Enhancing Scalability and Robustness of the Schur Complement Method Using Hierarchical Parallelism

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Acknowledgements

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<u>Solvers:</u>

- **TOPS (Towards Optimal Petascale Simulations)**
- **FASTMath (Frameworks, Algorithms, and Scalable Technologies for Mathematics)**

<u>Application partnership:</u>

- **CEMM (Center for Extended MHD Modeling, fusion energy)**
- **ComPASS (Community Petascale Project for Accelerator Science and Simulation)**

OUTLINE OF THE TALK

- **Hybrid solver based on Schur complement method**
  - Software: **PDSLin** (Parallel Domain decomposition Schur complement Linear solver)

- **Combinatorial problems in hybrid solver**
  - Sparse triangular solution with sparse right-hand sides
  - K-way graph partitioning with multiple constraints

… Focusing on scalability issues.

Schur complement method

- **a.k.a iterative substructuring method**
  or, non-overlapping domain decomposition

- **Divide-and-conquer paradigm . . .**
  - Divide entire problem (domain, graph) into subproblems (subdomains, subgraphs)
  - Solve the subproblems
  - Solve the interface problem (Schur complement)

- **Variety of ways to solve subdomain problems and Schur complement … lead to a powerful poly-algorithm or hybrid solver framework**

Algebraic view

1. **Reorder into 2x2 block system, A_{11} is block diagonal**

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

2. **Schur complement**

$$S = A_{22} - A_{21} A_{11}^{-1} A_{12} = A_{22} - (U_{11}^{-T} A_{21}^{T})^{T} (L_{11}^{-1} A_{12}) = A_{22} - W \cdot G$$

$$\text{where} \quad A_{11} = L_{11} U_{11}$$

S corresponds to interface (separator) variables, no need to form explicitly

3. **Compute the solution**

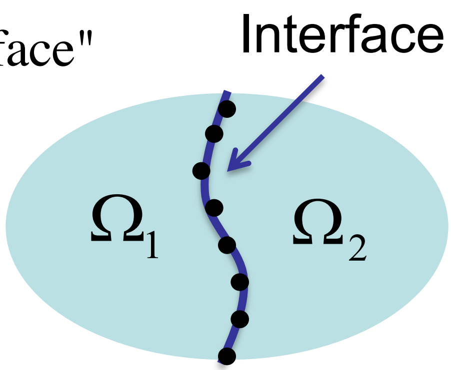
$$(1) \quad x_2 = S^{-1}(b_2 - A_{21} A_{11}^{-1} b_1) \quad \leftarrow \quad \text{iterative solver}$$

$$(2) \quad x_1 = A_{11}^{-1}(b_1 - A_{12} x_2) \quad \leftarrow \quad \text{direct solver}$$

Structural analysis view

- **Case of two subdomains**

Substructure contribution: $A^{(k)} = \begin{pmatrix} A_{ii}^{(k)} & A_{iI}^{(k)} \\ A_{Ii}^{(k)} & A_{II}^{(k)} \end{pmatrix}$ $\quad i = \text{"interior"}$, $I = \text{"Interface"}$



1. Assembled block matrix $A = \begin{pmatrix} A_{ii}^{(1)} & & A_{iI}^{(1)} \\ & A_{ii}^{(2)} & A_{iI}^{(2)} \\ A_{Ii}^{(1)} & A_{Ii}^{(2)} & A_{II}^{(1)} + A_{II}^{(2)} \end{pmatrix}$

2. Perform direct elimination of $A^{(1)}$ and $A^{(2)}$ independently,

   Local Schur complements: $S^{(k)} = A_{II}^{(k)} - A_{Ii}^{(k)} (A_{ii}^{(k)})^{-1} A_{iI}^{(k)}$

   Assembled Global Schur complement $S = S^{(1)} + S^{(2)}$

Solving the Schur complement system

- **SPD, conditioning property** [Smith/Bjorstad/Gropp'96]

  For an SPD matrix, condition number of a Schur complement is no larger than that of the original matrix.

