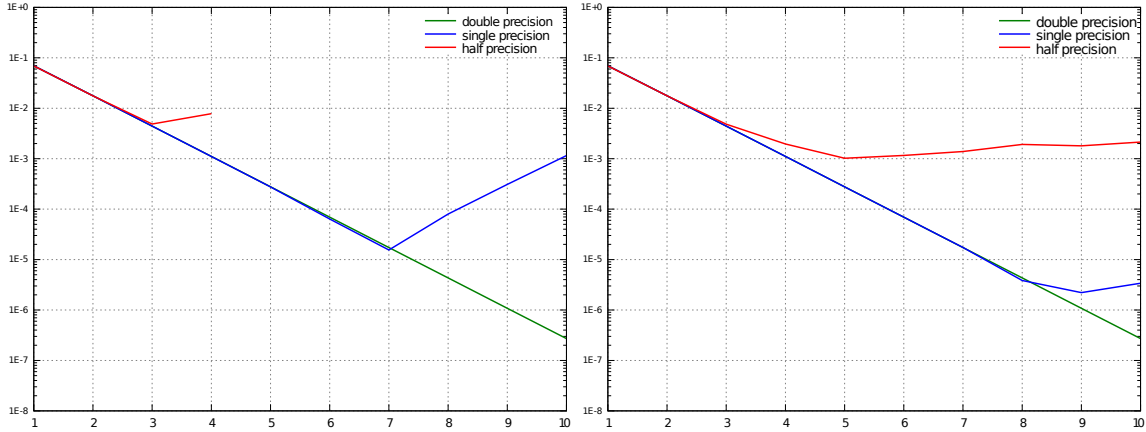
- Only candidate for prehandling so far: HFEM
- **Idea:** Use of **hierarchical** instead of **nodal basis** starting from a coarse grid
- Transform linear system $\widetilde{A} = S^{\mathsf{T}} A S$, $\widetilde{b} = S^{\mathsf{T}} b$, $x = S\widetilde{x}$



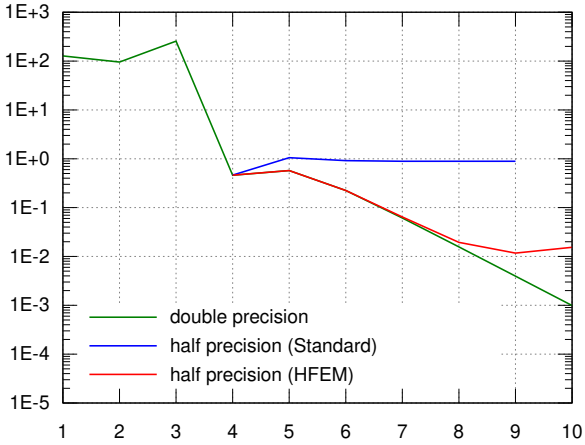
nodal (l) and hier. (r) basis
Source: Deuflhard et al., 1989

- $\operatorname{cond}\left(\widetilde{A}\right) = \mathcal{O}\left(\left(\log \frac{1}{h}\right)^2\right)$ in 1D, 2D; FEM: $\operatorname{cond}(A) = \mathcal{O}\left(\left(\frac{1}{h}\right)^2\right)$
- Add. partial Cholesky prehandling: $\begin{pmatrix} \widetilde{A}_0 & 0 \\ 0 & \widetilde{D} \end{pmatrix} = L^{\mathsf{T}} L \to L^{-1} \widetilde{A} L^{-\mathsf{T}}$
- Remark: in 3D $\operatorname{cond}\left(\widetilde{A}\right) = \mathcal{O}\left(\frac{1}{h} \log \frac{1}{h}\right)$ resp. $\mathcal{O}\left(\frac{1}{h}\right) \to$ Possible in SP

HFEM: Numerical results (errors)



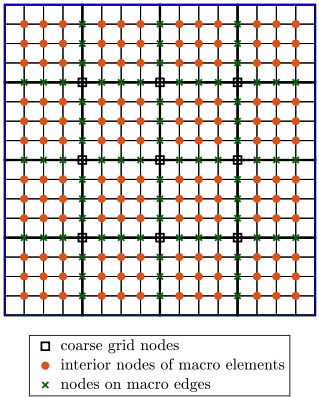
L^2-errors for different levels in 2D in DP, SP, HP without (left) and with (right) **prehandling via HFEM** for **"smooth"** solution. Source: Ruda et al., 2020



