Master of Science on Computational Science

Institute of Computational Science

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The linear system

After discretization in space or space and time we end up with

$$A\,x = b, \quad \text{or in the time dependent case,}$$
$$A_n\,x_n = b_n$$

Solution techniques

- Direct sparse methods
- Iterative methods

Direct sparse solvers

Complexity in 2D

- $O(N^{1.5})$ factorization
- $O(N \log N)$ solution

Complexity in 3D

- $O(N^2)$ factorization
- $O(N^{1.5})$ solution

Available Software

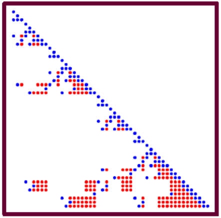
- PARDISO
- UMFPACK, CHOLMOD
- SUPERLU
- MUMPS

Efficient linear algebra

$$Ax = b \quad A \in R^{n\times n}$$

$$PQAP^T Px = PQb \quad A \in R^{n\times n}$$

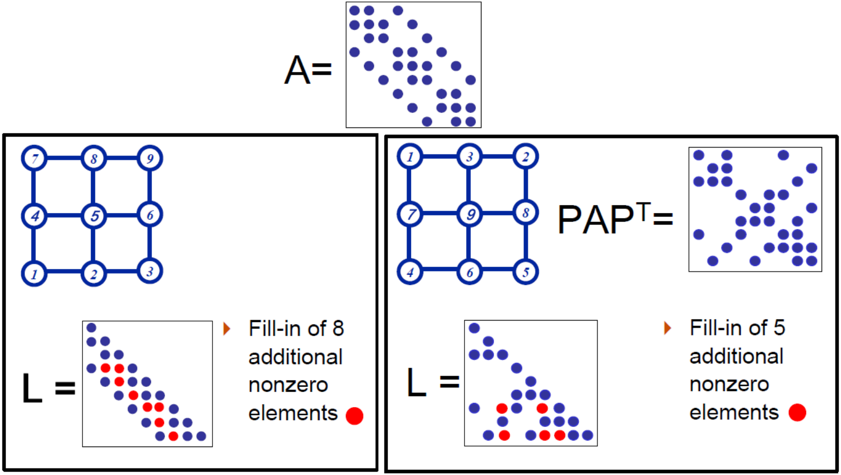
$$\begin{aligned} A &= LU \\ LUx &= b \\ Ly &= b \\ Ux &= y \end{aligned}$$



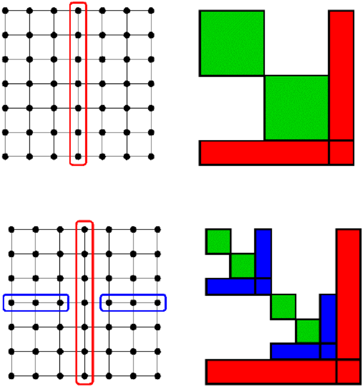
$$\begin{aligned} PQAP^T &= LU \\ LUPx &= PQb \\ Ly &= PQb \\ UPx &= y \end{aligned}$$

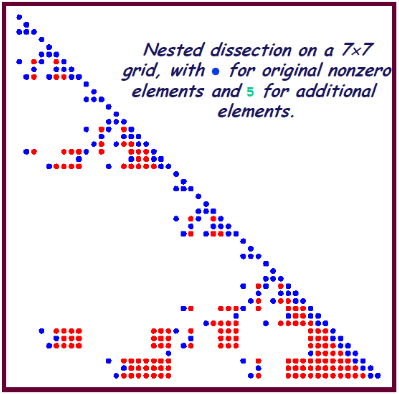
- Permutations P and Q chosen to preserve **sparsity** and **maintain stability** in $PAQ = LU$.
- L = Lower triangular, U = Upper triangular (**sparse**)

Nested dissection permutation P



Nested dissection ordering on a 7×7 grid





Direct Sparse Solvers

PARDISO performance in 2D

mesh	Elapsed time in seconds				memory
nodes	init	fact	back-sub	total	MB
65175	0.704	0.265	0.019	0.988	26.0
263838	3.199	1.539	0.111	4.849	117.5
1068112	14.766	9.518	0.535	24.819	527.7

PARDISO performance in 3D

mesh	Elapsed time in seconds				memory
nodes	init	fact	back-sub	total	MB
32002	0.636	2.783	0.069	3.488	80.4
256011	6.925	185.469	1.428	193.8	1438.3
2000396	76.625	11762.1	21.46	11860	24403.0