  - S is SPD, much reduced in size, better conditioned, but denser, solvable with preconditioned iterative solver

- **Two approaches to preconditioning S**

  1. Global S (e.g., PDSLin [Yamazaki/L.'10], HIPS [Henon/Saad'08])
     - **general algebraic preconditioner, e.g. ILU(S)**
  2. Local S (e.g. MaPHys [Giraud/Haidary/Pralet'09])
     - **restricted preconditioner; more parallel**
     - **e.g., additive Schwarz preconditioner** $S = S^{(1)} \oplus S^{(2)} \oplus S^{(3)} \ldots$

$$M = {S^{(1)}}^{-1} \oplus {S^{(2)}}^{-1} \oplus {S^{(3)}}^{-1} \ldots$$

Related work

PDSLin (LBNL)	MaPHyS (INRIA/CERFACS)	HIPS (INRIA)
Multiple procs/subdom, Smaller Schur compl.	Multiple procs/subdom, Smaller Schur compl.	Multiple subdoms/proc, Larger Schur compl., Good load balance.
Threshold based “ILU”, Global approx. Schur Robust precond.	Additive Schwartz, Local Schur Scalable precond.	Block level-based ILU, Global approx. Schur Scalable precond.

- **PDSLin**
  - Uses two levels of parallelization and load-balancing techniques for tackling large-scale systems
  - Provides a robust preconditioner for solving highly-indefinite or ill-conditioned systems
- **On-going work:** comparison of PDSLin and MaPHyS [Yamazaki et al.]

Parallelization with serial subdomain

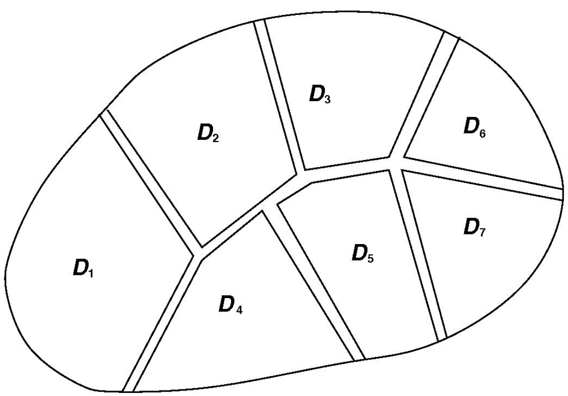
- **No. of subdomains increases with increasing core count.**
  ➔ Schur complement size and iteration count increase

- **HIPS (serial subdomain) vs. PDSLin (parallel subdomain)**
  - M3D-C[1], Extended MHD to model fusion reactor tokamak, 2D slice of 3D torus
  - Dimension 801k, 70 nonzeros per row, real unsymmetric

P	N_S	HIPS 1.0 sec (iter)	PDSLin sec (iter)
8	13k	284.6 (26)	79.9 (15)
32	29k	55.4 (64)	25.3 (16)
128	62k	--	17.1 (16)
512	124k	--	21.9 (17)

Parallelism – extraction of multiple subdomains

- **Partition adjacency graph of $|A|+|A^T|$**
  Multiple goals: reduce size of separator, balance size of subdomains
  - nested dissection (e.g., PT-Scotch, ParMetis)
  - k-way partition (preferred)

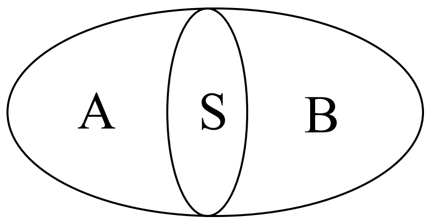


$$\left(\begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array}\right) = \left(\begin{array}{cccc|c} D_1 & & & & E_1 \\ & D_2 & & & E_2 \\ & & \ddots & & \vdots \\ & & & D_k & E_k \\ \hline F_1 & F_2 & \ldots & F_k & A_{22} \end{array}\right)$$

- **Memory requirement: fill is restricted within**
  - “small” diagonal blocks of A_{11}, and
  - ILU(S), maintain sparsity via numerical dropping

Graph partitioning

- Generalized nested dissection [Lipton/Rose/Tarjan '79]
  - **Top-down, divide-and-conquer, best for largest problems**
  - **Parallel codes : ParMetis, PT-Scotch**
  - **First level**



$$\longrightarrow \begin{bmatrix} A & 0 & x \\ 0 & B & x \\ x & x & S \end{bmatrix}$$

