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Recent Developments in Trilinos Linear Solvers

Sandia National Laboratories

Jonathan Hu

Trilinos User Group Meeting

HPSF Conference 2026

March 16-20, 2026, Chicago, IL

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U.S. Department of ENERGY NNSA National Nuclear Security Administration

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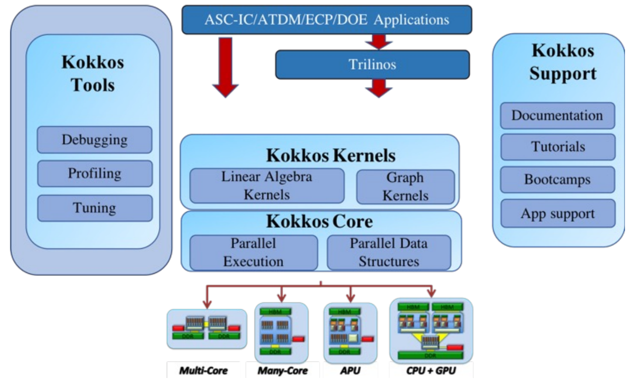
Trilinos Project

- Numerical libraries project
  - Relies on Kokkos ecosystem for on-node performance portability (github.com/kokkos)
  - Open source (github.com/trilinos/Trilinos)
  - Part of the High Performance Software Foundation (https://hpsf.io)
- Supports many architectures
  - CPUs (AMD, Intel)
  - Accelerators (Nvidia, AMD, Intel)
- Enabling technology for variety of simulations codes
  - Sandia internal (thermal fluid, plasma, multimaterial)
  - DOE Office of Science (energy, complex systems modelling)
  - University-led (multiphysics)



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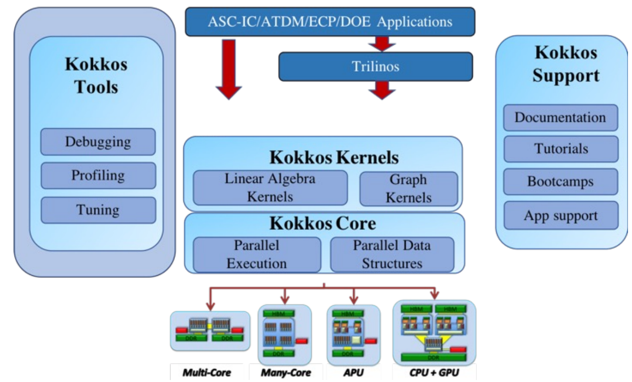
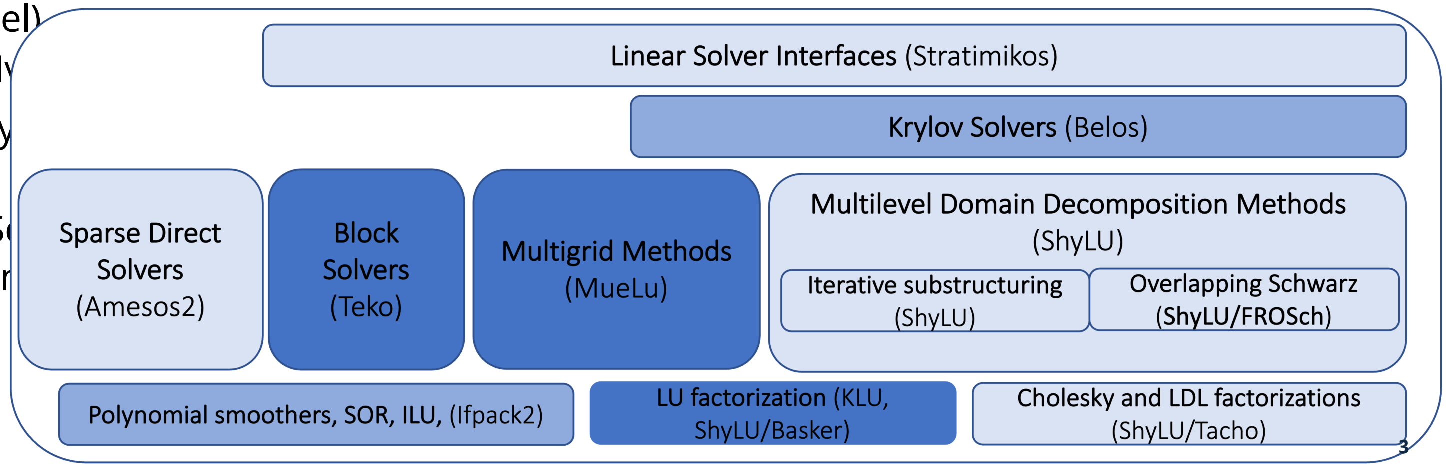
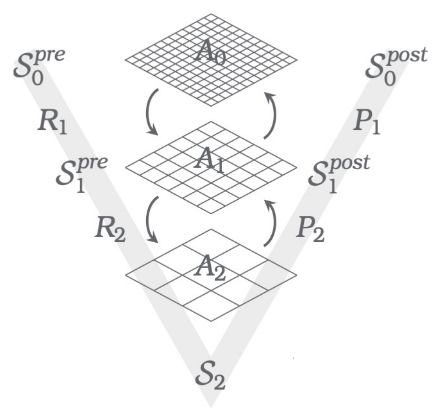




