Distributed Schur Complement Solvers for Real and Complex Block-Structured CFD Problems

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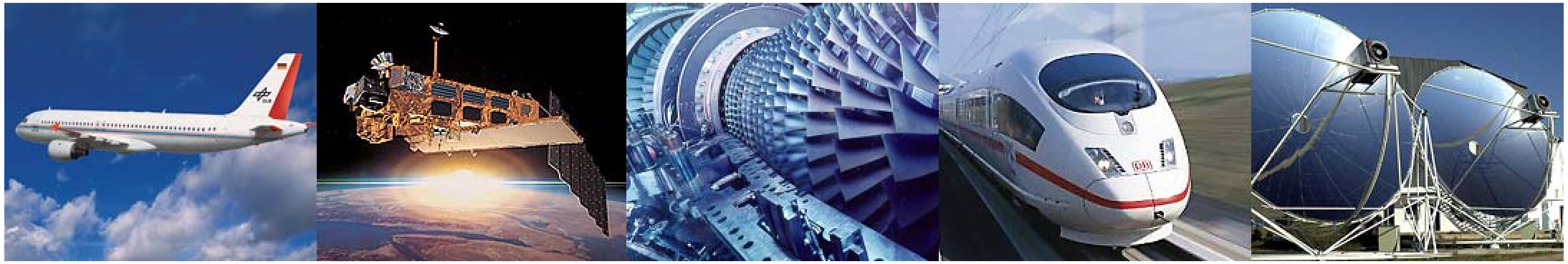


- Research Institution
- Space Agency
- Project Management Agency


DLR

Locations and employees

Germany: 6000 employees across 29 research institutes and facilities at

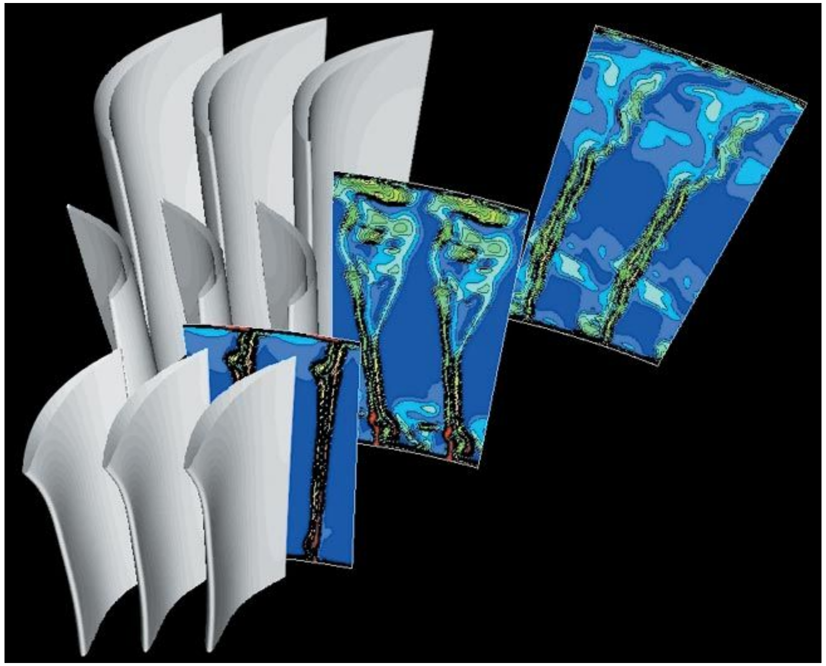
- 13 sites.

Offices in **Brussels**, **Paris** and **Washington**.

Survey

- Motivation
- The *Distributed Schur Complement* method (DSC)
- Complex and real problem formulation
- Experiments with TRACE matrices
- Conclusions