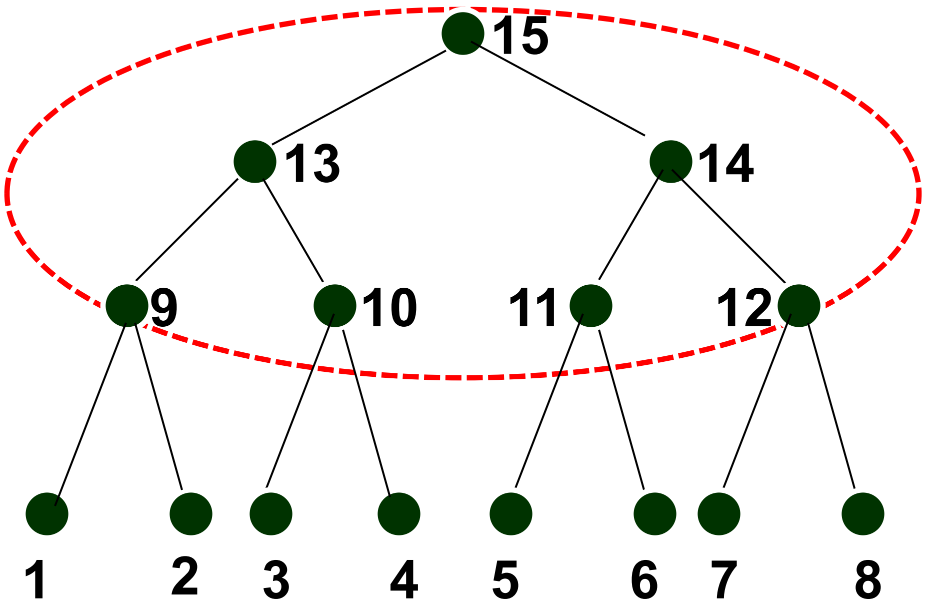
  - **Recurse on A and B**

- Goal: find the smallest separator S at each level
  - **Multilevel schemes:**
    - **ParMetis [Karypis et al.], PT-Scotch [Pellegrini et al.], PaToh [Catalyurek et al.]**
  - **Spectral bisection [Simon et al. `90-`95]**
  - **Geometric and spectral bisection [Chan/Gilbert/Teng `94]**

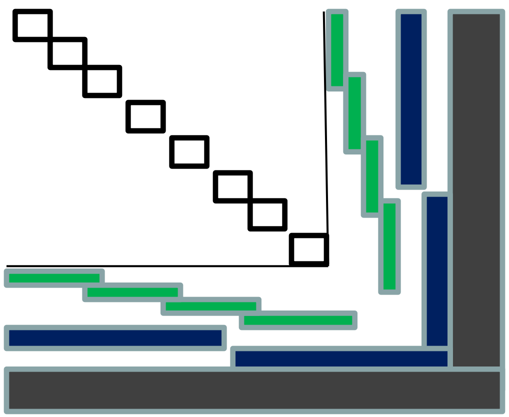
Ordering

- **Permute all the separators to the end**

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \left(\begin{array}{cccc|c} D_1 & & & & E_1 \\ & D_2 & & & E_2 \\ & & \ddots & & \vdots \\ & & & D_k & E_k \\ \hline F_1 & F_2 & \dots & F_k & A_{22} \end{array}\right)$$