Algebraic Multigrid (MueLu)

Multigrid in a nutshell

- Scalable solution method for linear systems arising from elliptic PDEs
- Typically used as preconditioner to Krylov method
- Idea: capture error at multiple resolutions:
  - **Smoothing** (S_i) reduces oscillatory error (high energy)
  - **Coarse grid correction** reduces smooth error (low energy)
- Algebraic multigrid
  - Generate grid transfers P_i & R_i and thus coarse matrices based on fine level matrix



Green's function inspired strength-of-connection coarsening for Algebraic Multigrid

by Firmbach, Phillips, Glusa, Popp, Siefert, Mayr; CIS LDRD {malphil, caglusa, csiefer}@sandia.gov

Slide courtesy of Christian Glusa

Observation & Idea

For constant diffusion tensor σ, the Green's function in $\mathbb{R}^d$, $d \geq 2$, is

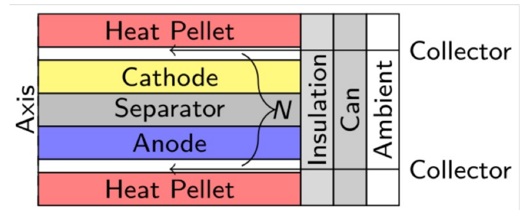
$$G(x, y) = \frac{1}{4\pi\sqrt{\det(\sigma)}} \frac{1}{\|x - y\|_\sigma},$$

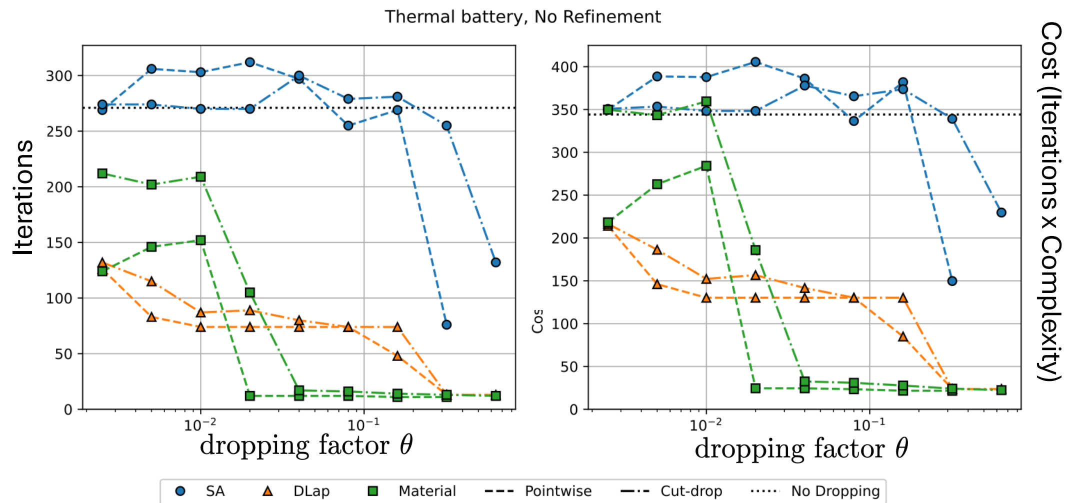
$$\text{where } \|z\|_\sigma := \sqrt{z^T \sigma^{-1} z}.$$

