Introduction to 3-D finite element computation

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Linear solvers for the system of the sparse matrix.

- linear equations
- direct method
  - LDL^T factorization
- iterative method
  - CG
  - Preconditioned CG
  - GMRES
- treatment of essential boundary conditions
  - Lagrange multiplier
  - orthogonal projection

Finite element equation (1/2)

bilinear form and functional:

$$a(u,v\,;\,\Omega) = 2\mu\int_\Omega \sum_{1\le i,j\le 3} [\epsilon(u)]_{i\,j}[\epsilon(v)]_{i\,j}\,dx + \lambda\int_\Omega \text{div}u\,\text{div}v\,dx,$$

$$l(v\,;\,\Omega) = \int_\Omega f\cdot v\,dx + \int_{\Gamma_N} h\cdot v\,ds$$

affine space and subspace:

$$V_h(g) := \{v_h \in Y_h\,;\,v_h(P_\alpha) = g(P_\alpha)\ \ \forall\alpha\in\Lambda_D\}$$

$$V_h := V_h(0) = \{v_h \in Y_h\,;\,v_h(P_\alpha) = 0\ \ \forall\alpha\in\Lambda_D\}$$

finite element equation:

Find $u_h \in V_h(g)$ such that

$$a(u_h, v_h) = l(v_h) \qquad \forall v_h \in V_h$$

Finite element equation (2/2)

stiffness matrix:

$$[A]_{\alpha\,\beta} = a(\varphi_\beta, \varphi_\alpha)$$

right-hand vector

$$[b]_\alpha = l(\varphi_\alpha) - \sum_{\beta \in \Lambda_D} a(\varphi_\beta, \varphi_\alpha) g_\beta \qquad (\,\alpha \in \Lambda_Y \setminus \Lambda_D\,)$$

$(N_Y - N_D) \times (N_Y - N_D)$ stiffness matrix: symmetric positive definite (SPD)

$$[A]_{\alpha\,\beta} = [A]_{\beta\,\alpha}, \qquad (Au, u) > 0 \quad (\,\forall u \in \mathbb{R}^{N_Y - N_D}\,).$$

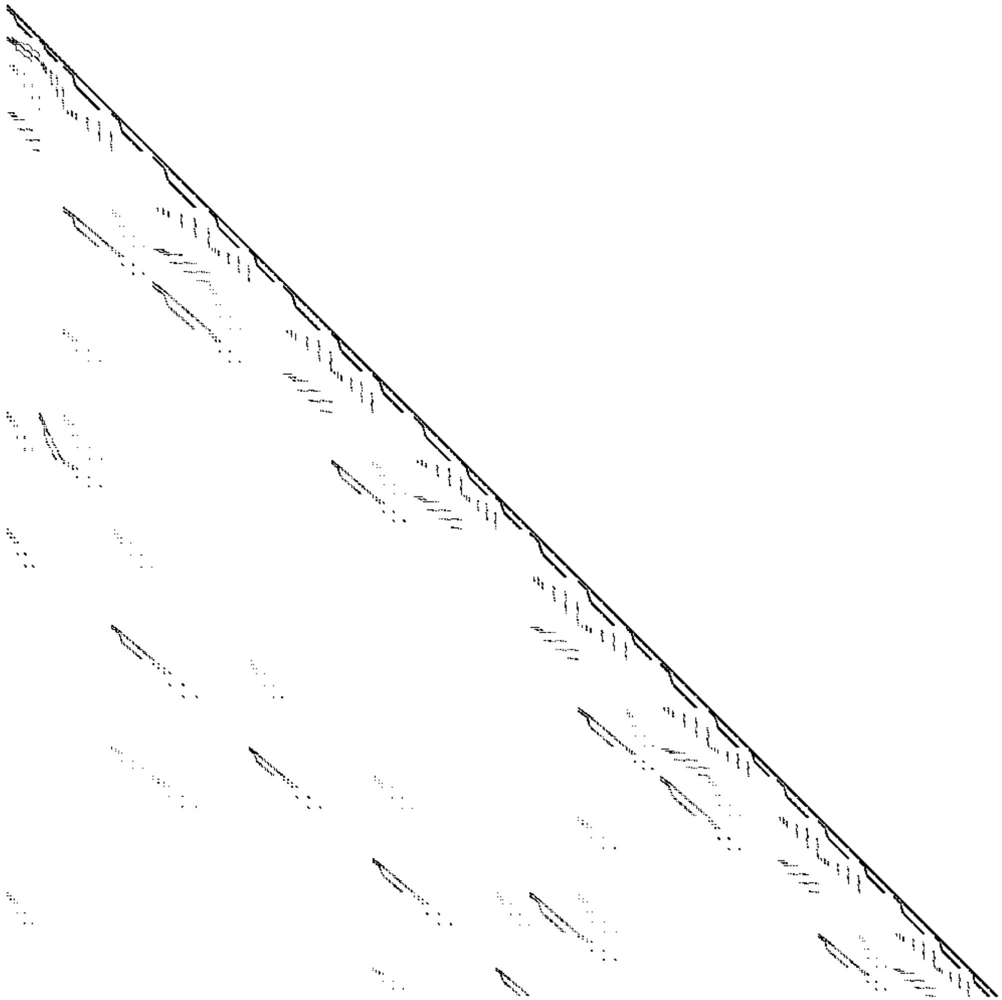
positive definiteness $\Leftarrow$ coercivity of $a(\cdot\,,\,\cdot)$