Parallel Simulation System TRACE

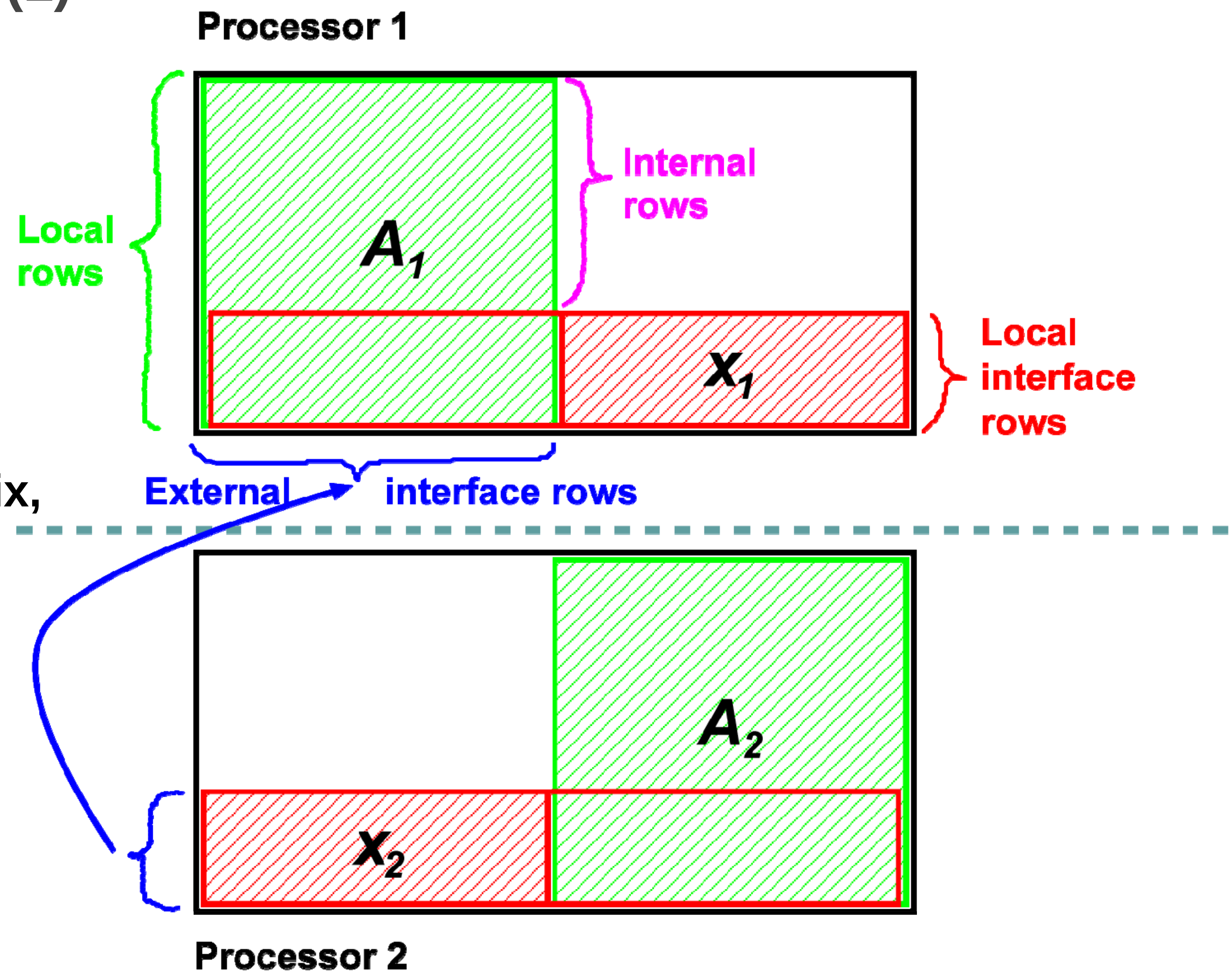


- TRACE: Turbo-machinery Research Aerodynamic Computational Environment
- Developed by the Institute for Propulsion Technology of the German Aerospace Center (DLR-AT)
- Calculates internal turbo-machinery flows
- Finite volume method with block-structured grids
- The linearized TRACE modules require the parallel, iterative solution of large, sparse non-symmetric systems of linear equations.

Preconditioners for TRACE: Background

- **Modules linearTRACE or adjointTRACE** $Ax = b$
  - ***A* non-symmetric, complex or real, sparse**
  - **Parallel iterative solver: (F)GMRes with preconditioning** $P^{-1}Ax = P^{-1}b$
    - **Distinctly dominates the time behavior**
    - **Matrix-vector and vector-vector operations**
    - **Preconditioning usually is the most time-consuming operation**
      - **Crucial for scalability**
      - **Status: Block-local preconditioning**
        - **ILU, SSOR**
        - **Scalability limited**
      - **Goal: global, scalable preconditioner**
        - **Experiments with Distributed Schur Complement (DSC) methods**

DSC Method (1)

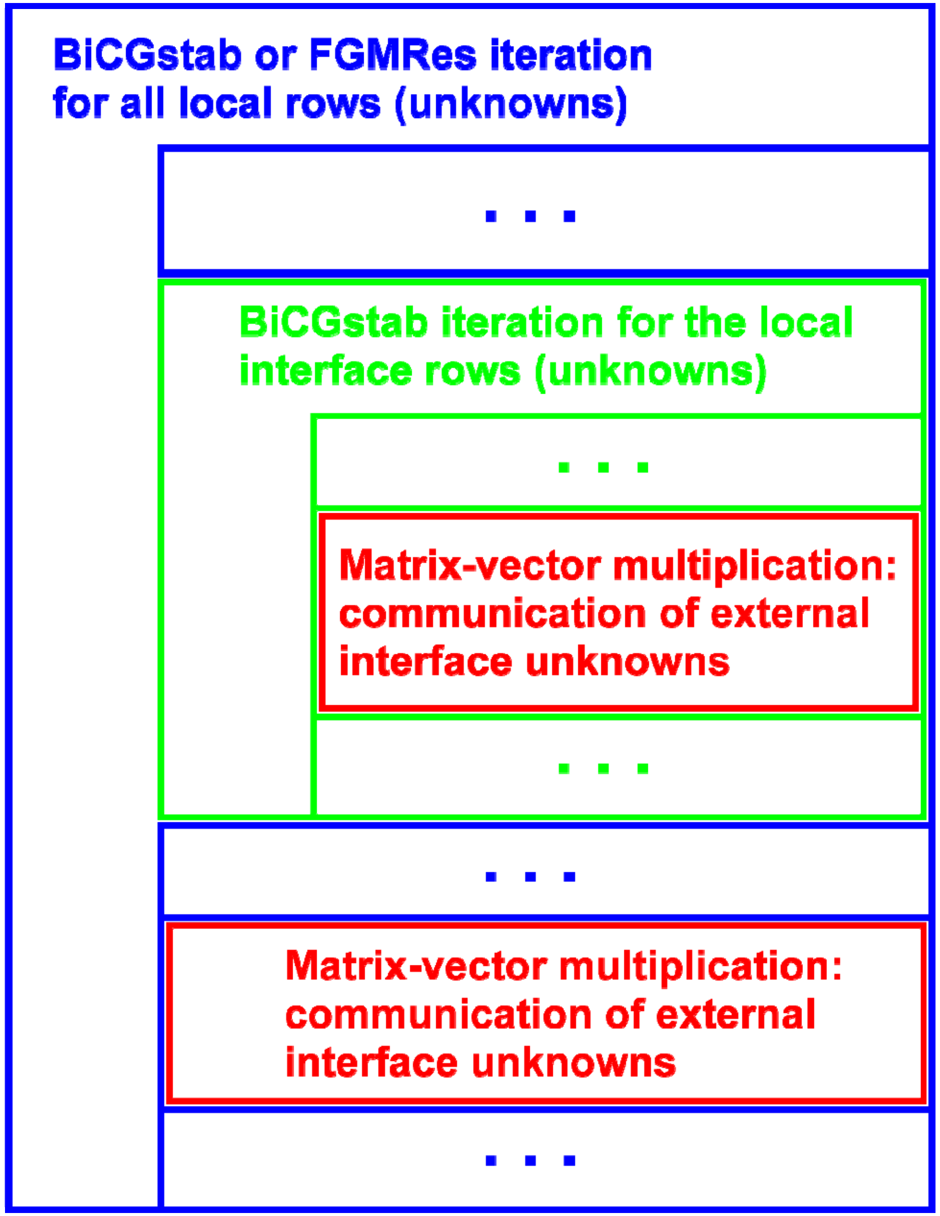


Distributed matrix, 2 processors

DSC Method (2)