Use distance Laplacian wrt metric $\|\cdot\|_\sigma$ for coarsening process.

- Effects from mesh stretching **and** material variations are tracked in coarsening process.
- Material effects are captured directly (and not via matrix entries),
- Providing material parameters poses no difficulty for applications.

$$\begin{aligned} -\nabla \cdot (\sigma(x)\nabla u) &= f && \text{in } \Omega, \\ u &= g && \text{on } \Gamma_D, \\ -(\sigma(x)\nabla u) \cdot n &= h && \text{on } \Gamma_N, \end{aligned}$$





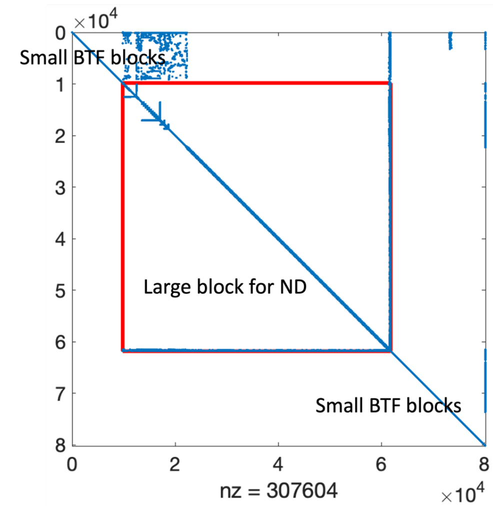
- MATERIAL strategy results in cheaper, more robust solves than previous choices (SA or DLAP).
- Implemented in Trilinos/MueLu.

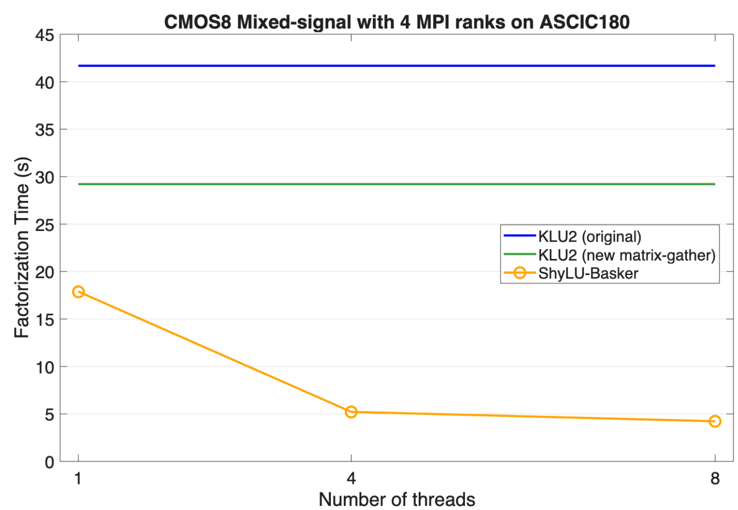
Direct Solvers (ShyLU-Basker)