A : $N \times N$ SPD matrix

b : N vector

How to find $x \in \mathbb{R}^N$ satisfying $A\,x = b$?

lower triangle part of symmetric stiffness matrix



$N_G = 4,692$
$N_A = 34,126$ (nonzeros = nnz)
max of nonzeros in the row $= 20$.

Direct solver : LDL^T factorization (1/6)

A : $N \times N$ SPD matrix

$$A = L\,D\,L^T$$

L : lower triangular matrix, $[L]_{i\,j} = 0\ (i < j)$, $[L]_{i\,i} = 1$,

D : diagonal matrix,

the factorization in unique.

Direct solver : LDL^T factorization (2/6)

A : $N \times N$ SPD matrix

$$A = L\,D\,L^T$$

L : lower triangular matrix, $[L]_{i\,j} = 0\ (i < j)$, $[L]_{i\,i} = 1$,

D : diagonal matrix,

$A^{(k)}$: $k \times k$-sub matrix of A ,

$L^{(k-1)} \in \mathbb{R}^{(k-1)\times(k-1)}$:$(k-1) \times (k-1)$-sub matrix of L,

$l = [\,l_{k\,1}\ l_{k\,2}\ \ldots\ l_{k\,k-1}\,]^T \in \mathbb{R}^{(k-1)}$

$$A^{(k)} = \begin{bmatrix} L^{(k-1)} & 0 \\ l^T & 1 \end{bmatrix} \begin{bmatrix} D^{(k-1)} & 0 \\ 0 & d_{k\,k} \end{bmatrix} \begin{bmatrix} L^{(k-1)T} & l \\ 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} L^{(k-1)} D^{(k-1)} L^{(k-1)T} & L^{(k-1)} D^{(k-1)} l \\ l^T D^{(k-1)} L^{(k-1)T} & l^T D^{(k-1)} l + d_{k\,k} \end{bmatrix}$$