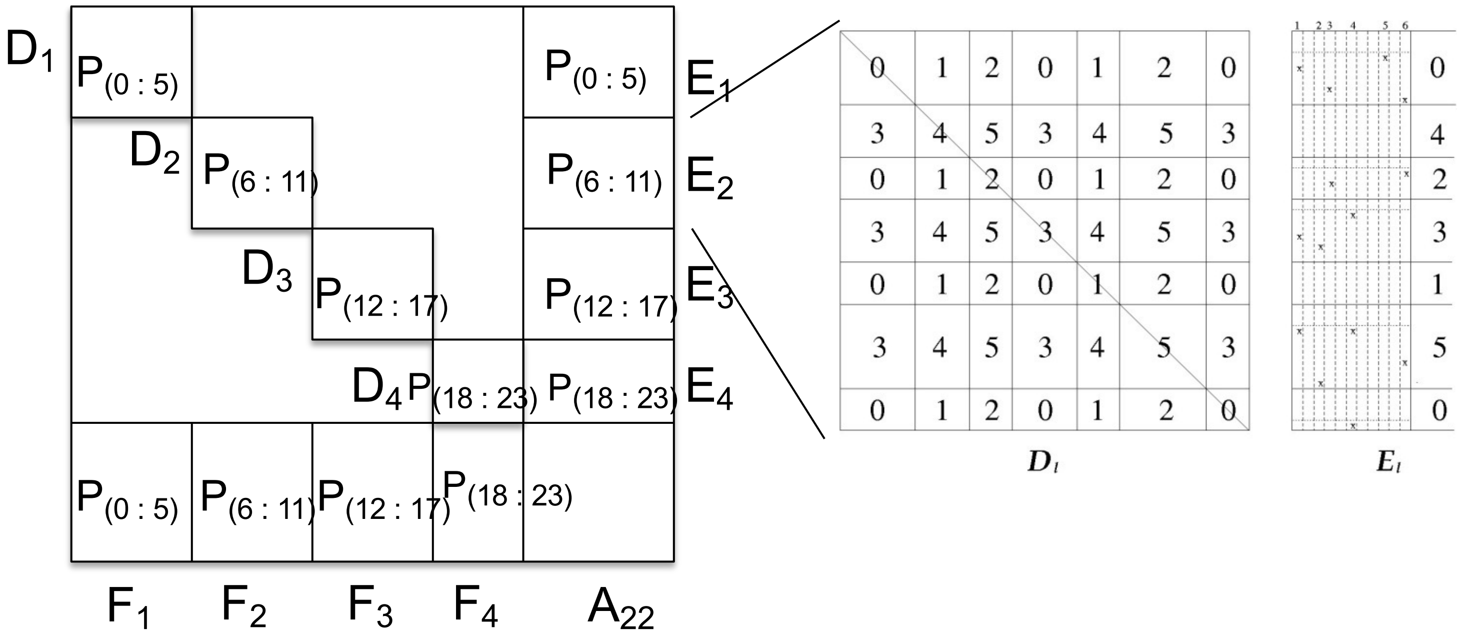


Separator tree



Hierarchical parallelism

- **Multiple processors per subdomain**
  - one subdomain with 2x3 procs (e.g. SuperLU_DIST, MUMPS)



- **Advantages:**
  - Constant #subdomains, Schur size, and convergence rate, regardless of core count.
  - Need only modest level of parallelism from direct solver.

PDSLin software

- **Parallel Domain decomposition Schur complement based Linear solver**
  - C and MPI, with Fortran interface.
  - Unsymmetric and symmetric, real and complex, multiple RHSs.
- **Requires the following external packages:**
  - parallel graph partitioning:
    - **PT-Scotch (http://labri.fr/perso/pelegrin/scotch), or**
    - **ParMetis (http://glaros.dtc.umn.edu/gkhome/views/metis)**
  - subdomain solver options:
    - **SuperLU (http://crd.lbl.gov/˜xiaoye/SuperLU)**
    - **SuperLU_DIST or SuperLU_MT: two levels of parallelization**
    - **MUMPS**
    - **PDSLin**
    - **Inexact subdomain solution: ILU**
  - Schur complement solver options:
    - **PETSc (http://mcs.anl.gov/petsc/petsc-as)**
    - **SuperLU_DIST**

PDSLin encompass Hybrid, Iterative, Direct

Hybrid

Default
Subdomain: LU
Schur: Krylov

Iterative

Options
(1) num_doms = 0
Schur = A: Krylov
(2) FGMRES Inner-Outer:
Subdomain: ILU
Schur: Krylov

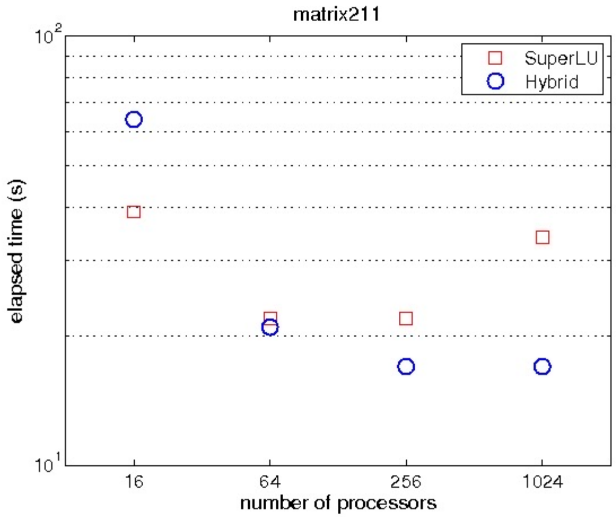
Direct

Options
(1) Subdomain: LU
Schur: LU
drop_tol = 0.0
(2) num_doms = 1
Domain: LU

$$\left(\begin{array}{cccc|c} D_1 & & & & E_1 \\ & D_2 & & & E_2 \\ & & \ddots & & \vdots \\ & & & D_k & E_k \\ \hline F_1 & F_2 & \dots & F_k & A_{22} \end{array}\right)$$