Sparse Direct Solver Improvements for Modern CMOS8 Circuit Simulations in Xyce

Ichitaro Yamazaki, Clark Dohrmann, Andrew Higgins ({iyamaza, ajhiggi}@sandia.gov)

- Xyce: open source, SPICE-compatible, high-performance analog circuit simulator
  - Linear systems in Xyce are difficult to solve
  - Preconditioned iterative solvers either perform poorly or fail
  - Sparse direct solvers are often only feasible method
    - KLU [T. Davis & E. Natarajan, 2010] is serial sparse direct solver designed for circuit simulation
    - Relies on block triangular form (BTF)
- **Challenge**: matrices arising from modern circuit simulations do not have BTF structures & are dominated by large diagonal block
- **Solution**: Trilinos/ShyLU-Basker (https://arxiv.org/abs/2506.05793)
  - CPU-based thread-parallel variant of KLU
  - Improved solver performance for large diagonal block
- **Impact**: Xyce's use of ShyLU-Basker has reduced overall mixed-signal CMOS8 simulation time from O(months) to O(weeks), a **4x improvement**
- **Ongoing research**: investigating distributed-memory sparse direct solver to further reduce the simulation time





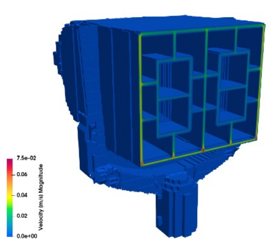
Slide courtesy of Ichitaro Yamazaki

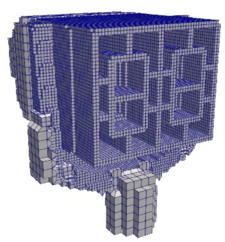
Multilevel Domain Decomposition (FROSch)

Multi-Level Monolithic Overlapping Schwarz

Within the StroemungsRaum project, we successfully integrated FROSch into the FEATFLOW software library and tested the (multi-level) monolithic overlapping Schwarz preconditioner.

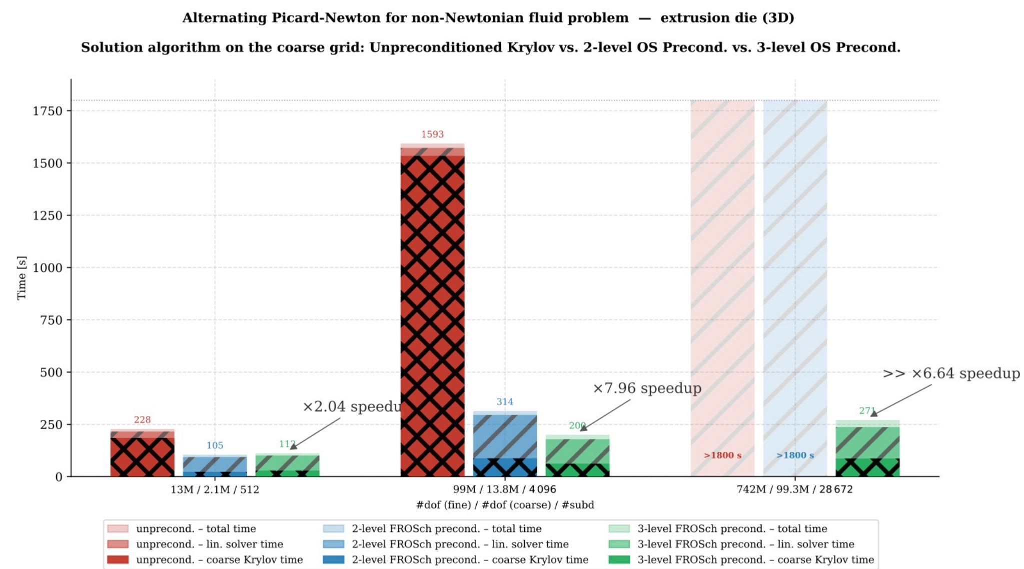
With funding from the:
Federal Ministry of Research, Technology and Space
German Initiative on “New Methods and Technologies for Exascale Computing”.