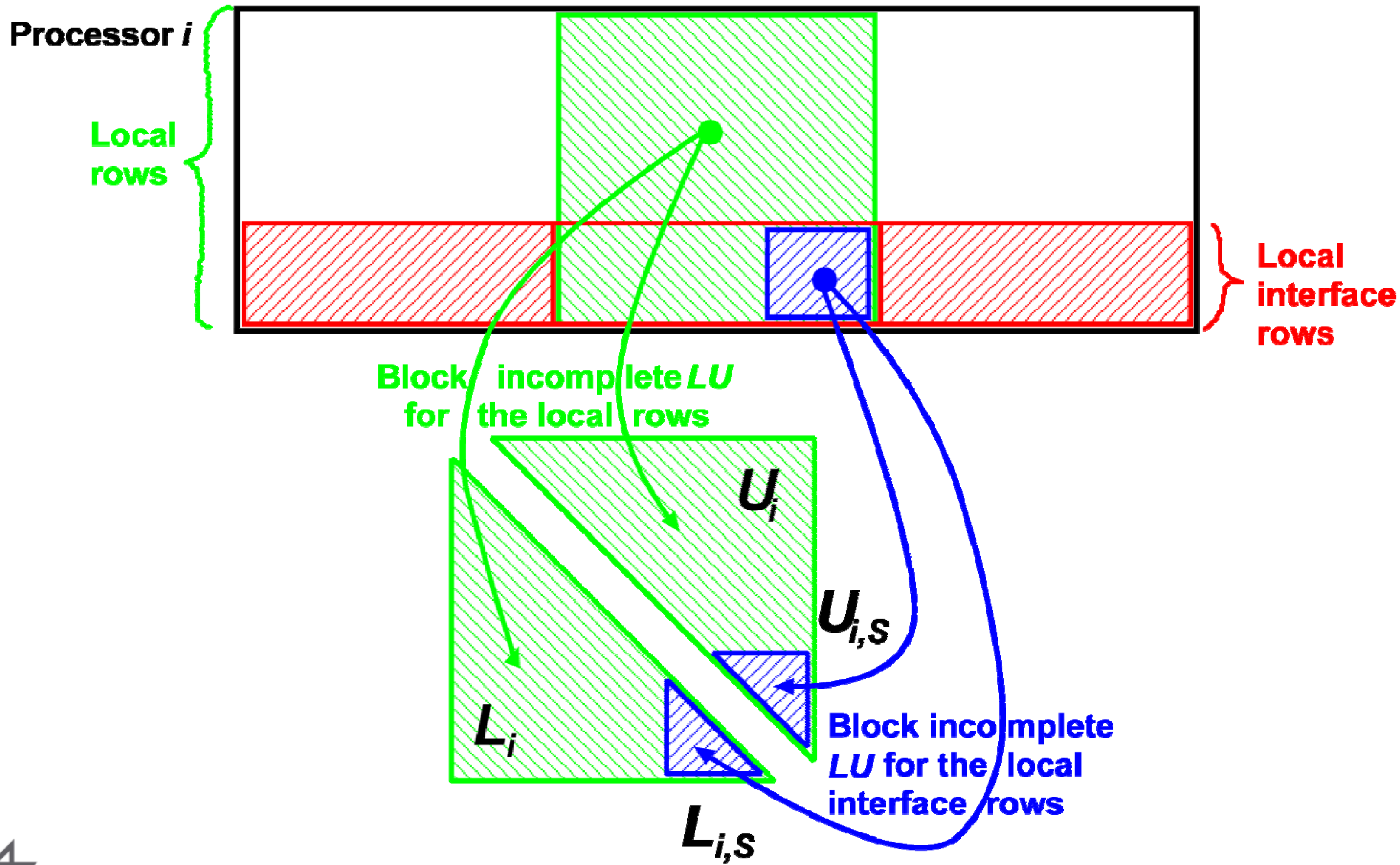
DSC Algorithm

Schematic view on each processor



DSC Method (3)

Preconditioning within the DSC algorithm



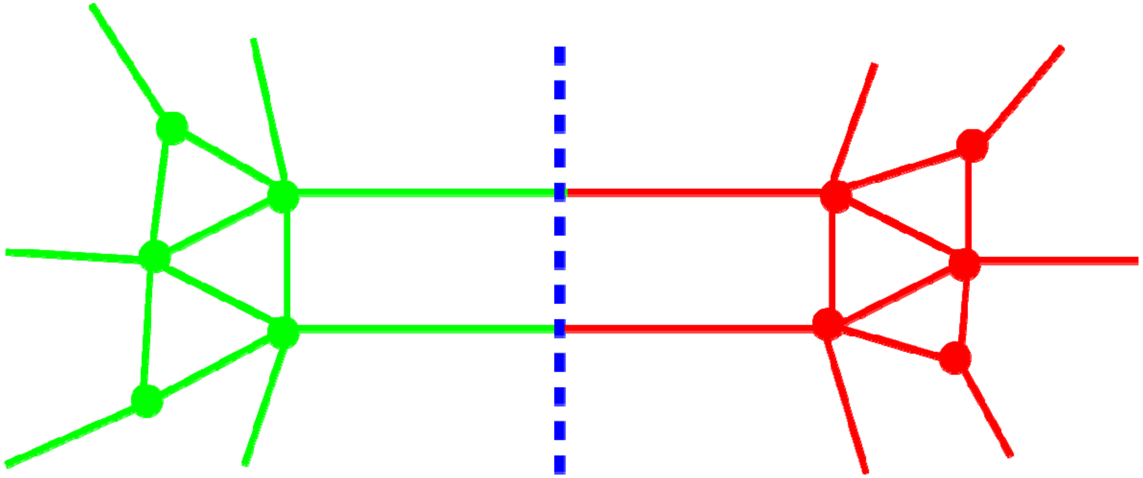
DSC Method (4): Effect of Partitioning

Graph partitioning: ParMETIS (University of Minnesota)

Goal:

Minimize the number of edges cut

⟷ Minimize the number of interface unknowns

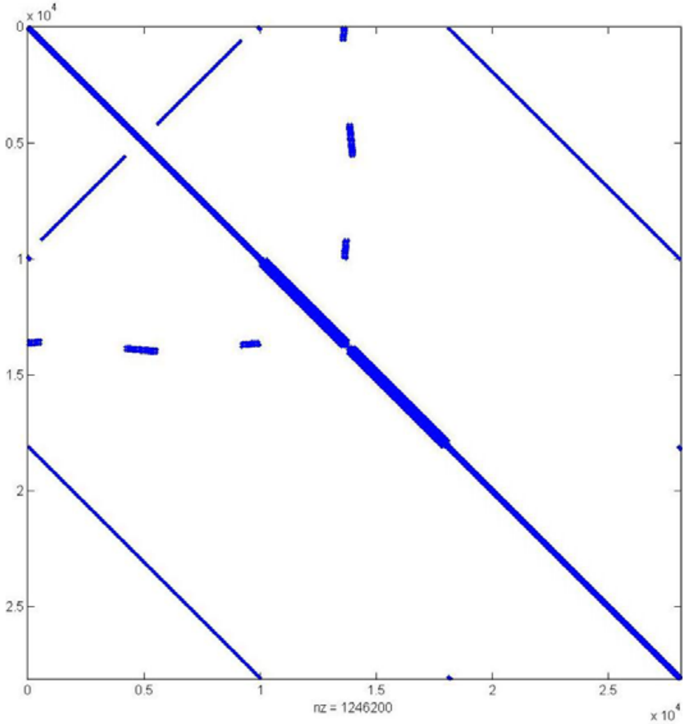


Undirected graph → Symmetrize the matrix structure

Matrix Experiments: Real or Complex Arithmetics?