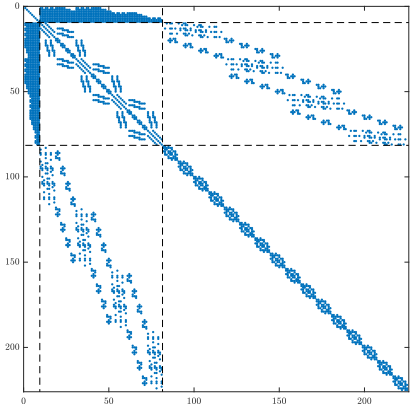
L^2-errors for different levels in 2D in DP, SP, HP without and with **prehandling via HFEM** for **strongly oscillating** solution
Source: Ruda et al., 2022

- Fine h for tolerance of $\approx 1\%$ for complex problems
  $\rightarrow$ large problems
  $\rightarrow$ requires HPC

- **Objective:** Construct solver consisting as much as possible on multiplications with **dense**, **well-conditioned matrices**
- **Starting Point:** Linear system after prehandling via **HFEM+Cholesky** $Ax = b$
- Subdivide nodes into 3 types ($\mathcal{C}$, $\mathcal{E}$, $\mathcal{I}$) and renumber A accordingly



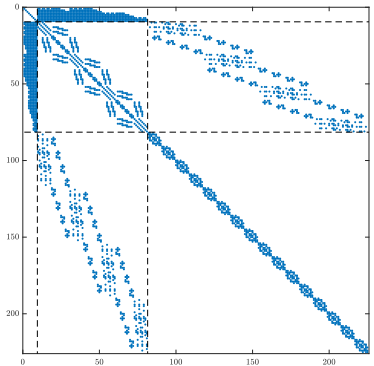
Source: Ruda et al., 2022



Source: Ruda et al., 2022

$$\begin{pmatrix} I & B & 0 \\ B^\mathsf{T} & E & D \\ 0 & D^\mathsf{T} & C \end{pmatrix} \begin{pmatrix} x_\mathcal{C} \\ x_\mathcal{E} \\ x_\mathcal{I} \end{pmatrix} = \begin{pmatrix} b_\mathcal{C} \\ b_\mathcal{E} \\ b_\mathcal{I} \end{pmatrix}$$

- D, E are sparse
- B is moderately dense
- C decomposes into **independent** blocks (as many as macro cells)



Source: Ruda et al., 2022

- **Blocks C_i of C are equal if they correspond to similar macro cells**
- **Only C grows like N** ($= \#\text{Dof}$)
- Applying **Schur complement** $\rightarrow$ semi-iterative method
- Applying further Schur complement $\rightarrow$ completely direct method

Semi-iterative Method

$\Lambda = E - DC^{-1}D^{\mathsf{T}}$

Use conjugate gradient method to solve

$$\underbrace{\begin{pmatrix} I & B \\ B^{\mathsf{T}} & \Lambda \end{pmatrix}}_{\Sigma} \begin{pmatrix} x_{\mathcal{C}} \\ x_{\mathcal{E}} \end{pmatrix} = \begin{pmatrix} b_{\mathcal{C}} \\ b_{\mathcal{E}} - DC^{-1}b_{\mathcal{I}} \end{pmatrix}$$

$$x_{\mathcal{I}} = C^{-1}\left(b_{\mathcal{I}} - D^{\mathsf{T}}x_{\mathcal{E}}\right)$$

Direct Method

$\Lambda = E - DC^{-1}D^{\mathsf{T}}$

$\Pi = \Lambda - B^{\mathsf{T}}B$

$$x_{\mathcal{E}} = \Pi^{-1}\left(b_{\mathcal{E}} - B^{\mathsf{T}}b_{\mathcal{C}} - DC^{-1}b_{\mathcal{I}}\right)$$

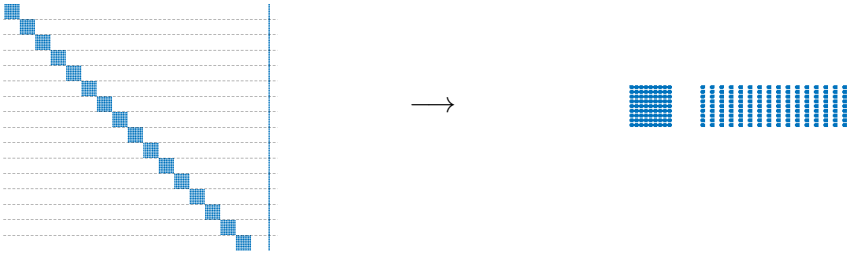
$$x_{\mathcal{C}} = b_{\mathcal{C}} - Bx_{\mathcal{E}}$$

$$x_{\mathcal{I}} = C^{-1}\left(b_{\mathcal{I}} - D^{\mathsf{T}}x_{\mathcal{E}}\right)$$

