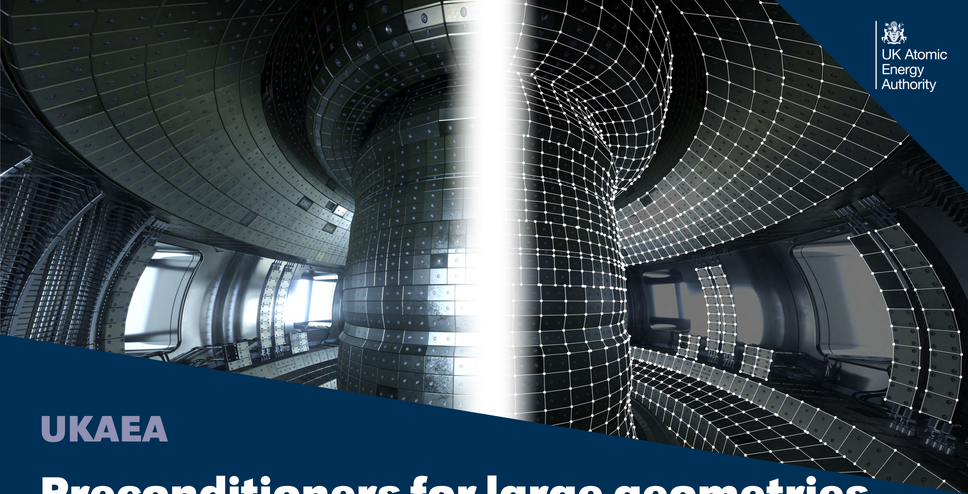

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Preconditioners for large geometries

November 27, 2020

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Overview

Introduction

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Multi-physics Simulations

`Modern science or engineering challenge`

Create & control nuclear fusion reactions

Analytical Solution	Numerical Solution	Computational Solution
↓	↓	↓
Exact analysis	Approximate solution	Framework & libraries
Theory, equations	PDE, FEM, Montecarlo	COMSOL,Ansys,MOOSE

Concepts

PDE problem -> Linear System Problem -> Matrix problem

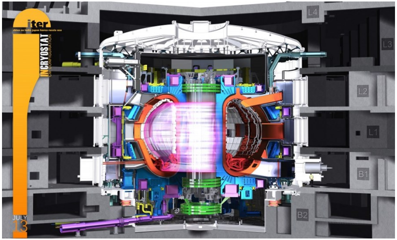
Direct Solver	Iterative Solver	Preconditioned Iterative Solver
↓	↓	↓
Gauss	Jacobi, Gauss-Seidel, SOR	Krylov subspace methods
Expensive	Approximate results, less cost	appropriate HPC resources

MOOSE

User-Focused
Finite Element Method
Massively parallelisation

HPC libraries:
PETSc * libMesh * Hypre

ITER[01]



Objective

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Determine a *suitable preconditioner* that helps iterative matrix solutions of multiphysics problems.

There are many factors that affect the preconditioner performance:

- Type of the PDE
- Dimensions
- Solver type
- Boundary Conditions
- Nature of the matrix
- Material used
- Degrees of freedom (DoF)

Metrics

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[01] Requirements for obtaining a good preconditioner (PC):

- The preconditioned matrix should have a clustered eigenspectrum away from 0, $n_{iter} \leq \frac{1}{2}\sqrt{\xi(G)}\ln\frac{2}{\epsilon} + 1$
- The PC should be as cheap to compute as possible,
- Its application to a vector should be cost-effective.

This work considers:

- Execution time (seconds)
- Memory usage (megabytes)
- Accuracy in the value of |R|
- Number of linear iterations

Methodology

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Preconditioners (PCs): (Based on PETSc [02] `-pc_type`)

asm , bjacobi , cholesky , eisenstat , exotic , gamg , hypre , hypre_boomeramg , hypre_euclid , hypre_parasails , hypre_pilut , icc , ilu , jacobi , ksp , lu , mg , ml , none , pfmg , redundant , sor , telescope , tfs , pbjacobi , vpbjacobi , shell , lsc , redistribute , svd , kaczmarz , gasm , composite , nn , mat , fieldsplit , galerkin , cp , patch , syspfmg , bddc , lmvm

Physical Characteristics: (Based on MOOSE Modules [03]):

- Thermal2D (Heat Conduction)
- Displacement3D (Finite Strain Elastic Stress)
- Pressure 3D (Finite Strain Elastic Stress)
- Fluid 3D (Navier-Stokes)

Methodology

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Execution mode:

- Serial
- Parallel
  - MPI (2p, 4p, 8p, 16p, 32p)
  - OpenMP (2t, 4t, 8t, 16t, 32t)
  - Hybrid (1t32p, 2t16p, 4p8t, 8t4p, 16t2p, 32t1p)

  p -> processes, t -> threads

PROCEDURE:

1- Running ten times the following combination:

42 preconditioners * 4 physical characteristics * 17 execution modes.

