

# 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

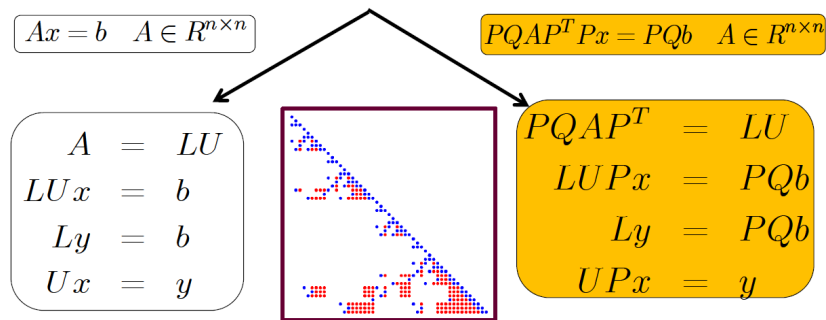
## Complexity in 3D

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

## Available Software

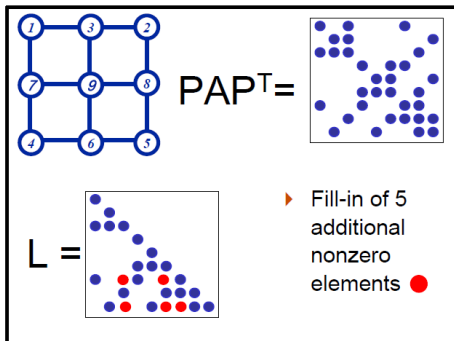
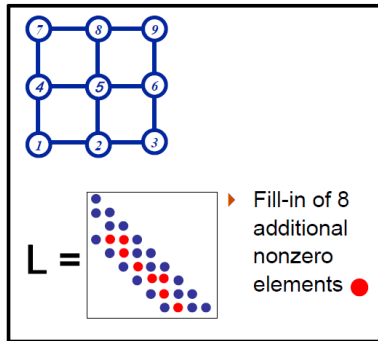
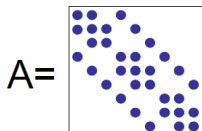
- PARDISO
- UMFPACK, CHOLMOD
- SUPERLU
- MUMPS

# Efficient linear algebra

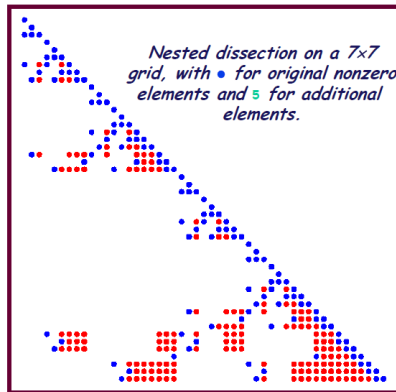
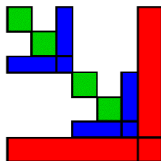
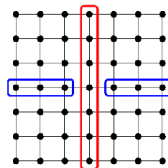
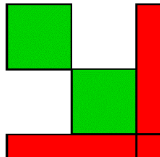
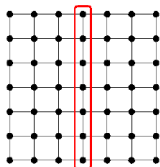


- Permutations  $P$  and  $Q$  chosen to preserve **sparsity** and **maintain stability** in  $PAQ = LU$ .
- $L$  = Lower triangular,  $U$  = Upper triangular (**sparse**)

# Nested dissection permutation $P$



# Nested dissection ordering on a $7 \times 7$ 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

$$A x = b$$

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

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



# 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  $n$ th 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)

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

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

while  $\|r_k\|_2 > \beta \text{ tol}$

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

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

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

end for

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

$$V_k = [v_1, \dots, v_k]$$

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

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

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

end while

## FGMRES(A,M,b,tol)

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

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

while  $\|r_k\|_2 > \beta \text{ tol}$

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

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

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

end for

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

$$V_k = [v_1, \dots, v_k], \quad Z_k = [z_1, \dots, z_k]$$

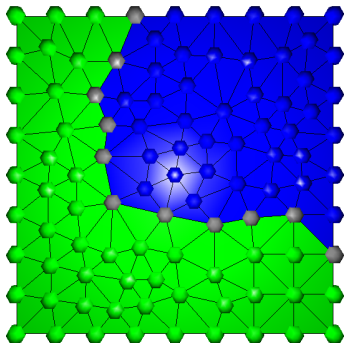
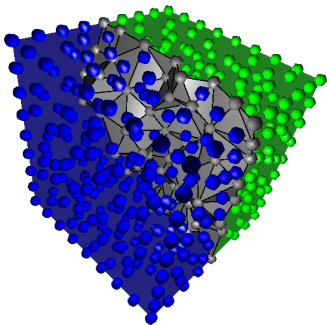
$$H_k = \{h_{i,j}\}, \quad 1 \leq i \leq j+1, \quad 1 \leq j \leq k$$

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

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

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**