- Matrices Σ, Λ, Π, C well-cond. (5–50 on unit square with Q1)
- Block structure of C: **Only C_i^{-1} computed and stored**
- Semi-iterative: Less storage consuming
- Direct: More storage consuming but even higher potential for TC, especially in case of many RHS

Multiplication with C^{-1}

- Both methods require 2 multiplications with C^{-1}
- Efficient implementation by transforming into dense matrix product (also if $\#\text{RHS} = 1$):



- Complexity $\mathcal{O}\left(N^{\frac{3}{2}}\right)$ but fast calculation by TC

Storage and Computational Cost of the Direct Method

- Consider equidistantly refined unit square, Q1
- Let $h_0 = 2^\ell \sqrt{h}$, $\ell = \ldots, -1, 0, 1, 2, \ldots$
- Relevant for **storage**: Π^{-1}, C_i^{-1}
- Relevant for **FLOP**: Π^{-1}, $C^{-1}(2\times)$

Direct Method

$\Lambda = E - DC^{-1}D^\mathsf{T}$, $\Pi = \Lambda - B^\mathsf{T}B$

$$x_\mathcal{E} = \Pi^{-1}\left(b_\mathcal{E} - B^\mathsf{T} b_\mathcal{C} - DC^{-1} b_\mathcal{I}\right)$$
$$x_\mathcal{C} = b_\mathcal{C} - B x_\mathcal{E}$$
$$x_\mathcal{I} = C^{-1}\left(b_\mathcal{I} - D^\mathsf{T} x_\mathcal{E}\right)$$

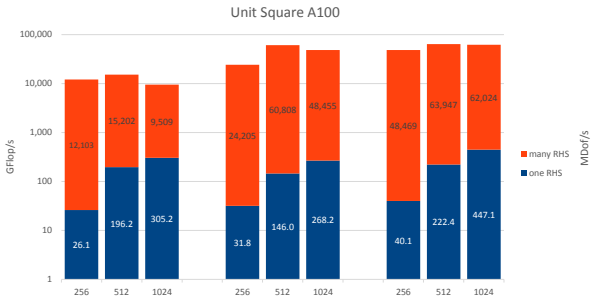
$h = \frac{1}{1024}$:

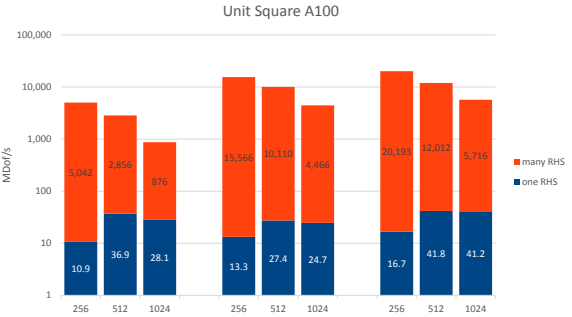
ℓ	-1	0	1	2	3
Total NNZ/N	16,400	14,100	1,000	500	4,200

ℓ	-1	0	1	2	3
#FLOP/$N^{3/2}$	33	**12**	18	65	256

- Best choice in terms of complexity: $h_0 = \sqrt{h}$ (or $\ell = 1$ considering storage)
- $\approx 12N^{3/2} \to$ 12,000 (SC) vs. 1,000 FLOP (MG) for $h = \frac{1}{1024}$

Direct Method: Unit Square on A100



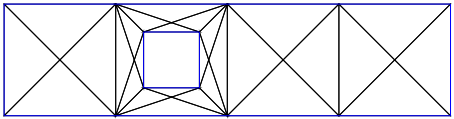


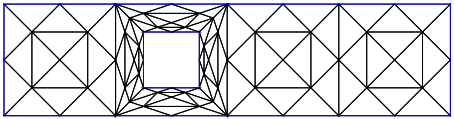
GFLOP/s (left) and **MDof/s** (right) with direct method on **A100** with one and many RHS depending on h^{-1} in **DP**, **SP** and **HP** (left, middle and right 3 columns, respectively)

→ **Up to 60 TFlop/s (for problems with many RHS)**

→ More arithmetic work ($\times 12$), but still much faster than standard MG solver on x64 AMD CPU (8 MDof/s for many rhs)