Iterative Krylov subspace methods

They work with matrix-vector products Ay for given vectors y

Symmetric systems

- **PCG**
- **MINRES**
- **SYMMLQ**
- **LSMR**
- **SQMR**

Nonsymmetric systems

- **GMRES**
- **CGS**
- **BICGSTAB**
- **QMR**
- **LSQR**

Preconditioners

$$A\,x = b$$

$$\text{left:} \quad P^{-1}A\,x = P^{-1}b$$

$$\text{right:} \quad AP^{-1}\,y = b, \quad P\,x = y$$

Iterative Krylov subspace methods

At each timestep of the simulation whether we solve linear or nonlinear PDEs we need to solve until convergence one or several linear systems:

At the nth timestep

$$A_n\, x_n = b_n$$

Left preconditioning

$$P_n^{-1}(A_n\, x_n) = P_n^{-1}\, b_n$$

High condition number

Lower condition number

Iterative Krylov subspace methods require only matrix-vector products Ay for given vectors y and depending on the type of the matrix we have

Symmetric matrices

- **PCG**
- **MINRES**

Nonsymmetric matrices

- **GMRES**
- **BICGSTAB**

Generalized minimum residual methods

GMRES(A,M,b,tol)

$x_0 = M^{-1}b,\ r_0 = b - Ax_0,$

$\beta = \|r_0\|_2\ u_1 = \dfrac{r_0}{\beta},\ k = 0$

while $\|r_k\|_2 > \beta\ tol$

$k = k + 1\ z_k = M^{-1}v_k,\ w = Az_k$

for $i = 1, 2, \ldots, k$ do

$h_{i,k} = u_i^T w,\ w = w - h_{i,k}u_i$

end for

$h_{k+1,k} = \|w\|_2,\ u_{k+1} = \dfrac{w}{h_{k+1,k}}$

$V_k = [u_1, \ldots, u_k]$

$H_k = \{h_{i,j}\},\ 1 \le i \le j + 1,\ 1 \le j \le k$

$y_k = \text{argmin}_y \|\beta e_1 - H_k\, y\|_2$

$x_k = x_0 + M^{-1}V_k\, y_k,\ r_k = b - A\, x_k$

end while

FGMRES(A,M,b,tol)

$x_0 = M_0^{-1}b,\ r_0 = b - Ax_0,$

$\beta = \|r_0\|_2\ u_1 = \dfrac{r_0}{\beta},\ k = 0$

while $\|r_k\|_2 > \beta\ tol$

$k = k + 1, z_k = M_k^{-1}v_k,\ w = Az_k$

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$h_{i,k} = u_i^T w,\ w = w - h_{i,k}u_i$

end for

$h_{k+1,k} = \|w\|_2,\ u_{k+1} = \dfrac{w}{h_{k+1,k}}$

$V_k = [u_1, \ldots, u_k],\ Z_k = [z_1, \ldots, z_k]$

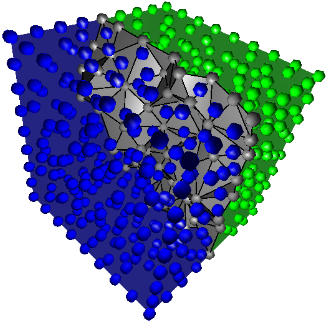
$H_k = \{h_{i,j}\},\ 1 \le i \le j + 1,\ 1 \le j \le k$

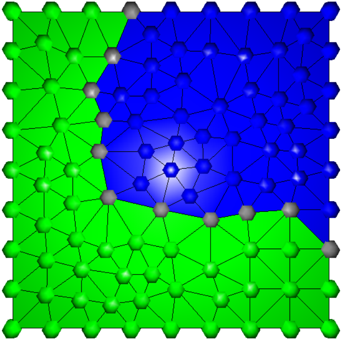
$y_k = \text{argmin}_y \|\beta e_1 - H_k\, y\|_2$

$x_k = x_0 + Z_k\, y_k,\ r_k = b - A\, x_k$

end while

Preconditioning methods: domain decomposition





$$\begin{pmatrix} A_{11} & 0 & A_{1B} \\ 0 & A_{22} & A_{2B} \\ A_{1B}^T & A_{2B}^T & A_{BB} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_B \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_B \end{pmatrix}$$

Preconditioning methods: multigrid

Multigrid methods

- **Geometric MG**
- **Algebraic MG**

Software

- **PETSc**
- **SAMG/XAMG**