Solution of an incompressible Stokes problem with a non-Newtonian fluid on an extrusion die.

https://www.stroemungsraum.mathematik.tu-dortmund.de/



Universität zu Köln
technische universität dortmund
FAU Friedrich-Alexander-Universität Erlangen-Nürnberg
JÜLICH Forschungszentrum
TUBAF Die Ressourcenuniversität. Seit 1765.
IANUS Simulation
Stephan Köhler, Oliver Rheinbach, TU Freiberg

STROEMUNGSRAUM FROSch TRILINOS

With funding from the: Federal Ministry of Research, Technology and Space

TU BERGAKADEMIE FREIBERG

Slide courtesy A. Heinlein, A.Heinlein@tudelft.nl

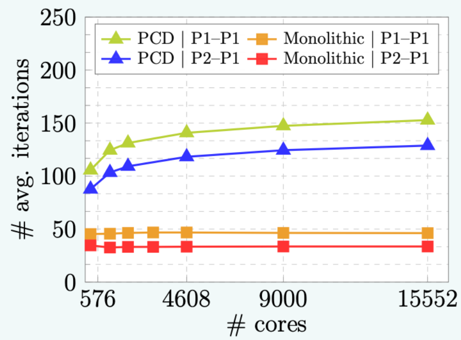
Current Research in FROSch at the University of Cologne

K. Ho, A. Klawonn, J. Knepper, M. Lanser, L. Saßmannshausen | Center for Data and Simulation Science

UNIVERSITY OF COLOGNE

Monolithic Schwarz Preconditioners for Fluid Flow Problems

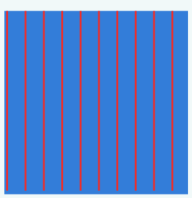
- 3D stationary Navier-Stokes *Backward-facing Step* Problem
- For 15552 cores: number of dofs $\approx 3{\cdot}10^8$
- Full comparison of monolithic and block preconditioners from `FROSch` and `Teko` package for Navier-Stokes fluid flow



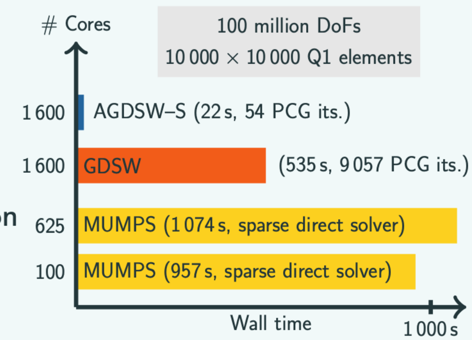
DFG

Parallel Implementation: Adaptive Coarse Spaces for Overlapping Schwarz Applied to Heterogeneous Diffusion Problems

- AGDSW–S: Adaptive coarse space
- Adaptive with respect to coefficients (→ eigenvalue problems)

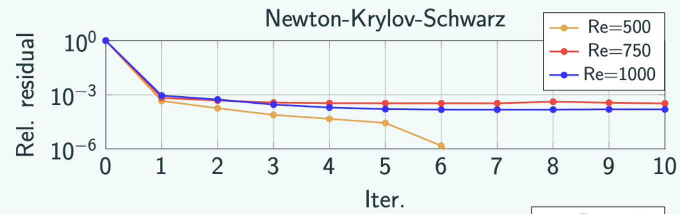


- Example coefficient function for 100×100 elements
- blue $= 1$, red $= 10^6$



Nonlinear Schwarz Preconditioners for CFD

- 2D stationary Navier-Stokes *Lid-driven Cavity* Problem on 4096 subdomains
- $67.5{\cdot}10^3$ dofs per subdomain
- Scalability tested up to 9216 subdomains and MPI ranks