Unstructured Coarse Grids

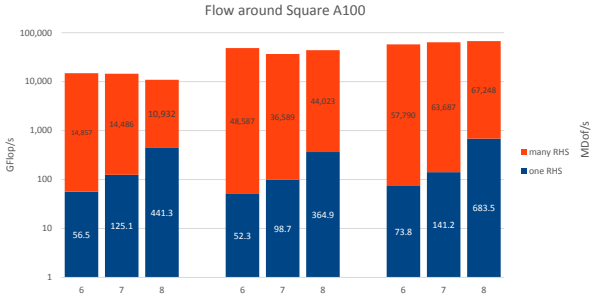


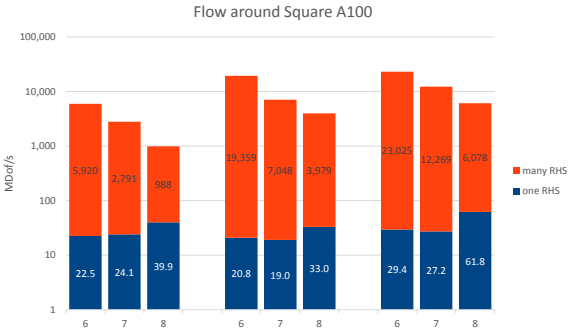


- So far: Analysis and numerical tests on unit square
- **Direct method** also applicable to "arbitrary" P1 grids
- Coarse grids with many similar cells are advantageous $\rightarrow$ few different C_i
- Example "flow around a square"
  - 3 Groups of similar cells $\rightarrow$ $C_1^{-1}, C_2^{-1}, C_3^{-1}$ must be calculated and stored

L (L_0) N	$\frac{\#\text{FLOP}}{N^{\frac{3}{2}}}$	$\frac{\text{NNZ}}{N}$
6 (1) 56,896	10.5	410
7 (2) 228,480	10.9	1,750
8 (2) 915,712	11.6	1,810

Direct Method: Flow around a Square on A100





GFLOP/s (left) and **MDof/s** (right) with direct method on **A100** with one and many RHS depending on h^{-1} in **DP**, **SP** and **HP** (left, middle and right 3 columns, respectively)

Limitations of the Direct Method

- High storage requirement of $\mathcal{O}\left(N^{\frac{3}{2}}\right)$ due to Π^{-1}
- Limit of fine grid width in our tests: $h = \frac{1}{1024}$ (on one GPU)
- Hardly applicable to 3D because storage requirement of $\mathcal{O}\left(N^{\frac{5}{3}}\right)$
- Requirement for simple form of the direct method: No coupling between nodes in $\mathcal{C}$ and $\mathcal{I}$ (coarse grid and interior nodes)
  - Rectangular Q1 grids
  - "arbitrary" P1 grids
- **Less memory consuming, more versatile but also less performant variant: Semi-iterative method**

Semi-iterative Method: Storage Requirement

$\frac{1}{h}$	$\frac{N}{10^6}$	$\frac{1}{h_0}$	Σ	C_i^{-1}	D	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**

Number of nonzero entries relative to N

Semi-iterative Method

$\Lambda = E - DC^{-1}D^{\mathsf{T}}$
Use conjugate gradient method to solve

$$\underbrace{\begin{pmatrix} I & B \\ B^{\mathsf{T}} & \Lambda \end{pmatrix}}_{\Sigma} \begin{pmatrix} x_{\mathcal{C}} \\ x_{\mathcal{E}} \end{pmatrix} = \begin{pmatrix} b_{\mathcal{C}} \\ b_{\mathcal{E}} - DC^{-1}b_{\mathcal{I}} \end{pmatrix}$$

$$x_{\mathcal{I}} = C^{-1}\left(b_{\mathcal{I}} - D^{\mathsf{T}}x_{\mathcal{E}}\right)$$

- Storage requirement: $30N - 40N$ in SP (in comparison: $9N$ with standard FEM in DP)

Semi-iterative Method: Performance Estimate

- **Basic composition of the method**:
  - $1 \times D$ and $1 \times C^{-1}$ to compute RHS
  - **Iterative step**: $1 \times \Sigma$, 3 AXPY and 2 dot products per iteration
    $\rightarrow \#\text{iter}\,[2\mathrm{NNZ}(\Sigma) + 6\#\text{rows} + 4\#\text{rows}]$,
    $\#\text{rows} = \mathcal{O}\left(N^{\frac{3}{4}}\right)$
  - Intermediate step: $1 \times D^{\mathsf{T}}$
  - **Direct step**: $1 \times C^{-1}$

