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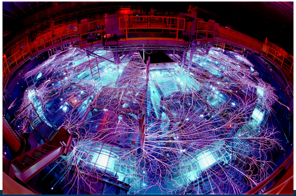

Higher-order geometric-algebraic multigrid

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Deliverable for EMPIRE

Scalable solution of curl-curl problems in higher order Nedelec spaces

- MueLu has an AMG preconditioner for 1st order elements (RefMaxwell); EMPIRE already uses that.
- Geometric multigrid for curl-curl is comparatively easy to set up compared to AMG. (de Rham complex is automatically preserved.)

Proposed hybrid (geometric-algebraic) multigrid approach:

- Coarsen from polynomial degree p down to 1 (potentially with intermediate steps, e.g. $p \to p/2 \to 1$), using nestedness of FE spaces.
- Apply Hiptmair smoothing (subspace relaxation on kernel of curl and complement) on geometric multigrid levels.
- Apply AMG solver starting from first order discretization.

Additional operators no problem for EMPIRE because they are all assembled on the same mesh.

Implementation:

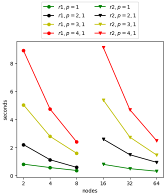
- Assembly of strong form operators (gradient, curl, interpolations) leverages Intrepid2 interpolation tools.
- Improved “geometric” interface in MueLu.
- Implemented in MiniEM driver in Panzer.

Lots of support by Mauro Perego, Nate Roberts and Roger Pawlowski!

Solve times: combined weak/strong scaling

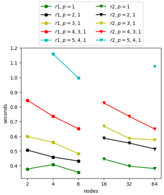
Uniform tetrahedral meshes for unit cube; 2 problem sizes: r1 @ 2.3M unknowns, r2 @ 18.7M unknowns; 1 time step

Solo (36 Broadwell CPUs / node)



poly orders	nnz / row	iterations r1	iterations r2
1	16	31	31
$2 \to 1$	43	23	23
$3 \to 1$	84	24	24
$4 \to 1$	144	31	31

Lassen (4 V100 GPUs / node)



poly orders	nnz / row	iterations r1	iterations r2
1	16	30	31
$2 \to 1$	43	24	24
$3 \to 1$	84	27	26
$4 \to 3 \to 1$	144	21	20
$5 \to 4 \to 1$	224	32	32

Observations:

- Good weak scalability (in iterations & time).
- Strong scalability improves with polynomial order.
- Selection of schedule for p-coarsening by trial-and-error.
- Missing data points: memory usage is a limiting factor.
- Not shown: Assembly time deteriorates with p, but that is to be expected.
  Evaluation of element matrix in $\mathcal{O}(p^{3d})$, apply in $\mathcal{O}(p^{2d})$.

Matrix-free multigrid

The “geometric”, $p > 1$ part of the multigrid hierarchy lends itself to matrix-free approach:

- Entirely pre-computed, no need to perform any matrix-matrix products.
- All operations are wrt standard FE spaces.

Goal

Save memory, improve apply performance

Implemented so far

- Matrix-free interpolation and strong form differential operators in MiniEM.
- Ifpack2 smoothing using `Tpetra::Operator` with attached diagonal (Jacobi, Chebyshev, Hiptmair)
- MueLu plumbing for operators instead of matrices

In progress:

- Matrix-free weak form operators, apply in $\mathcal{O}(p^{2d})$ ops per element (Graham Harper)
- Sum factorization improvements, apply in $\mathcal{O}(p^{d+1})$ ops per element (Nate Roberts)

Next steps

- Outstanding items:
  - special implementation of 2nd order elements is incomplete, n-th order elements are not a drop-in replacement (Intrepid2)
  - need an implementation of `Basis::getValues` for multiple elements (Intrepid2)
  - matrix assembly performance for higher order elements (Intrepid2, Panzer)
    $\rightarrow$ sum factorization will also help here $\mathcal{O}(p^{2d+1})$ ops per element
  - support for non-trivial initial conditions using Intrepid2 projection tools (Panzer)
- Additional verification problems for FEM convergence
- Integration into EMPIRE
- Multigrid performance improvements (e.g. (re)balancing for “geometric” hierarchy)