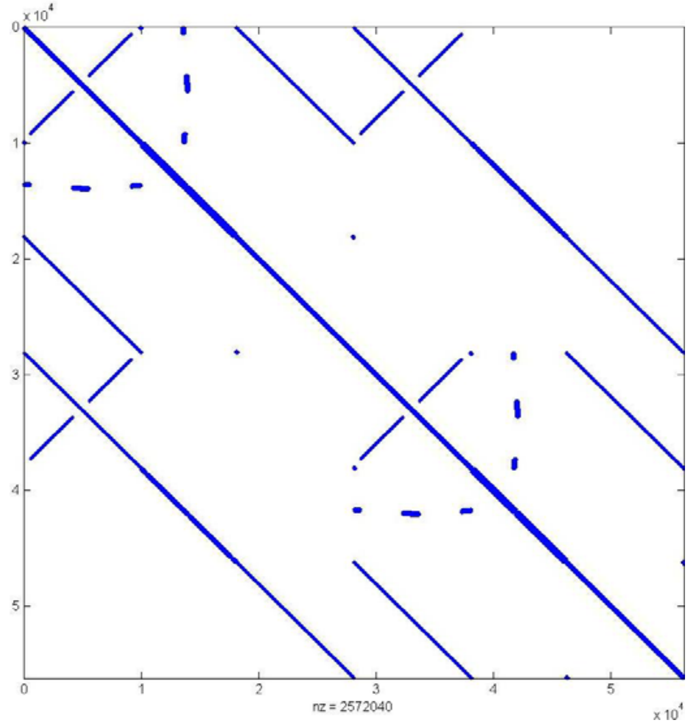
Complex TRACE matrix
(n=28,120; nz=1,246,200; Cond.: $6.7 \cdot 10^6$)

$$Ax = b$$
$$\Leftrightarrow (C + iD)(y + iz) = c + id$$



Real TRACE matrix
(n=56,240; nz=2,572,040; Cond.: $8.4 \cdot 10^6$)

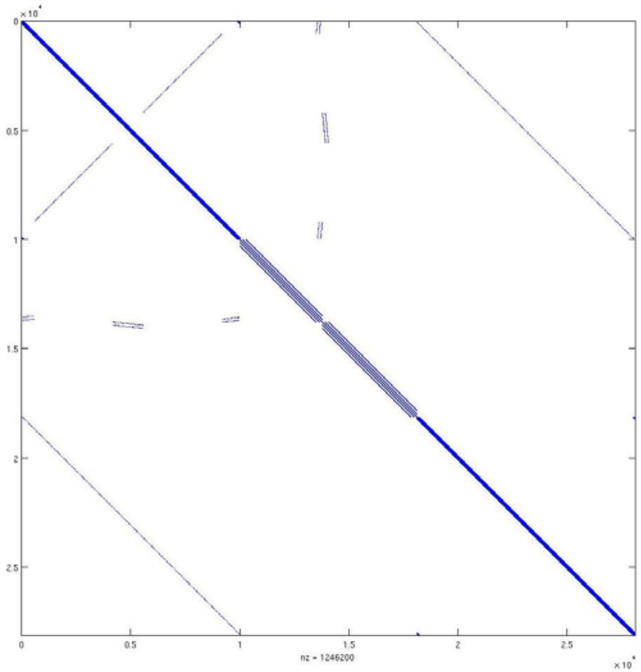
$$\begin{pmatrix} C & -D \\ D & C \end{pmatrix} \begin{pmatrix} y \\ z \end{pmatrix} = \begin{pmatrix} c \\ d \end{pmatrix}$$
$$\Leftrightarrow Gw = e$$



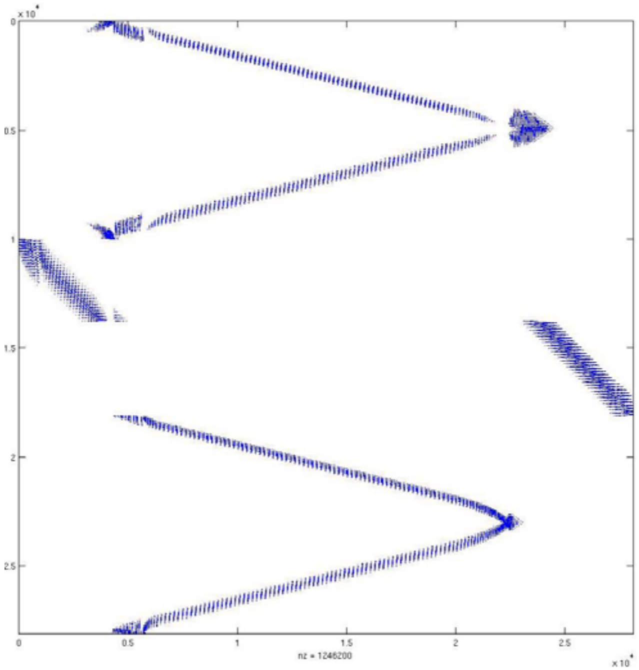
DSC Preconditioner: Matrix Permutation (complex)

Background: Fill-in reduction for ILUT preconditioning

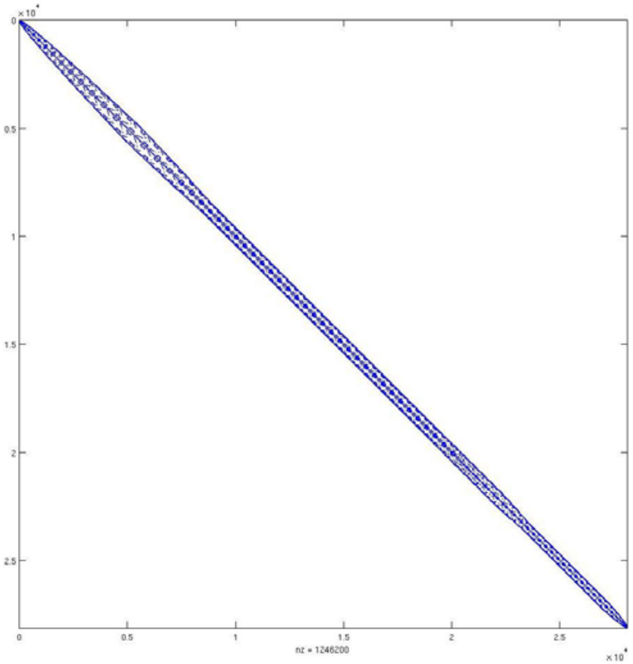
Original



Minimum Degree (MD)