Direct solver : LDL^T factorization (3/6)

$$A^{(k)} = \begin{bmatrix} L^{(k-1)} & 0 \\ l^T & 1 \end{bmatrix} \begin{bmatrix} D^{(k-1)} & 0 \\ 0 & d_{k\,k} \end{bmatrix} \begin{bmatrix} L^{(k-1)T} & l \\ 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} L^{(k-1)} D^{(k-1)} L^{(k-1)T} & L^{(k-1)} D^{(k-1)} l \\ l^T D^{(k-1)} L^{(k-1)T} & l^T D^{(k-1)} l + d_{k\,k} \end{bmatrix}$$

find $\{l_{i\,j}\}_{1 \leq j < i \leq N}$ and $\{d_{k\,k}\}_{1 \leq k \leq N}$

$$\begin{bmatrix} a_{k\,1} \\ a_{k\,2} \\ \vdots \\ a_{k\,k-1} \end{bmatrix} = L^{(k-1)} D^{(k-1)} \begin{bmatrix} l_{k\,1} \\ l_{k\,2} \\ \vdots \\ l_{k\,k-1} \end{bmatrix}$$

$$a_{k\,k} = l^T D^{(k-1)} l + d_{k\,k}$$

Algorithm: LDL^T factorization

do $k = 1, 2, \ldots, N$

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

$$l_{k\,i} d_{i\,i} = a_{k\,i} - \sum_{j=1}^{i-1} l_{i\,j} d_{j\,j} l_{k\,j}$$

enddo

$$d_{k\,k} = a_{k\,k} - \sum_{j=1}^{k-1} l_{k\,j} d_{k\,k} l_{k\,j}$$

envelop method

Algorithm: LDL^T factorization

do $k = 1, 2, \ldots, N$

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

$$\lambda_{k\,i} = a_{k\,i} - \sum_{j=1}^{i-1} l_{i\,j} \lambda_{k\,j}$$

$$l_{k\,i} = \lambda_{k\,i} / d_{i\,i}$$

enddo

$$d_{k\,k} = a_{k\,k} - \sum_{j=1}^{k-1} l_{k\,j} \lambda_{k\,j}$$

Direct solver : LDL^T factorization (6/6)

To find x satisfying $L\,D\,L^T x = b$,

$$Ly = b$$

$$DL^T = y$$

are solved sequentially.

A : sparse $\Rightarrow$ $L\,D\,L^T$ factorization is only needed on some nonzero components.