2- If converged:

Calculate the standard deviation of the execution time of each run.

Plot execution time, memory, number of iterations, and |R|.

Apply the Pareto efficiency in the data already plotted.

HPC Resources

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Cumulus cluster at UKAEA

Hardware

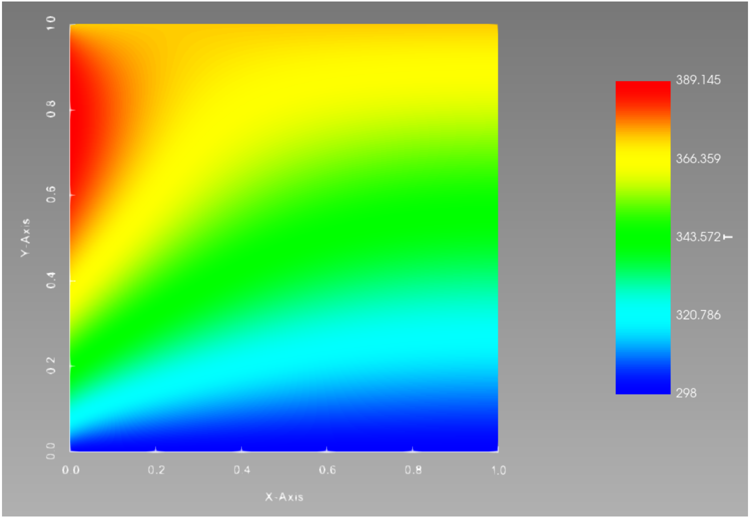
The cumulus nodes have 65 general worker nodes in cumulus, and 6 GPU nodes. Each node has 32 CPU cores of spec - Intel(R) Xeon(R) CPU E5-2683 v4 @ 2.10GHz
Each has 512GB of RAM, and are connected to each other via a FDR Infiniband network.
The home file system is Lustre.

Software

Python 3.6.4
cmake 3.16.4
GCC 7.3.0
Openmpi 3.1.1

Heat Conduction 2D

Steady state on steel 1cm x 1cm - Mesh 128 x 128



Compute Finite Strain Elastic Stress

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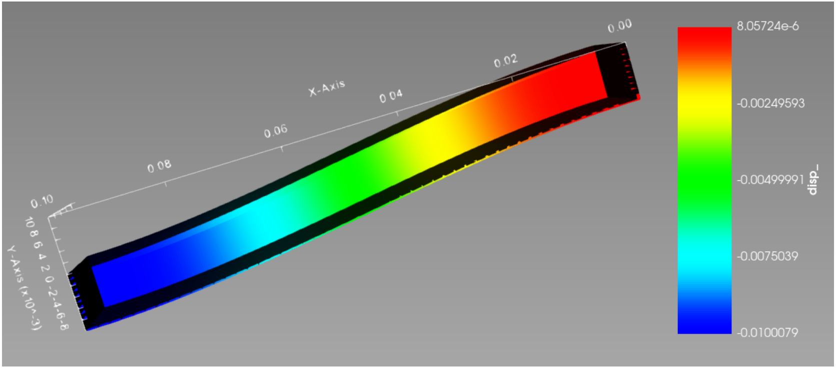
Displacement in 3D (x = 0.10cm, y = 0.01cm, z = 0.02cm)