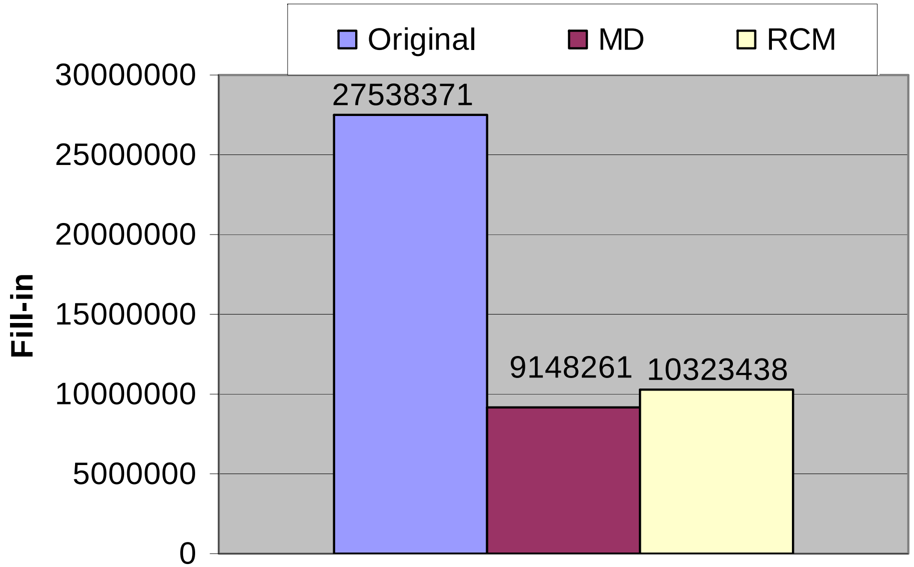


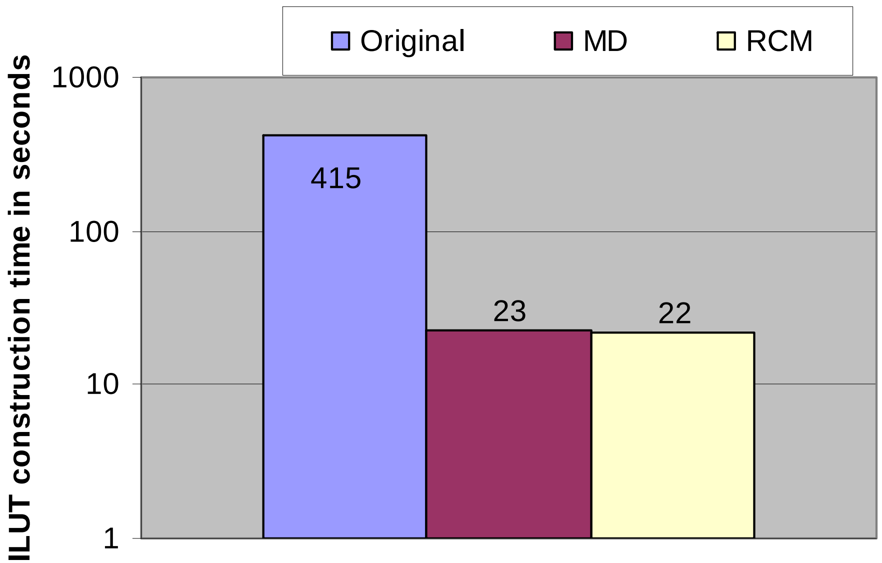
Reverse Cuthill-McKee (RCM)



ILU Preconditioner: Fill-in in *L* and *U* (complex)

MATLAB: ILUT preconditioner; threshold = 10^{-3}

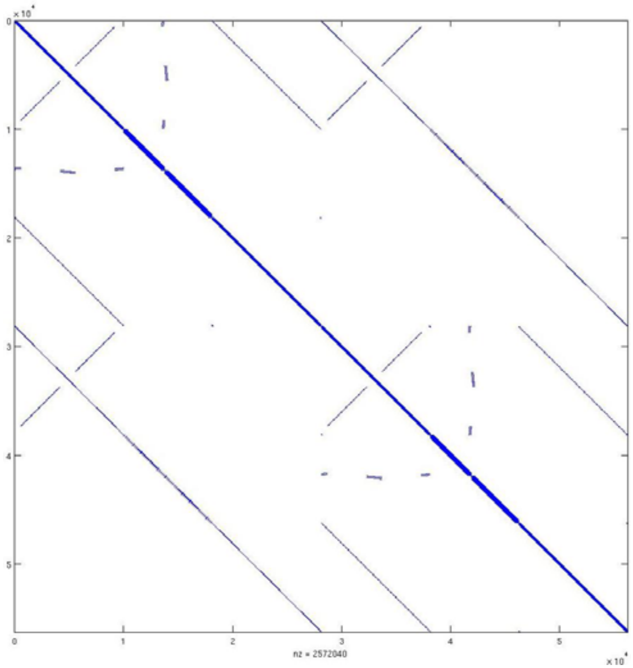




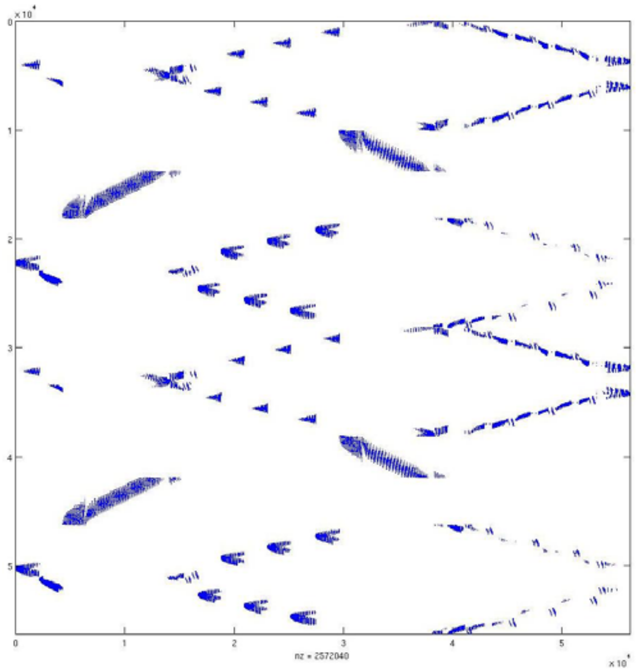
ILU Preconditioner: Matrix Permutation (real)