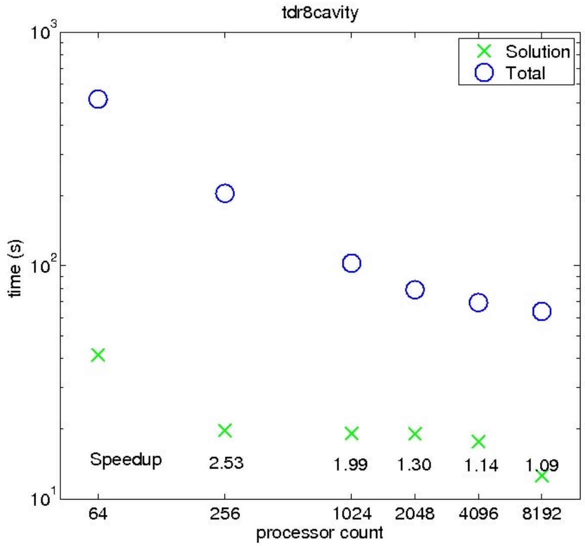
PDSLin vs. SuperLU_DIST

- **Cray XT4 at NERSC**
- **Matrix211 : extended MHD to model burning plasma**
  - dimension = 801K, nonzeros = 56M, real, unsymmetric
  - PT-Scotch extracts 8 subdomains of size ≈ 99K, S of size ≈ 13K
  - SuperLU_DIST to factorize each subdomain, and compute preconditioner LU($\widetilde{S}$)
  - BiCGStab of PETSc to solve Schur system on 64 processors with residual < 10^{-12} , converged in 10 iterations
- **Needs only 1/3 memory of direct solver**



PDSLin for RF cavity (strong scaling)

- **Cray XT4 at NERSC; used 8192 cores**
- **Tdr8cavity : Maxwell equations to model cavity of International Linear Collider**
  - dimension = 17.8M, nonzeros = 727M
  - PT-Scotch extracts 64 subdomains of size ≈ 277K, S of size ≈ 57K
  - BiCGStab of PETSc to solve Schur system on 64 processors with residual < 10^{-12}, converged in 9 ~ 10 iterations
- **Direct solver failed !**



PDSLin for largest system

- Matrix properties:
  - 3D cavity design in Omega3P, 3rd order basis function for each matrix element
  - dimension = 52.7 M, nonzeros = 4.3 B (~80 nonzeros per row), real, symmetric, highly indefinite
- Experimental setup:
  - PT-Scotch extracts 128 subdomains of size ~410k
  - SuperLU DIST factors each subdomain, computes preconditioner LU($\widetilde{S}$) of size 247k (32 cores)
  - BiCGStab of PETSc to solve Sy = d
- Performance:
  - Fill-ratio (nnz(Precond.)/nnz(A)): ~ 250
  - Using 2048 cores:
    - preconditioner construction: 493.1 sec.
    - solution: 108.1 second (32 iterations)

Combinatorial problems

[Yamazaki, L., Rouet, Ucar]

Computing approximate Schur preconditioner

Combinatorial problems . . .

- **Sparse triangular solution with many sparse RHS**

$$S = A_{22} - \sum_{l} (U_l^{-T} F_l^T)^T \, (L_l^{-1} E_l), \text{ where } D_l = L_l U_l$$

- **Sparse matrix–matrix multiplication**

$$\widetilde{G} \leftarrow \text{sparsify}(G, \sigma_1); \quad \widetilde{W} \leftarrow \text{sparsify}(W, \ \sigma_1)$$

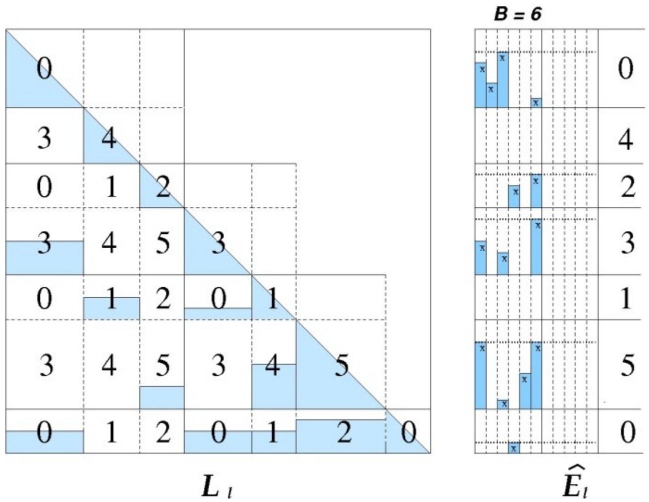
$$T^{(p)} \leftarrow \widetilde{W}^{(p)} \times \widetilde{G}^{(p)}$$

$$\hat{S}^{(p)} \leftarrow A_{22}{}^{(p)} - \sum\nolimits_q T^{(q)}(p); \quad \widetilde{S} \leftarrow \text{sparsify}(\hat{S}, \ \sigma_2)$$

