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A Matrix-Free Approach for Algebraic Multigrid

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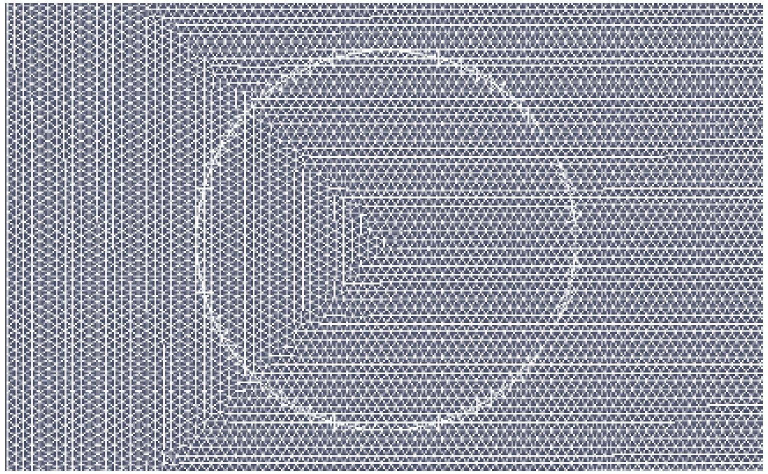
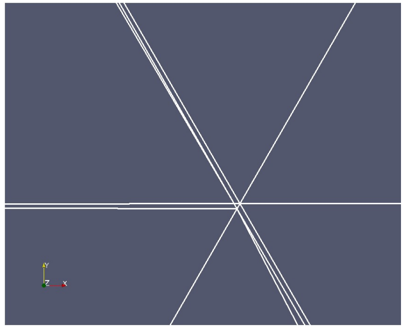
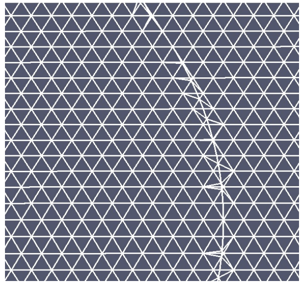
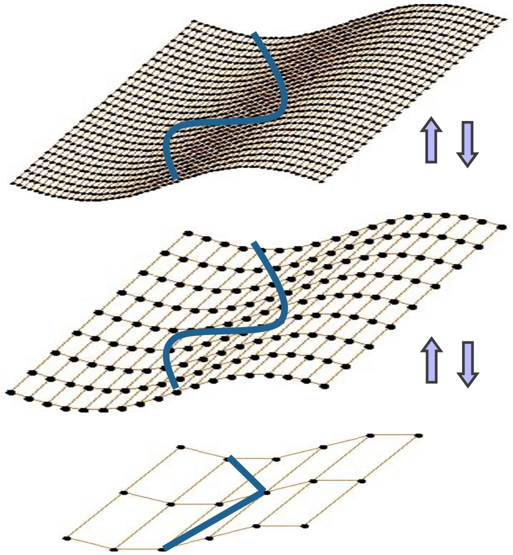
Introduction

- ASCR-funded research
- Software: Trilinos/MueLu, Sierra/Aria
- Collaborators: Ray Tuminaro, David Noble





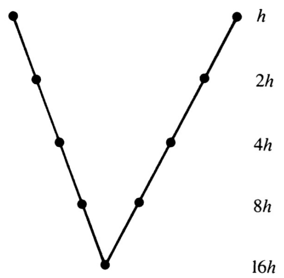




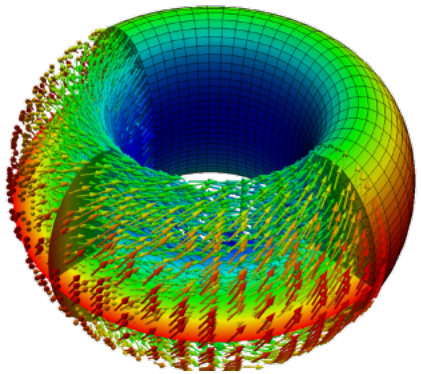
- Algebraic multigrid (AMG):
  - An approach for solving a linear system by smoothing errors on multiple grids
- Matrix-free method:
  - An approach for solving a linear system without explicitly storing the values of the matrix