Navier-Stokes

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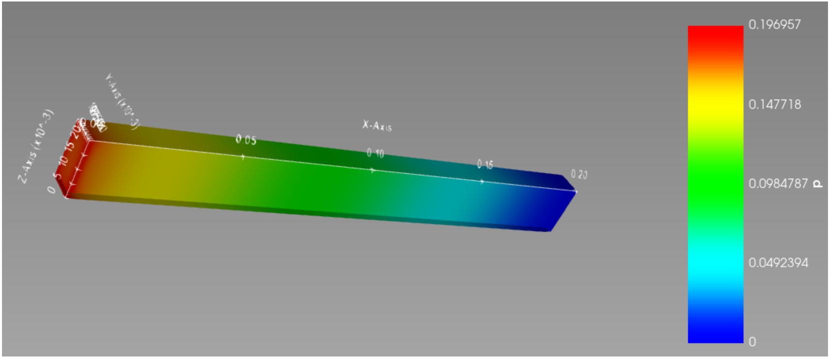
Fluid in 3D (x = 0.20cm, y = 0.01cm, z = 0.02cm)

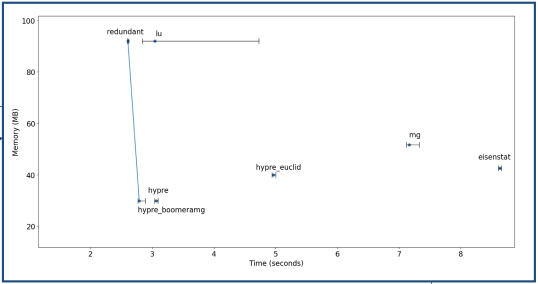


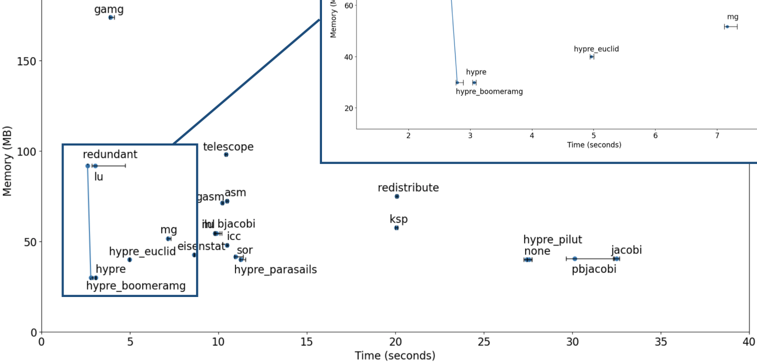
Results

* gamg (3.893 s, 174.026 MB, 1.425356e-06, 23 iterations)

Heat Conduction 2D (serial)

redundant: 2.606s, 91.99 MB, 9.919 113e-10, 2 iter
hypre_boomeramg: 2.79s, 29.91 MB, 3.567015e-07, 12 iter
lu: 3.041s, 91.98 MB, 9.919 113e-10, 2 iter
hypre: 3.061s, 29.91 MB, 3.567015e-07, 24 iter





Results

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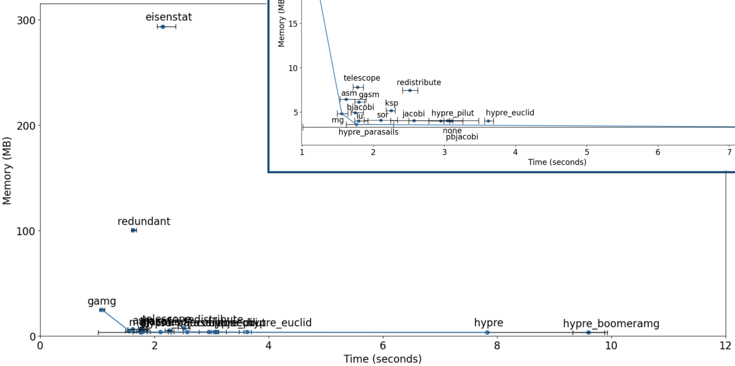
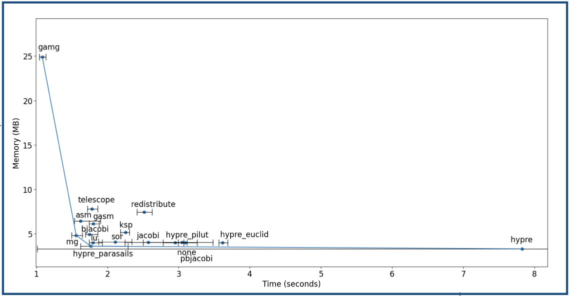
MPI 16 proc: gamg (1.290s) | OpenMP 16 threads: hypre(1.384s)