Background: Fill-in reduction for ILUT preconditioning

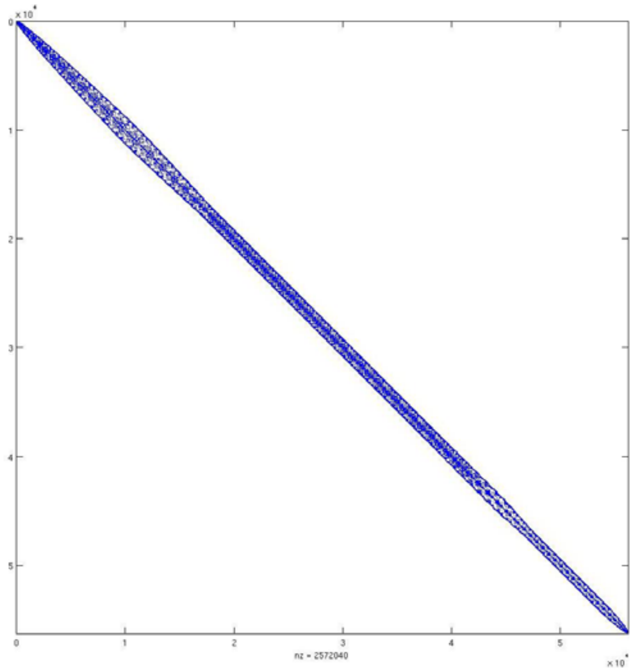
Original



Minimum Degree (MD)

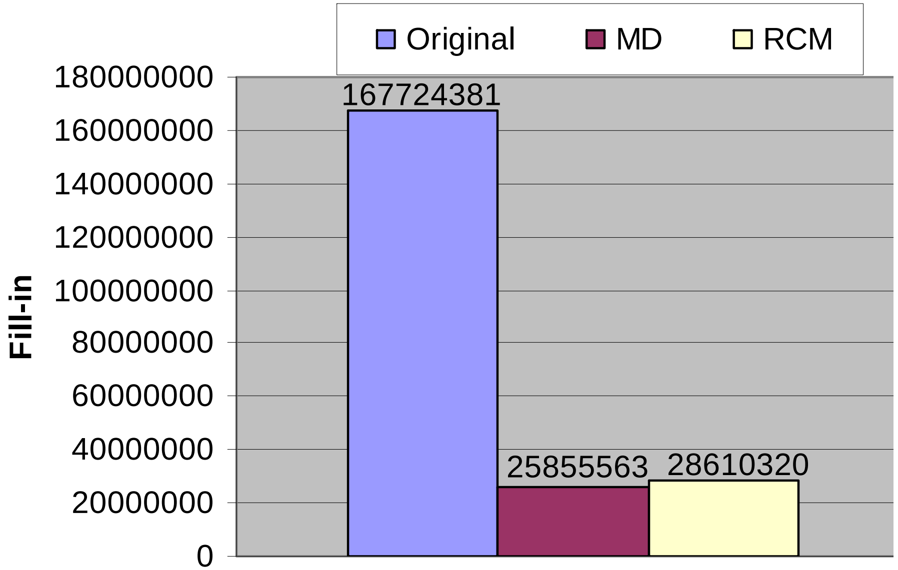


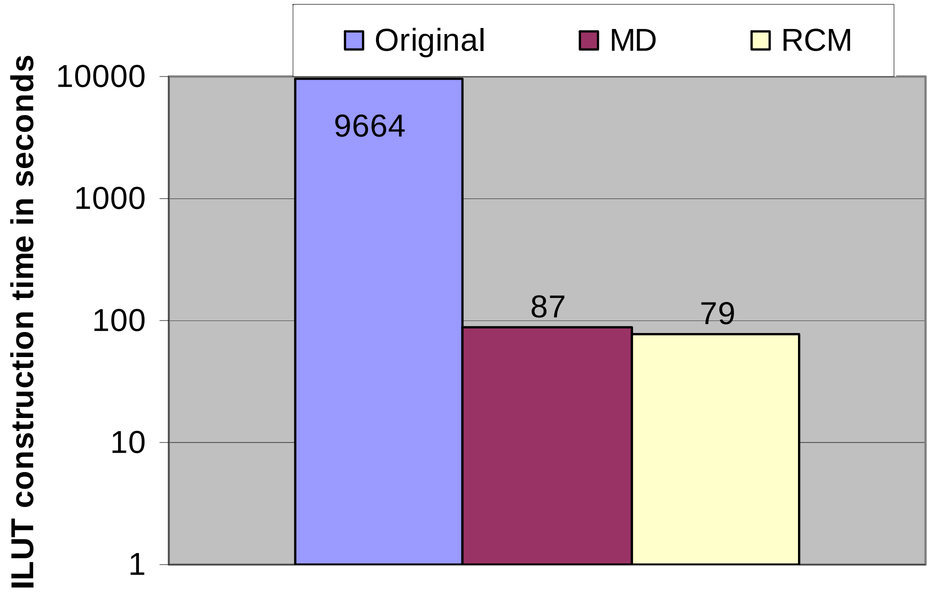
Reverse Cuthill-McKee (RCM)



ILU Preconditioner: Fill-in in *L* and *U* (real)