Motivation

- Algebraic multigrid works well “out of the box” for many problems meeting certain requirements
  - Classic AMG (Ruge, Stuben)
  - Smoothed Aggregation (Vanek, Brezina, Mandel, 1998)



- Many multiphysics problems involve collocated DOFs
  - Problems with multiple species
  - Stabilized equal-order discretizations



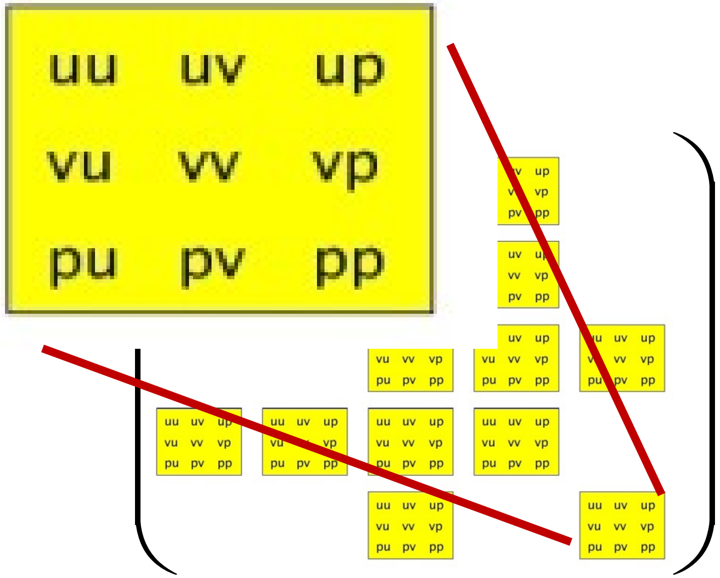
- Matrix-free methods reduce the memory burden but increase the computational burden
  - Excellent for FEMs on GPUs (Kronbichler, 2013)