Semi-iterative Method

$\Lambda = E - DC^{-1}D^{\mathsf{T}}$
Use conjugate gradient method to solve

$$\underbrace{\begin{pmatrix} I & B \\ B^{\mathsf{T}} & \Lambda \end{pmatrix}}_{\Sigma} \begin{pmatrix} x_{\mathcal{C}} \\ x_{\mathcal{E}} \end{pmatrix} = \begin{pmatrix} b_{\mathcal{C}} \\ b_{\mathcal{E}} - DC^{-1}b_{\mathcal{I}} \end{pmatrix}$$

$$x_{\mathcal{I}} = C^{-1}\left(b_{\mathcal{I}} - D^{\mathsf{T}}x_{\mathcal{E}}\right)$$

- Entire method in SP on A100
- Majority of the work: Dense matrix operations; Small part: sparse $\times$ dense and BLAS1

Semi-iterative Method: Performance Estimate

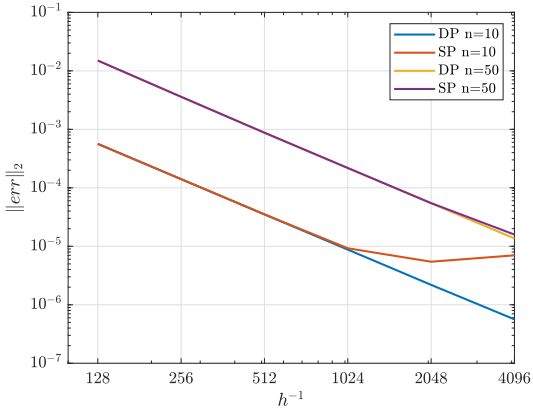
$\Sigma *$ dense	AXPY	dot product	dense $*$ dense	$D *$ dense
2,375	227	321	**150,000**	1,200

GFlop/s in benchmarks on A100 in SP

$\frac{1}{h}$	$\frac{1}{h_0}$	#iter	FLOP/N it.	FLOP/N dir.	time it.+dir.	GFLOP/s	MDof/s
1024	16	30	913	15,400	0.43 + 0.11	31,445	**1,926**
	32	24	1,217	3,615	0.60 + 0.03	8,206	1,698
2048	32	28	1,085	15,400	2.04 + 0.43	27,919	**1,694**
	64	23	1,881	3,611	3.53 + 0.10	6,333	1,153
4096	32	31	1,011	63,543	7.43 + 7.10	74,476	1,154
	64	25	1,374	15,391	10.17 + 1.72	23,636	**1,410**

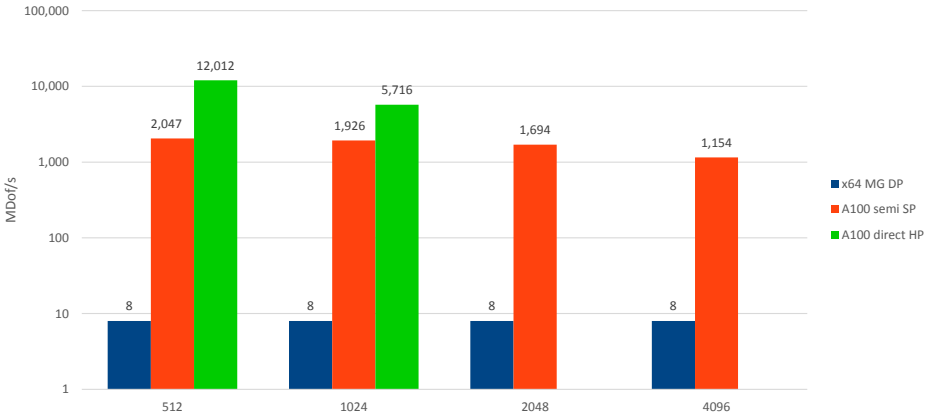
Performance estimate

Semi-iterative Method: Accuracy



Relative error with semi-iterative method in DP and SP for differently smooth solutions

Comparison: MG – semi-iterative – direct



Comparison of **MDof/s** for many RHS with **MG** in **DP** on **AMD CPU**, **direct** method in **HP** on **A100** and **semi-iterative** in **SP** on **A100** (estimate)

Outlook and Conclusion

- Implementation of the semi-iterative method on GPU
- Prehandling in 3D
- Analysis of suitable preconditioners for the iterative step and initial guesses for the solution vector to reduce number of iterations
- Testing semi-iterative Method for other FE spaces and in 3D
- Implementation into FEATFLOW software

- **Conclusion: It is possible to exploit Lower-Precision Accelerator Hardware for PDE computing** (under certain conditions)

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