MATLAB: ILUT preconditioner; threshold = 10^{-3}

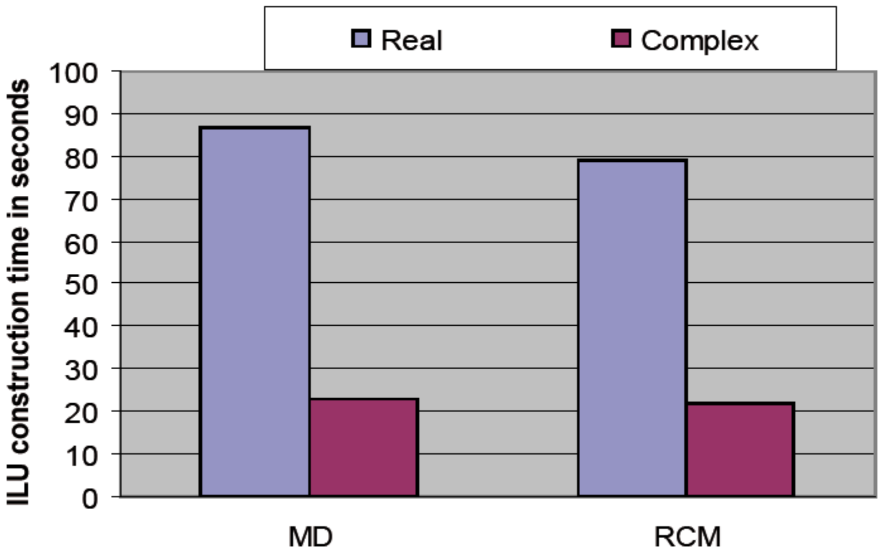


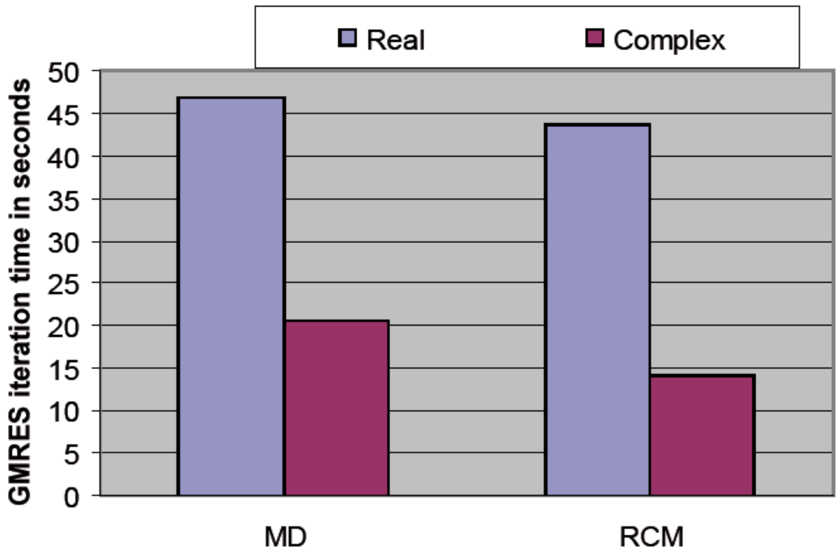


Performance: Complex or real Arithmetics?

MATLAB: ILUT preconditioning;

threshold = 10^{-3}; |rel. residual| < 10^{-10}

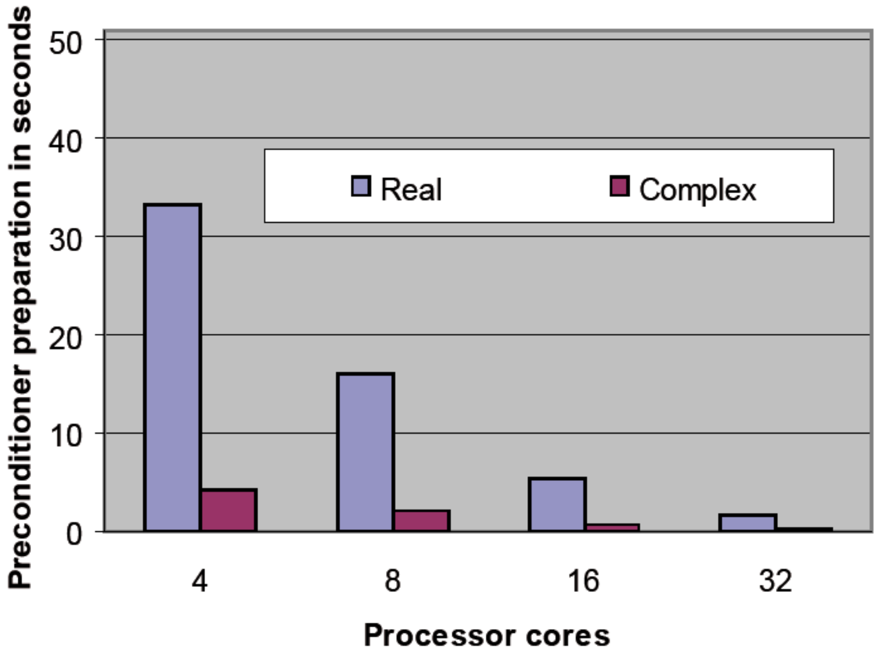


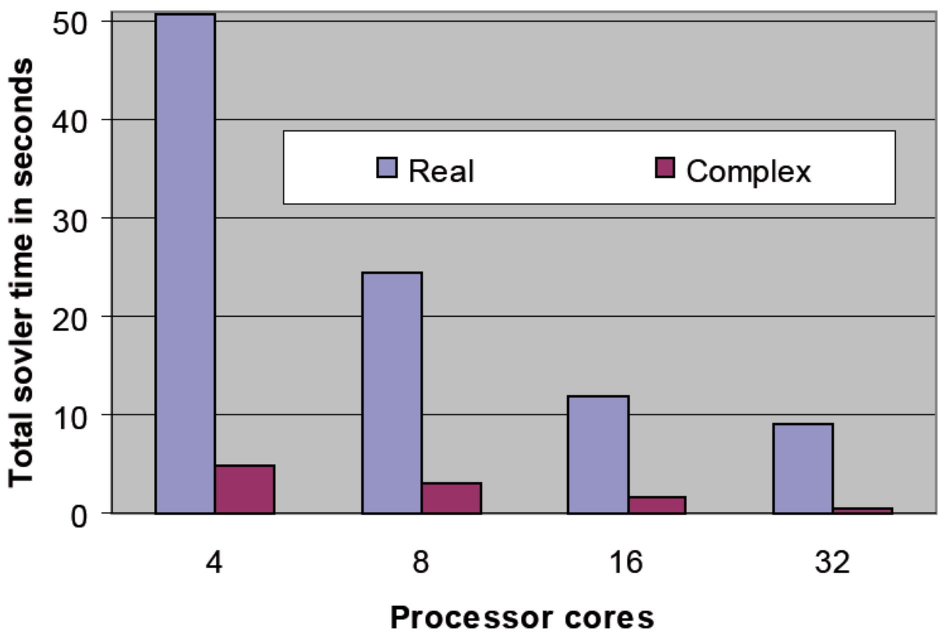


Performance on the AeroGrid Cluster of DLR

(Dual-processor nodes; Quad-Core Intel Harpertown; 2.83 GHz)