$$m + \frac{1}{27}m + \frac{1}{27^2}m + \cdots + \frac{1}{27^L}m$$

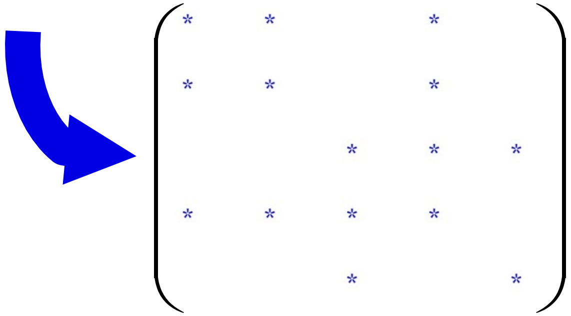
AMG for Multiphysics

Consecutive DOFs within nodes

$$[u_1\ v_1\ p_1\ \ \cdots\ \ u_n\ v_n\ p_n]$$

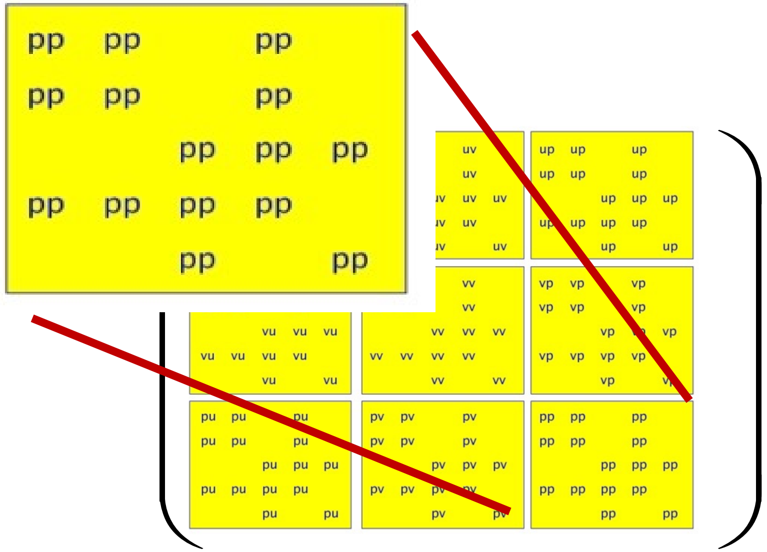


- Graph algorithms on nodes



Consecutive DOFs within fields

$$[u_1\ \cdots\ u_n\ \ v_1\ \cdots\ v_n\ \ p_1\ \cdots\ p_n]$$



- Leads to blocked prolongator structure

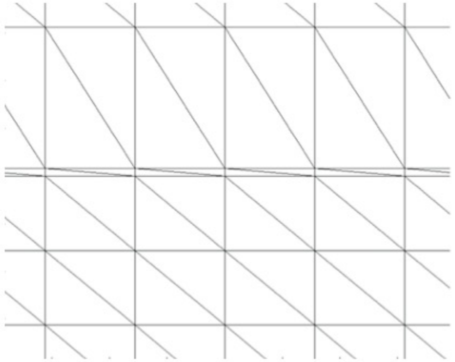
The Distance Laplacian

- Consider a multiphysics system where the DOFs are collocated

- The distance Laplacian is defined by

$$L_{ij} = \begin{cases} -1/d(i,j), & i \neq j, A_{ij} \neq 0 \\ -\sum_{k \neq i} L_{ik}, & i = j \\ 0, & \text{otherwise} \end{cases}$$

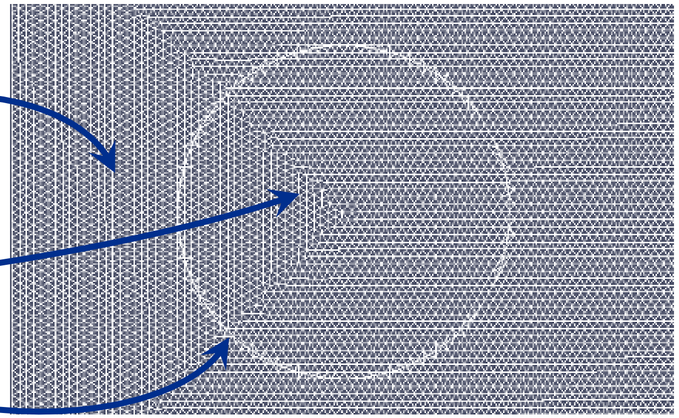
$$\begin{bmatrix} A & B^T \\ B & -D \end{bmatrix}$$



- Only requires A, coordinates for each DOF

- Implemented in MueLu/ML with more features in progress

  – 3 dofs/node (velocities, water pressure)
  – 3 dofs/node (velocities, air pressure)
  – 4 dofs/node (velocities, air & water pressure)