fill-in : components with 0 become nonzeros during factorization

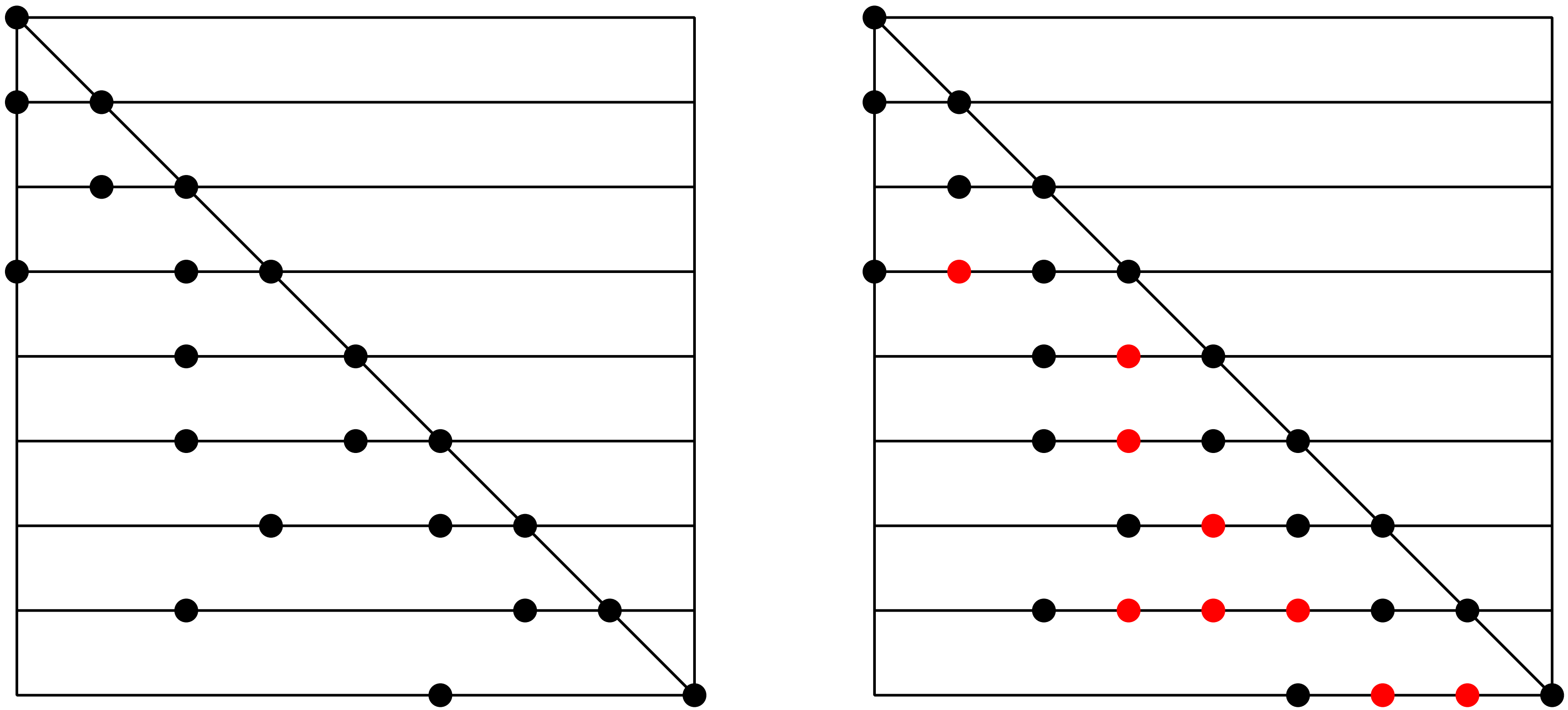
SKS (Skyline Storage) : factorization begins with the minimum column index of nonzero in a row

ordering : technique to reduce fill-in by renumbering of nodes

Skyline Storage (SKS) format

minimum column index of nonzero index on k-th row:

$$\beta(\mu) = \min\{\nu \in \{1, 2, \ldots, N\}\,;\, [\,A\,]_{\mu\,\nu} \neq 0\}$$



$$v_A^S \in \mathbb{R}^{N_A^{(S)}}, \;\beta \in \mathbb{R}^{N_G}, \quad N_A^{(S)} = \sum_{1 \leq \mu \leq N_G} (\mu - \beta[\mu] + 1)$$

$$v_A^S[k] = A_{\mu\,\nu}\,,\; \beta[\mu] \leq \nu \leq \mu\,,$$

$$\sum_{1 \leq \nu < \mu} (\nu - \beta[\nu] + 1) < k \leq \sum_{1 \leq \nu \leq \mu} (\nu - \beta[\nu] + 1)$$

minimum column index of nonzero index on k-th row:

$\beta(k) = \min\{\mu \in \{1, 2, \ldots, N\}\,;\, [\,A\,]_{k\,\mu} \neq 0\}$

Algorithm:

do $k = 1, 2, \ldots, N$

do $i = \beta(k), \ldots, k-1$

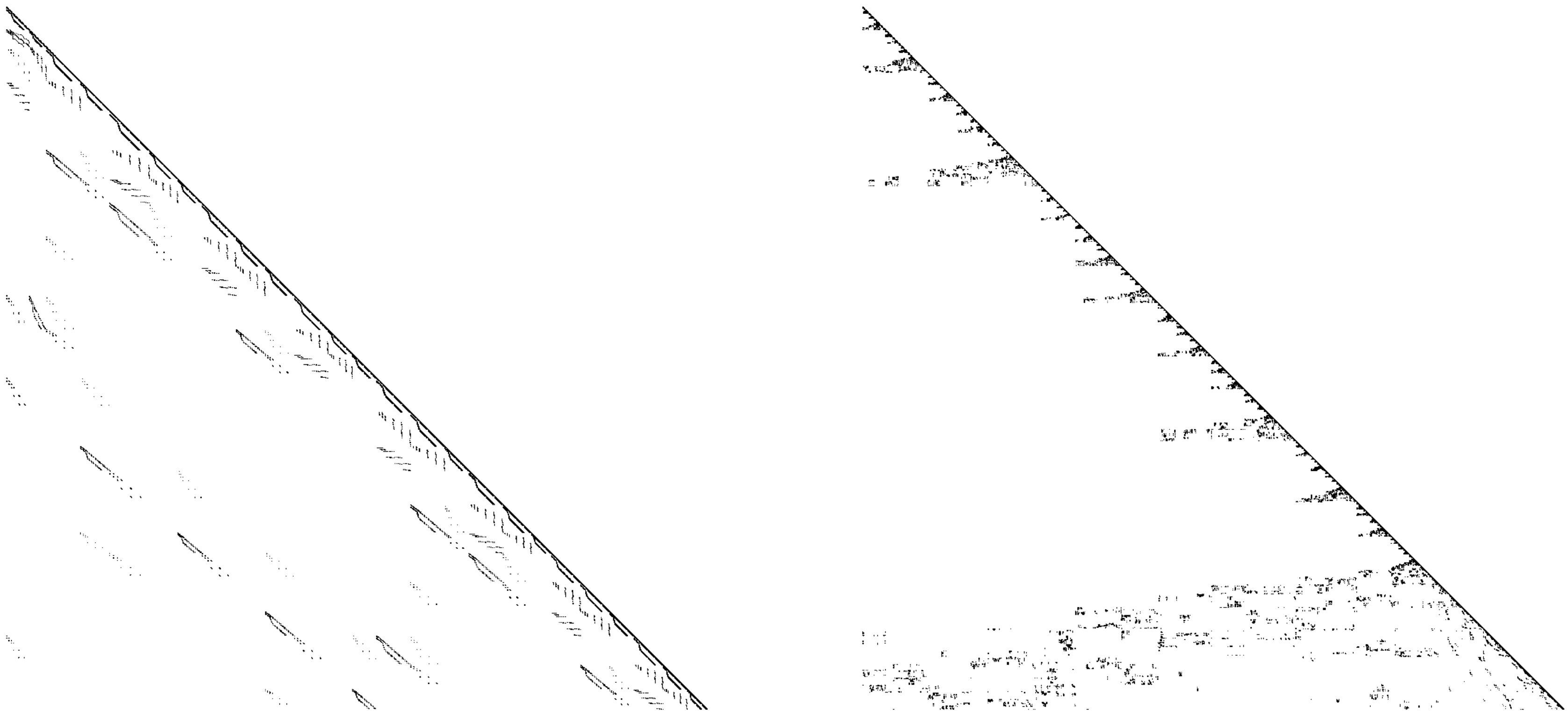
$$\lambda_{k\,i} = a_{k\,i} - \sum_{j=\max(\beta(k),\beta(i))}^{i-1} l_{i\,j}\lambda_{k\,j}$$

$$l_{k\,i} = \lambda_{k\,i}/d_{i\,i}$$

enddo

$$d_{k\,k} = a_{k\,k} - \sum_{j=\max(\beta(k),\beta(i))}^{i-1} l_{k\,j}\lambda_{k\,j}$$

lower triangle part of symmetric stiffness matrix



AMD : An approximate minimum degree ordering

$N_G = 4,692$
$N_A = 34,126$ (nonzeros $=$ nnz)

total memory for elasticity solver: 344.4M $\rightarrow$ 235.1M.

for unsymmetric matrix:

$$A^{(k)} = \begin{bmatrix} L^{(k-1)} & 0 \\ l^T & 1 \end{bmatrix} \begin{bmatrix} U^{(k-1)T} & u \\ 0 & d_{k\,k} \end{bmatrix}$$

$$= \begin{bmatrix} L^{(k-1)}U^{(k-1)T} & L^{(k-1)}u \\ l^T L^{(k-1)T} & l^T u + d_{k\,k} \end{bmatrix}$$

find $\{l_{i\,j}\}_{1\leq j<i\leq N}$, $\{u_{j\,i}\}_{1\leq j<i\leq N}$, and $\{d_{k\,k}\}_{1\leq k\leq N}$.