- **K-way graph partitioning with multiple objectives**
  - Small separator
  - Similar subdomains
  - Similar connectivity

1. Sparse triangular solution with sparse RHS

- **RHS vectors E_ℓ and F_ℓ are sparse (e.g., about 20 nnz per column); There are many RHS vectors (e.g., $O(10^4)$ columns)**

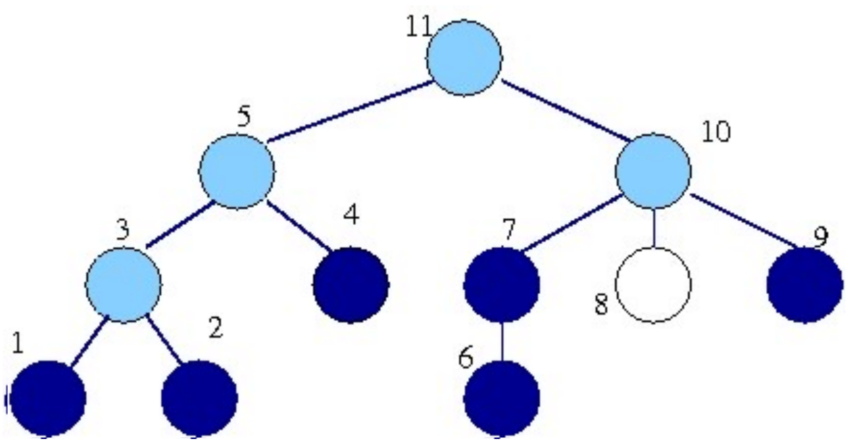


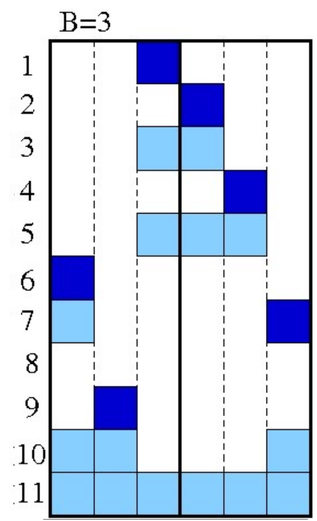
- **Blocking the RHS vectors**
  - Reduce number of calls to the symbolic routine and number of messages, and improve read reuse of the LU factors
  - ➢ Achieved over 5x speedup
  - ✖ zeros must be padded to fill the block

Sparse triangular solution with sparse RHSs

- **Combinatorial question: Reorder columns of E_ℓ to maximize structural similarity among the adjacent columns.**
- **Where are the fill-ins?**

  <u>Path Theorem</u> [Gilbert'94] **Given the elimination tree of D_l, fill will be generated in G_l at the positions associated with the nodes on the path from nodes of the nonzeros in E_l to the root**