References

BMFTR

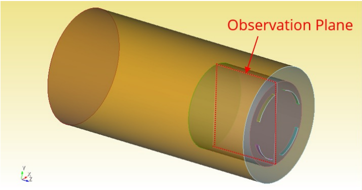
Center for Data and Simulation Science

Application Solver Development (GEMMA)

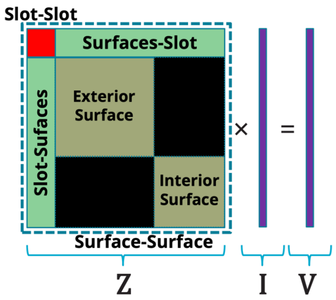
Preconditioners for Iterative Multi-Region Solution of High-Q Cavity Problems

Developers: Vinh Dang, Joe Kotulski {vqdang, jdkotul}@sandia.gov

- GEMMA: freq. domain simulation code, boundary element formulation
  - Characterization of electromagnetic fields in cavities
  - Computation challenge: dense, complex-valued linear systems
- Multi-region distributed-memory solver framework
  - Select appropriate solver for different regions
  - Uses fast numerical technique, adaptive cross approximation
  - Depends on Kokkos, Kokkos Kernels.
  - Uses Trilinos/Belos Krylov solvers.
- Current preconditioner: additive Schwarz using local block-diagonal preconditioners from self-interaction blocks
- New local prec. approach: multi-iteration Simple Algebraic Approximate Inverse (SAAI)
  - Zero two blocks closest to diagonal blocks and transform diagonal blocks
  - Approximate $X = M^{-1}Y \approx Z^{-1}Y$ via multiple iterations in each preconditioner apply



D-cavity problem (126,976 unknowns) at 1200MHz



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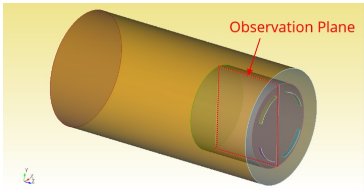

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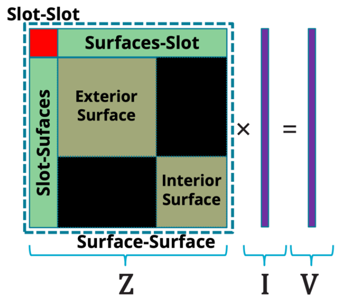

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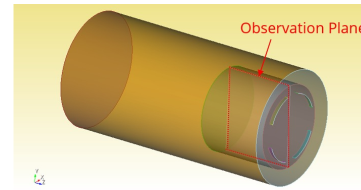

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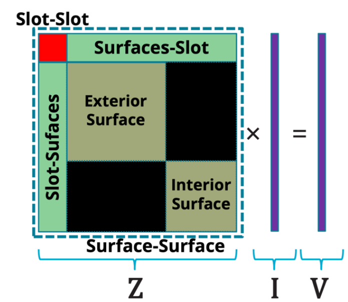

Unrestarted GMRES, (tol. 1e-10), 4 MPI ranks	Block-diagonal	2-iteration SAAI
Preconditioner build time	2.57s	**6.62s**
Number of GMRES iterations	1092	**296**
Solve time	189.73s	**33.17s**

Slide courtesy of V. Dang & J. Kotulski

Solvers R&D and Application Impact

- 11:40am , Malachi Phillips
  - *Block-based Algebraic Multigrid Preconditioners in Trilinos/Teko*
- 1:35pm, Roger Pawlowski
  - *Scalability and Performance of the Empire Plasma Physics Code on the El Capitan Platform*
- 2:00pm, Heidi Thornquist
  - *Enabling Scalable Predictive Circuit Simulation Using Trilinos*
- 2:25pm, Marco Delchini
  - *Leveraging Trilinos Scientific Computing Library for Computational Fluid Dynamics Applications*
- 3:40pm, Christian Glusa
  - *Multigrid Solvers for Maxwell's Equations in Trilinos*