Heat Conduction 2D (Hybrid 2t 16 p)

gamg: 1.083s, 24.89 MB, 4.194201e-06, 23 iter
mg: 1.559s, 4.81 MB, 5.027078e-06, 1092 iter
hypre_parasails: 1.793s, 3.98 MB, 4.943789e-06, 1702 iter
hypre: 7.826s, 3.29 MB, 1.119766e-06, 11 iterations





Results

Heat Conduction 2D

"Good preconditioners"
asm bjacobi eisenstat gamg hypre hypre_boomeramg hypre_euclid hypre_parasails hypre_pilut icc ilu jacobi ksp lu mg ml none redundant sor telescope pbjacobi redistribute gasm

"Bad Preconditioners"
cholesky exotic pfmg tfs vpbjacobi shell lsc svd kaczmarz composite nn mat fieldsplit galerkin cp patch syspfmg bddc lmvm

Results

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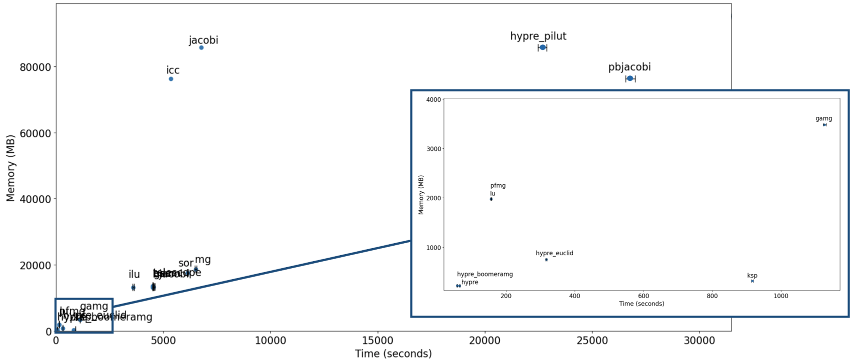
Compute Finite Strain Elastic - Displacement 3D (serial)

hypre_boomeramg: 57.652 seconds, 219.74 MB, 0.004452565, 50 iterations
hypre: 65.037 seconds, 216.06 MB, 0.005185383, 46 iterations
lu: 156.239 seconds, 1977.42 MB, 0.01921162, 2 iterations
ksp: 822.979 seconds, 316.84 MB, 0.005962132, 6 iterations
gamg: 1126.2 seconds, 3482.23 MB, 0.009540412, 659 iterations

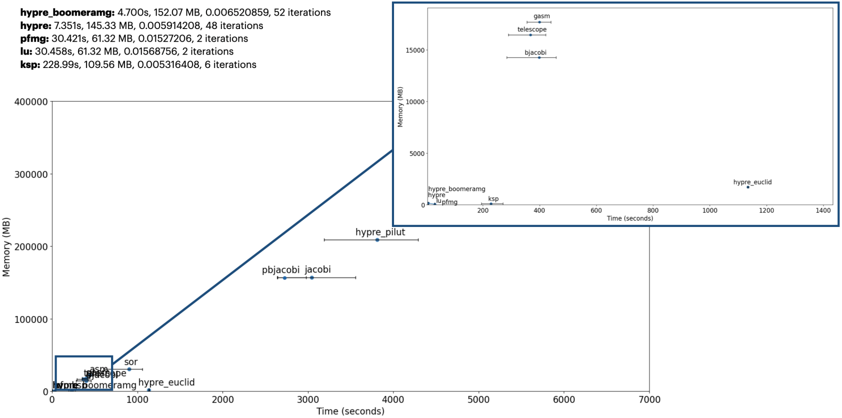


Results

MPI 32 processes: hypre_boomeramg (5.476s)
OpenMP 32 threads: hypre_boomeramg(8.275s)

Compute Finite Strain Elastic - Displacement 3D (Hybrid - 8t4p)

hypre_boomeramg: 4.700s, 152.07 MB, 0.006520859, 52 iterations
hypre: 7.351s, 145.33 MB, 0.005914208, 48 iterations
pfmg: 30.421s, 61.32 MB, 0.01527206, 2 iterations
lu: 30.458s, 61.32 MB, 0.01568756, 2 iterations
ksp: 228.99s, 109.56 MB, 0.005316408, 6 iterations



Results

Finite Strain Elastic Stress 3D

"Good preconditioners"

asm bjacobi cholesky gamg hypre hypre_boomeramg hypre_euclid hypre_pilut icc ilu jacobi ksp lu mg ml none pfmg sor telescope pbjacobi gasm mat cp