In envelope method l and u are stored with SKS format.

Stiffness matrix of finite element has symmetric pattern of nonzeros.

Direct solver for fast computation

– ordering : Reverse Cuthill-McKee, Minimum degree

– factorization :

UMFPACK T. Davis, 1997

SuperLU X. Li, 1999

PARDISO O. Schenk, 2000 $\in$ Intel compiler

– parallelization for SMP : SuperLU, PARDISO

large scale problem $\rightarrow$ Krylov subspace methods

$x_0 \;\longrightarrow\; x_1 \;\longrightarrow\; x_2 \;\longrightarrow \cdots \;\longrightarrow\; x_m \longrightarrow \cdots$ (iteratively)

Krylov subspace

$$K_n(A,\, r) := \text{span}[r, A\,r, A^2\,r, \ldots, A^{n-1}\,r]$$

dim$K_n(A,\, r) \leq N$, depends on $r \in \mathbb{R}^N$.

$$M = \min\{n\,;\; K_n(A,\, r) = K_{n+1}(A,\, r)\}$$

$$K_1(A,\, r) \subset K_2(A,\, r) \subset \cdots \subset K_M(A,\, r) = K_{M+1}(A,\, r) = \cdots$$

$x_0 \in \mathbb{R}^N$: initial guess, $r_0 = b - A\,x_0$: initial residual

CG method finds $u_n \in K_n(A, r_0)$ satisfying

$$(A\,(x_0 + u_n), y) = (b, y) \qquad \forall y \in K_n(A, r_0)\,.$$

A : SPD $\Rightarrow$ unique solution exists in each Krylov subspace

$$K_n(A, r_0) \;(1 \leq n \leq M).$$

Algorithm : CG method

$$x_0 \in \mathbb{R}^N \, ,$$

$$r_0 := b - Ax_0 \, ,$$

$$p_0 := r_0 \, ,$$

do $n = 0, 1, \ldots,$ until $||r_n||/||r_0|| < \varepsilon$

$$\alpha_n := (r_n,\, r_n)/(A\,p_n,\, p_n) \, ,$$

$$x_{n+1} := x_n + \alpha_n p_n \, ,$$

$$r_{n+1} := r_n - \alpha_n A p_n \, ,$$

$$\beta_n := (r_{n+1},\, r_{n+1})/(r_n,\, r_n) \, ,$$

$$p_{n+1} := r_{n+1} + \beta_n p_n \, .$$

$\varepsilon > 0$: stopping criteria

Iterative solver : CG method (3/3)

CG minimizes the functional $J(u) = \dfrac{1}{2}(A\,u,\ u) - (b,\ u)$ on $K_n(A, r_0) + x_0$.

the minimizer $x_n \in K_n(A, r_0) + x_0$:

$$J(x_n) \leq J(y) \qquad \forall y \in K_n(A, r_0) + x_0\ .$$

Iterative solver : preconditioned CG method (1/3)

Q : $N \times N$ SPD, $AQ \sim I$, $QA \sim I$

Krylov subspace

$$K_n(QA,\, Qr) := \text{span}[Qr, (QA)\, Qr, (QA)^2\, Qr, \ldots, (QA)^{n-1}\, Qr]$$