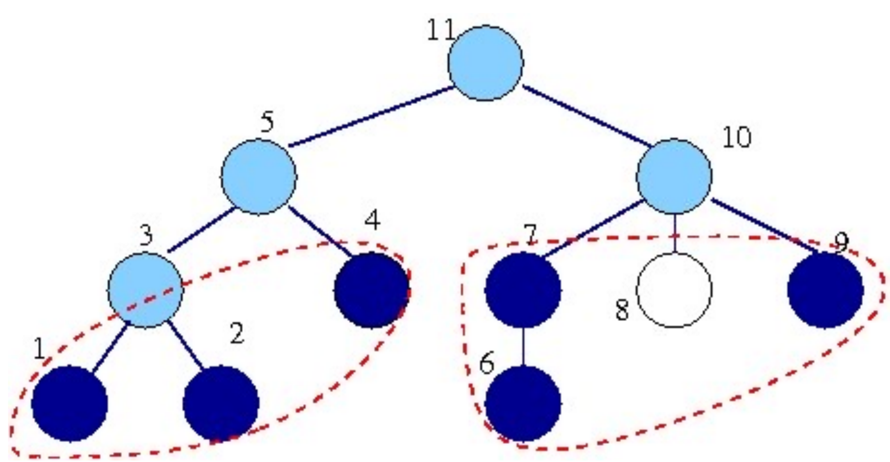


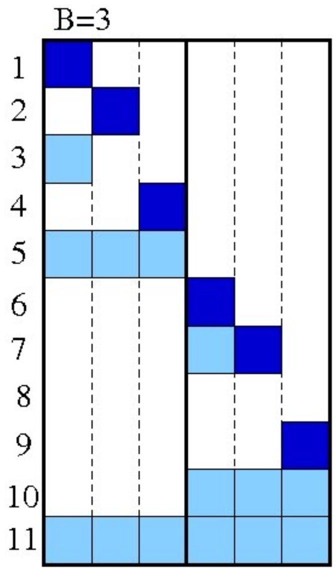


24 padded zeros

Sparse triangular solution … postordering

- **Postorder-conforming ordering of the RHS vectors**
  - Postorder the elimination tree
  - Permute the columns of E_I such that the row indices of the first nonzeros are in ascending order
- **Increased overlap of the paths to the root, fewer padded zeros**
- **20 – 40% reduction in solution time . . . improved over ND.**





13 padded zeros

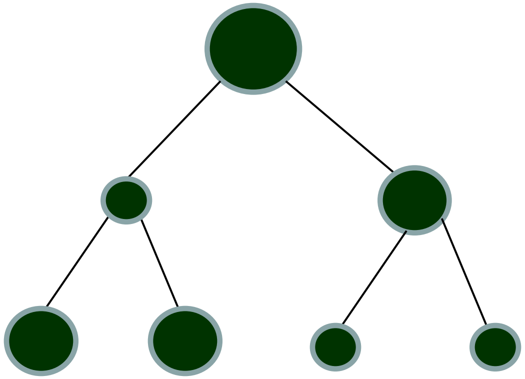
Sparse triangular solution … further optimization

- **Define a cost function that measures the dissimilarity of the sparsity pattern within a partition.**
- **Reordering based on a hypergraph partitioning model which minimizes the cost function above.**
- **Led to additional 10% reduction in time.**

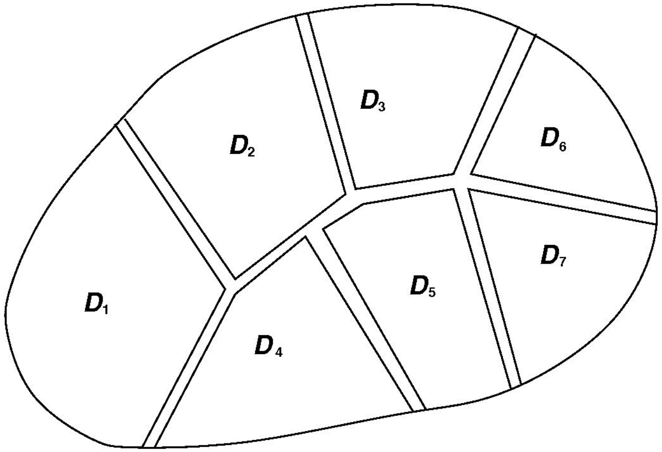
2. K-way subdomain extraction

- **Problem with ND:**

  Imbalance in separator size at different branches → Imbalance in subdomain size

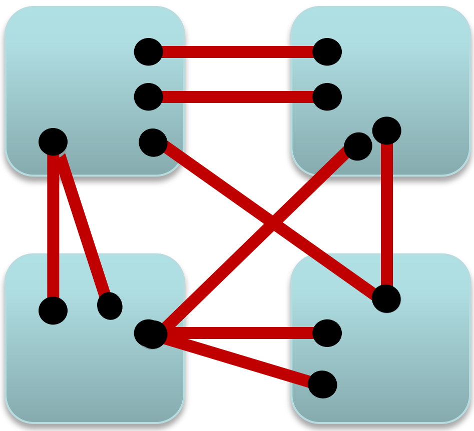


- **Alternative: directly partition into K parts, meet multiple constraints:**
  1. **Compute k-way partitioning → balanced subdomains**
  2. **Extract separator → balanced connectivity**



Experimenting several heuristics

- **Direct partition**
  1. Scotch: k-way edge partition
     - **Parts have similar size; minimize number of edge cuts**
  2. Form edge-induced subgraph
     - **Two end-points form wide vertex separator**
     - **Find smaller vertex separator via minimal vertex cover**