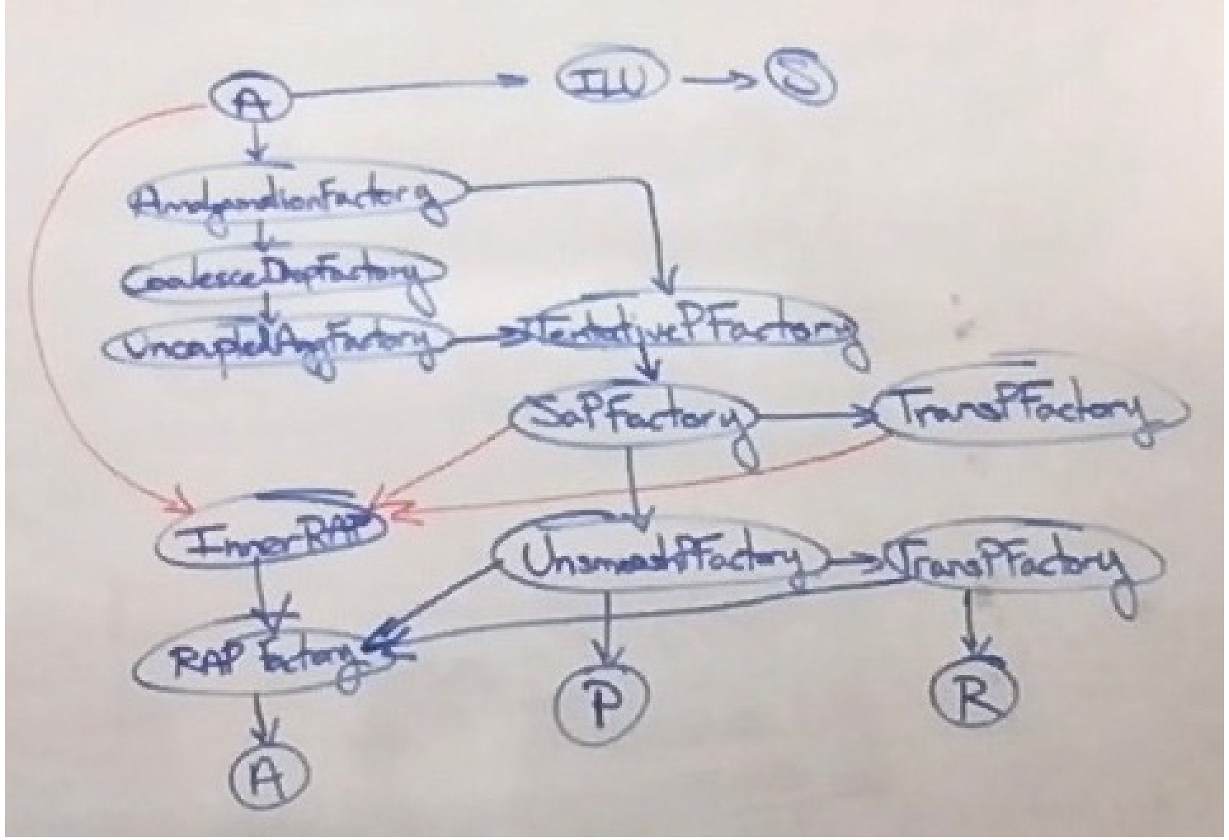


The Multigrid Strategy

- We propose an auxiliary operator multigrid method using the distance Laplacian
  - Compressed representation of A
  - No need to store entries of A
  - L is SPSD
  - DOF group splitting

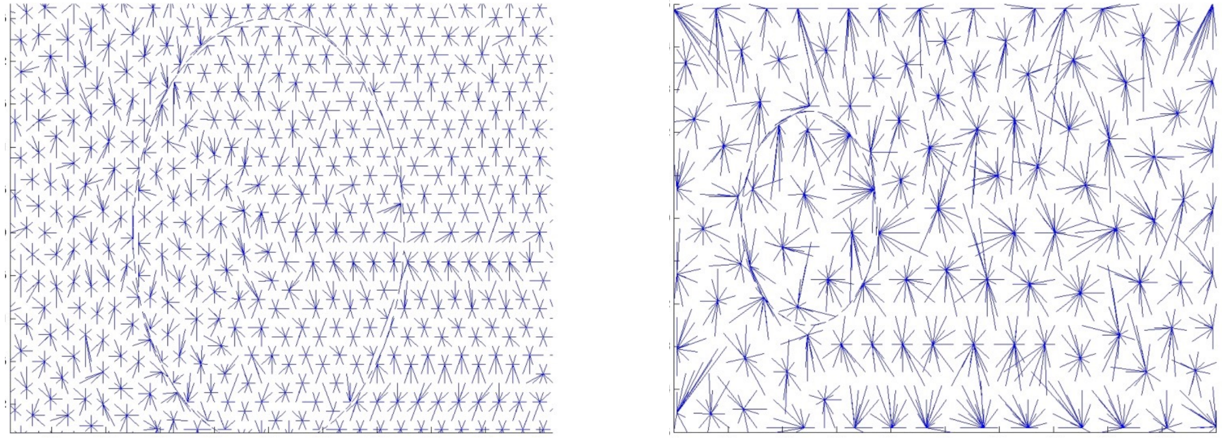
- Apply smoothed aggregation to L, and then “unsmoosh”

$$\begin{array}{ccc} A & & P_A \\ \downarrow & & \uparrow \\ L & \longrightarrow & P_L \end{array}$$