$x_0 \in \mathbb{R}^N$: initial guess, $r_0 = b - A\, x_0$: initial residual

Preconditioned CG method finds $u_n \in K_n(QA, Qr_0)$ satisfying

$$(A\,(x_0 + u_n), y) = (b, y) \qquad \forall y \in K_n(QA, Qr_0)$$

A, Q : SPD $\Rightarrow$ unique solution exists in each Krylov subspace

$$K_n(QA, Qr_0) \ (1 \leq n \leq M).$$

Algorithm : p-CG method

$$x_0 \in \mathbb{R}^N \,,$$

$$r_0 := b - Ax_0 \,,$$

$$p_0 := Qr_0 \,,$$

do $n = 0, 1, \ldots,$ until $||r_n||/||r_0|| < \varepsilon$

$$\alpha_n := (Qr_n,\, r_n)/(A\,p_n,\, p_n) \,,$$

$$x_{n+1} := x_n + \alpha_n p_n \,,$$

$$r_{n+1} := r_n - \alpha_n A p_n \,,$$

$$\beta_n := (Qr_{n+1},\, r_{n+1})/(Qr_n,\, r_n) \,,$$

$$p_{n+1} := Qr_{n+1} + \beta_n p_n \,.$$

Q : incomplete $L\,D\,L^T$ factorization ignoring fill-in.

Lemma:

for $1 \leq l \leq N_1(Q\mathcal{A}, Qr_0)$

(a) $(r_l, z) = 0 \quad \forall z \in K_l(Q\mathcal{A}, Qr_0)$,

(b) $(\mathcal{A}p_l, z) = 0 \quad \forall z \in K_l(Q\mathcal{A}, Qr_0)$,

(c) $\text{span}[Qr_0, Qr_1, ..., Qr_l] = \text{span}[p_0, p_1, ..., p_l] = K_{l+1}(Q\mathcal{A}, Qr_0)$.

proof $\leftarrow$ induction.

nonzero column index on k-th row:

$I(k) = \{\mu \in \{1, 2, \ldots, N\}\,;\, [\,A\,]_{k\,\mu} \neq 0\}$

Algorithm: incomplete LDL^T factorization

do $k = 1, 2, \ldots, N$

do $i \in I(k)$

$$\lambda_{k\,i} = a_{k\,i} - \sum_{j \in I(i) \cap I(k)} l_{i\,j} \lambda_{k\,j}$$

$$l_{k\,i} = \lambda_{k\,i} / d_{i\,i}$$

enddo

$$d_{k\,k} = a_{k\,k} - \sum_{j \in I(k)} l_{k\,j} \lambda_{k\,j}$$

Arnoldi method (1/2)

A : $N \times N$ matrix (general non-singular)

Arnoldi method + finding minimizer on Krylov subspaces

Algorithm : Arnoldi method

$$||v_1|| = 1$$

do $j = 1, 2, \dots, m$

do $i = 1, 2, \dots, j$

$$h_{i\,j} := (A\,v_j, v_i)$$

$$w_j := Av_j - \sum_{1 \le i \le j} h_{i\,j} v_i$$

$$h_{j+1\,j} := ||w_j||$$

$$v_{j+1} := w_j / h_{j+1\,j}\ .$$

generating orthonormal basis : $\{v_j\}$ in $K_n(A, v_1)$ by Gram-Schmidt method.

Arnoldi method (2/2)

$$[H_m]_{i\,j} := h_{i\,j}$$

$$\bar{H}_m := \begin{bmatrix} H_m \\ 0 \cdots 0 \; h_{m+1\,m} \end{bmatrix} \in \mathbb{R}^{(m+1)\times m}$$

$$V_m := [v_1, v_2, \ldots, v_m], \;\; V_{m+1} := [v_1, v_2, \ldots, v_m, v_{m+1}] .$$

$$V_m^T V_m = I_m,$$

$$A\,V_m = V_m H_m + w_m e_m^T = V_{m+1} \bar{H}_m,$$

$$V_{m+1}^T A\,V_m = \bar{H}_m .$$

$$V_{m+1}^T\, r_0 = \begin{bmatrix} (v_1, r_0) \\ (v_2, r_0) \\ \vdots \\ (v_{m+1}, r_0) \end{bmatrix} = \begin{bmatrix} \beta \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \beta\, e_1 . \quad (\beta = ||r_0||)$$