- **Recursive hypergraph partitioning**

- **Results**

+ improved balance of subdomains and interface
– larger Schur complement & interfaces
→ total time improved a little

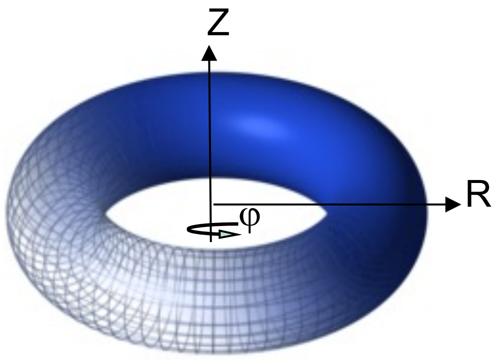
Final remarks

- **Direct solvers can scale to 1000s cores**
- **Domain-decomposition type of hybrid solvers can scale to 10,000s cores**
  - Can maintain robustness too
- **Expect to scale more with low-rank structured factorization preconditioner**

Extra Slides

Application 1: Burning plasma for fusion energy

- DOE SciDAC project: Center for Extended Magnetohydrodynamic Modeling (CEMM),   PI: S. Jardin, PPPL
- **Develop simulation codes to predict microscopic MHD instabilities of burning magnetized plasma in a confinement device (e.g., tokamak used in ITER experiments).**
  - Efficiency of the fusion configuration increases with the ratio of thermal and magnetic pressures, but the MHD instabilities are more likely with higher ratio.
- **Code suite includes M3D-C^1, NIMROD**



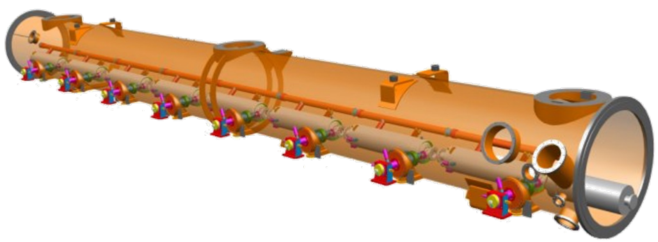
(S. Jardin)

- At each φ = constant plane, scalar 2D data is represented using 18 degree of freedom quintic triangular finite elements Q_{18}
- Coupling along toroidal direction

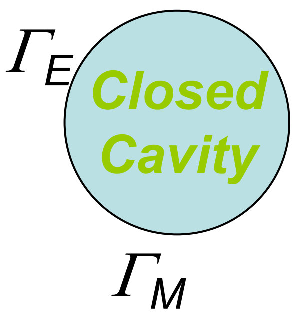
Application 2: Accelerator cavity design

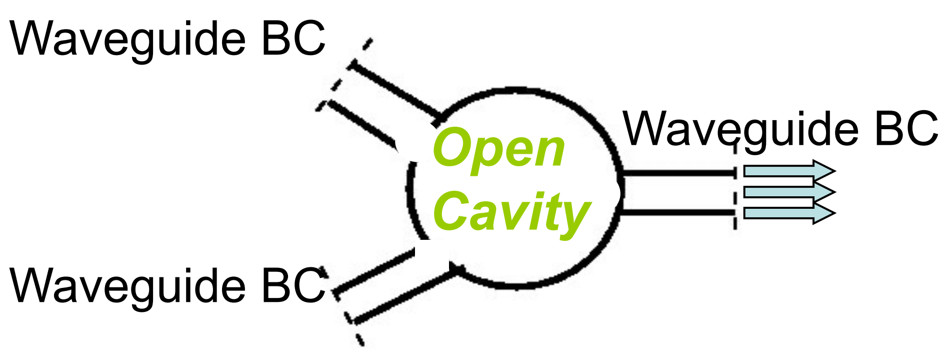
- DOE SciDAC: Community Petascale Project for Accelerator Science and Simulation (ComPASS), PI: P. Spentzouris, Fermilab
- **Development of a comprehensive computational infrastructure for accelerator modeling and optimization**
- **RF cavity: Maxwell equations in electromagnetic field**
- **FEM in frequency domain leads to large sparse eigenvalue problem; needs to solve shifted linear systems**

(L.-Q. Lee)



RF unit in ILC





linear eigenvalue problem

$$(K_0 - \sigma^2 M_0)\, x = M_0\, b$$

nonlinear complex eigenvalue problem

$$(K_0 + i\,\sigma W - \sigma^2 M_0)\, x = b$$