Results

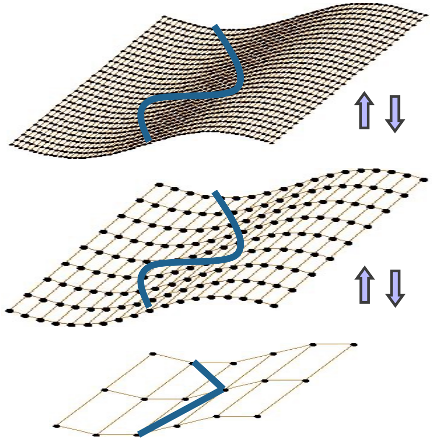
- Rising bubble problem in Aria:

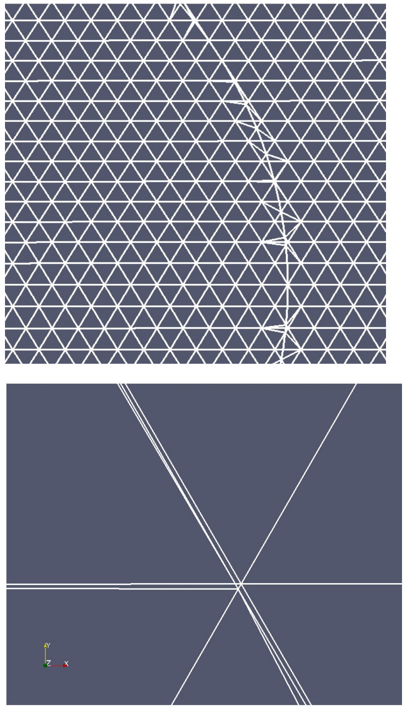


1st level aggregates   2nd level aggregates

- ILU relaxation to address smoothing concerns
  - associated with incompressibility constraint
  - tiny mesh spacing @ interface

method	iterations
ILU only	180
Unsmoothed/plain aggregation	25
Smoothed aggregation	19





Developments in Matrix-Free Multigrid

- Martin Kronbichler – matrix-free GMG for FEMs (2012)
  - As high as 70% of theoretical GPU arithmetic throughput
- Matrix-free in deal.II library (2019)
- Modified matrix-free PCG with an emphasis on data locality (2021)

- Matrix-free methods are often invasive
- No need for the entire multigrid hierarchy to be matrix-free
- Basis function storage and Jacobian re-use
- Trades memory for computation

$$m + \frac{1}{27}m + \frac{1}{27^2}m + \cdots + \frac{1}{27^L}m$$

Matrix-Free Operator Structure in Trilinos

- Tpetra::Operator
  - Panzer::STK_Interface (mesh)
  - Panzer::DOFManager
  - Intrepid2::BasisValues
  - A kernel describing the physics
  - Kokkos used for each object

- Used to create Belos::LinearProblem
- Solved by Belos::SolverFactory

- Alternatively, send to MueLu

Conclusion

- Distance Laplacian:
  - Auxiliary operator
  - Collocated multiphysics problems
  - Avoid aspects of physics that cause AMG to fail
  - Algebraic multigrid

- Future directions:
  - Theoretical explanations for distance Laplacian
  - Implement the full matrix-free chain in MueLu
  - More complex applications

Thank You!

Questions?

Aggregation

- Constructing aggregates for the distance Laplacian can be done with only the mesh graph and information about the discretization
  - Greedy approach is a classic
  - Take clever stencils like [0,…,0,1,0,…,0,-1,0,…,0] and apply it to off-diagonal nonzeros
    - Use a graph coloring to do these simultaneously for all colors in one group at a time (with care)