DSC method, real versus complex problem formulation

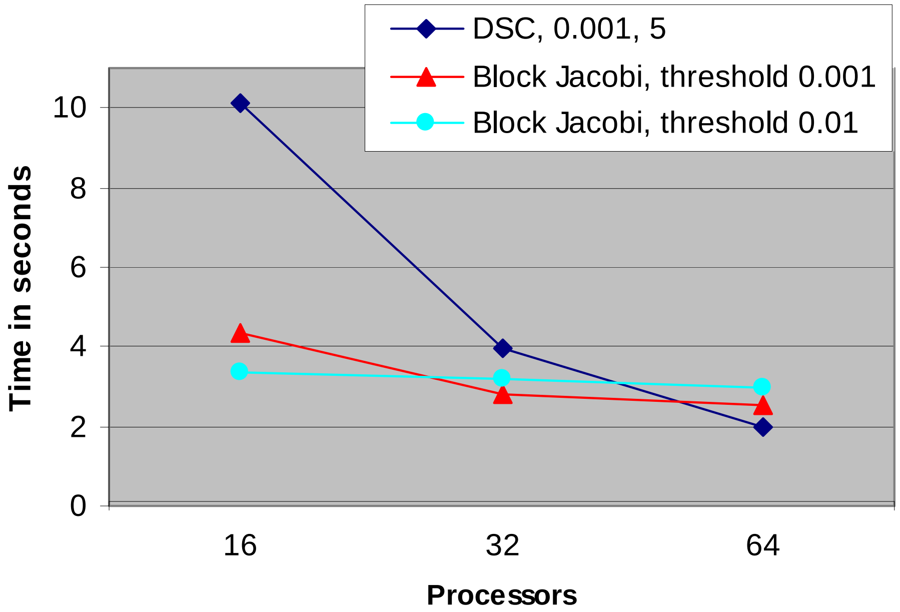


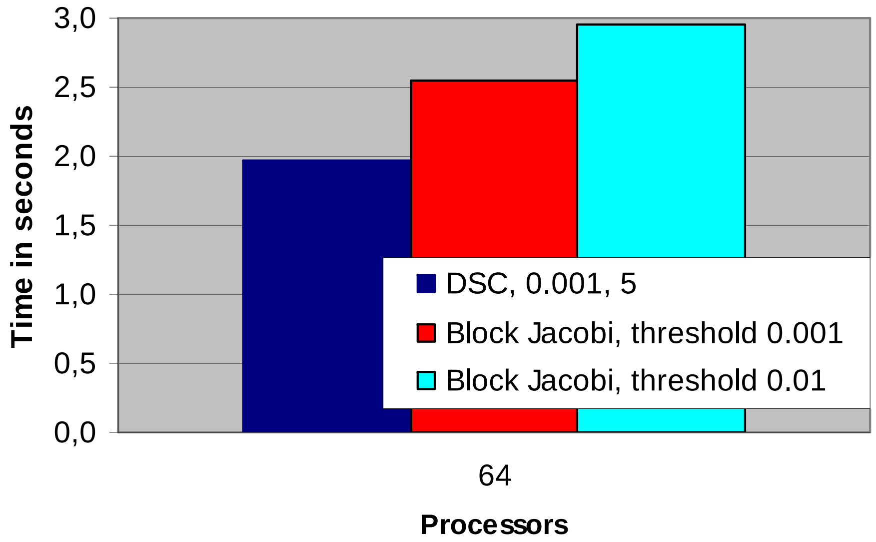


DSC Method: Performance (real)

(Dual-processor nodes; AMD Opteron 250; 2.4 GHz)

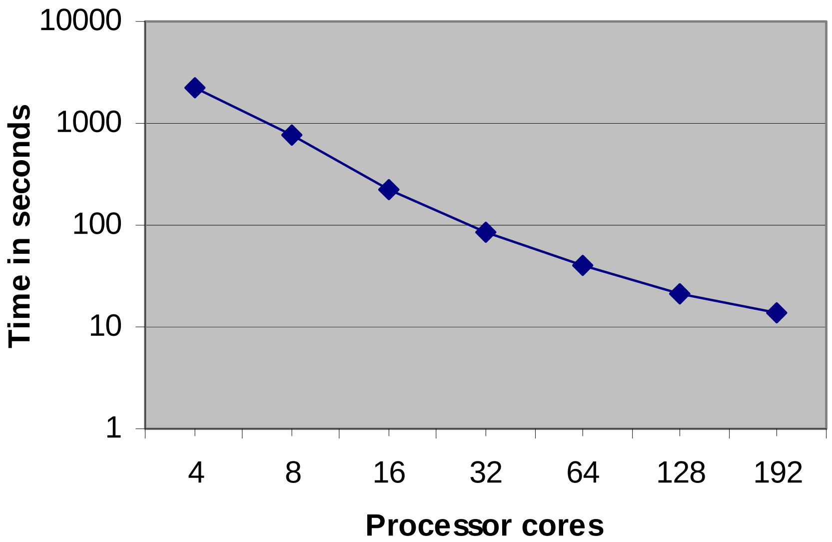
DSC method versus Block-Jacobi preconditioning (with RCM)



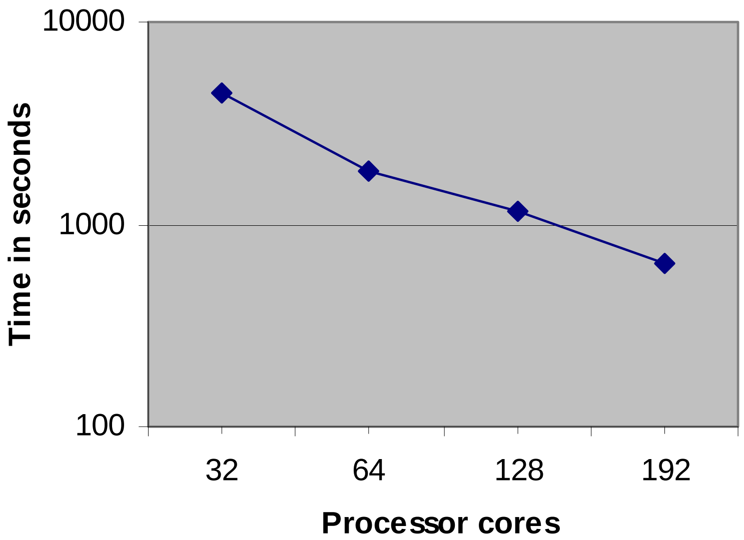


For a high processor count,
the DSC method appears to pay off.

DSC Method: Strong Scaling (complex)
(Dual-processor nodes; Quad-Core Intel Harpertown; 2.83 GHz)



TRACE matrix THD
(n=378,400; nz=45,456,500;
threshold = 10^{-3}; |rel. residual| < 10^{-5})



TRACE matrix UHBR
(n=4,497,520; nz=552,324,700;
threshold = 10^{-3}; |rel. residual| < 10^{-10})

Conclusions

- **Permutation (MD, RCM) crucial for ILUT performance; slight advantages for RCM (higher locality)**
- **Complex computations significantly faster than real ones (higher locality, better ratio of calculation to memory access)**
- **DSC method lets expect higher scalability than block-local methods.**
- **Future work**
  - **Development of an intelligent solver for TRACE with problem- and convergent-dependent parameter control and preconditioning**
  - **Application of the DSC method as robust smoother in Multigrid methods**

Questions?

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10 JAHRE DLR-PARABELFLÜGE