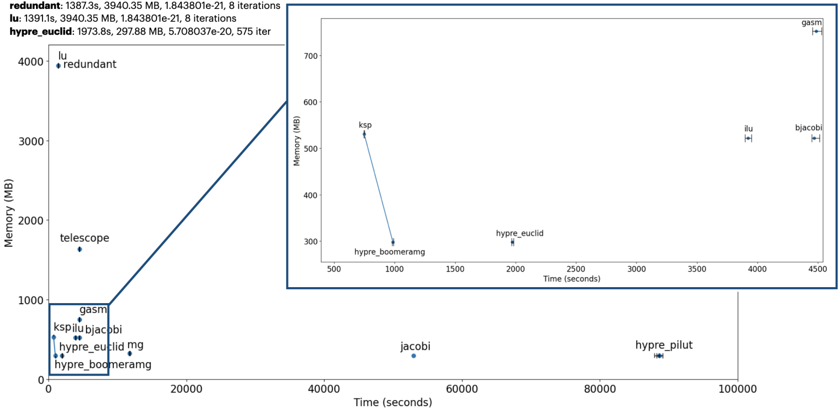
"Bad Preconditioners"

hypre_parasails redundant tfs vpbjacobi shell lsc redistribute svd kaczmarz composite nn fieldsplit galerkin

Results

Navier-Stokes 3D (serial)

ksp: 748.22s, 530.58 MB, 1.699691e-20, 8 iterations
hypre_boomeramg: 985.9s, 297.88 MB, 5.766776e-20, 173 iter
redundant: 1387.3s, 3940.35 MB, 1.843801e-21, 8 iterations
lu: 1391.1s, 3940.35 MB, 1.843801e-21, 8 iterations
hypre_euclid: 1973.8s, 297.88 MB, 5.708037e-20, 575 iter

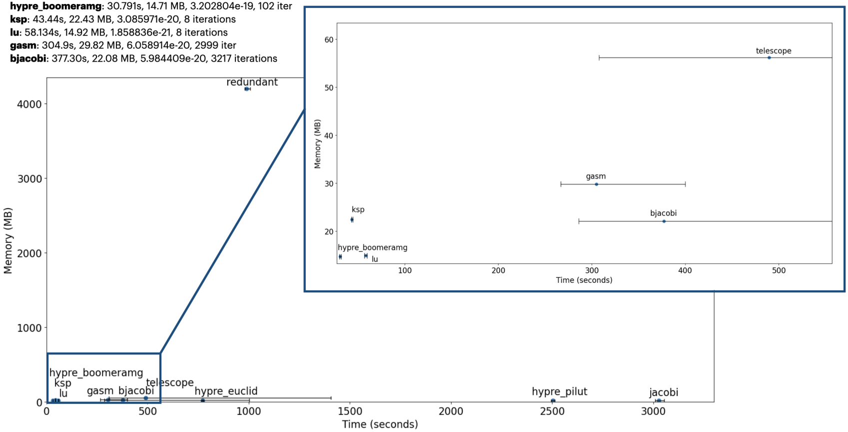


Results

MPI 32 processes: hypre_boomeramg (30.792 seconds)
OpenMP 32 threads: telescope(191.00 seconds)

Navier-Stokes (Hybrid - 1t32p)

hypre_boomeramg: 30.791s, 14.71 MB, 3.202804e-19, 102 iter
ksp: 43.44s, 22.43 MB, 3.085971e-20, 8 iterations
lu: 58.134s, 14.92 MB, 1.858836e-21, 8 iterations
gasm: 304.9s, 29.82 MB, 6.058914e-20, 2999 iter
bjacobi: 377.30s, 22.08 MB, 5.984409e-20, 3217 iterations



Results

Navier -Stokes 3D

"Good preconditioners"
asm bjacobi cholesky hypre_boomeramg hypre_euclid hypre_pilut icc ilu jacobi ksp lu mg ml none redundant telescope redistribute gasm composite cp

"Bad Preconditioners" eisenstat exotic gamg hypre hypre_parasails pfmg sor tfs pbjacobi vpbjacobi shell lsc svd kaczmarz nn mat fieldsplit galerkin

Open questions and next steps

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- Parallelisation behaviour (communication, synchronization)
- Scalability of each preconditioner
- Other HPC architectures
- Solver types
- Finer grids
- Internode
- Optimization flags
- MultiPDEs simulations

Acknowledgement

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@yulwitter

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