GMRES (General Minimum Residual) method

$r_0 = b - Ax_0$

Find $u \in K_m(A, r_0)$

$$||A(u + x_0) - b|| \leq ||A(v + x_0) - b|| \quad \forall v \in K_m(A, r_0)\,.$$

$u = V_m y$, $y \in \mathbb{R}^m$.

$$\begin{aligned} J(y) &:= ||AV_m y - r_0|| \\ &= ||V_{m+1}^T (AV_m y - r_0)|| \\ &= ||(V_{m+1}^T AV_m) y - (V_{m+1}^T r_0)|| \\ &= ||\bar{H}_m y - \beta e_1||\,. \qquad (\beta = ||r_0||) \end{aligned}$$

Find $y \in \mathbb{R}^m$

$$J(y) \leq J(z) \quad \forall z \in \mathbb{R}^m\,.$$

Full Orthogonalization Method (FOM)

$r_0 = b - Ax_0$

Find $u \in K_m(A, r_0)$

$$(A(u + x_0) - b, v) = (A\,u - r_0, v) = 0 \quad \forall v \in K_m(A, r_0)\,.$$

$u = V_m y$, $v = V_m z$, $(y, z \in \mathbb{R}^m)$.

$$\begin{aligned} 0 &= (A\,u - r_0, v) \\ &= (AV_m y - r_0, V_m z) \\ &= (V_m^T A V_m y - V_m^T r_0, z) \\ &= (H_m y - \beta e_1, z) \end{aligned}$$

Find $y \in \mathbb{R}^m$ s.t. $H_m y = \beta e_1$.

Remark

A : coercive ($(A\,v, v) > 0 \;\; \forall v \neq 0$) $\Rightarrow \exists H_m^{-1}$, otherwise $\Rightarrow$?

GMRES method (minimization problem)

Givens rotation matrices $\Omega_i \in \mathbb{R}^{(m+1)\times(m+1)}$

$$\Omega_i := \begin{bmatrix} I_{i-1} & & & \\ & c_i & s_i & \\ & -s_i & c_i & \\ & & & I_{m-i} \end{bmatrix}, \; c_1 := \frac{h_{1\,1}}{\sqrt{h_{1\,1}^2 + h_{2\,2}^2}}, \; s_1 := \frac{h_{2\,1}}{\sqrt{h_{1\,1}^2 + h_{2\,2}^2}}.$$

$Q_m := \Omega_m \Omega_{m-1} \cdots \Omega_1 \in \mathbb{R}^{(m+1)\times(m+1)}$,

$\bar{R}_m := Q_m \bar{H}_m$: upper triangular,

$\bar{g}_m := Q_m(\beta e_1) = [\,\gamma_1 \; \gamma_2 \; \cdots \; \gamma_{m+1}\,]^T$,

$$\bar{R}_m := \begin{bmatrix} R_m \\ 0 \; \cdots \; 0 \end{bmatrix} \; (R_m \in \mathbb{R}^{m\times m}), \; \bar{g}_m := \begin{bmatrix} g_m \\ \gamma_{m+1} \end{bmatrix} \; (g_m \in \mathbb{R}^m).$$

$\min ||\beta e_1 - \bar{H}_m y|| = \min ||\bar{g}_m - \bar{R}_m y|| = |\gamma_{m+1}| = |s_1 s_2 \cdots s_m| \beta$.

$y_m = R_m^{-1} g_m$ attains the minimum.

Remark : $\exists R_m^{-1}$ $(1 \le m \le M)$ for all non-singular matrix A .

FOM method using Givens rotation matrices

$Q_{m-1} := \Omega_{m-1}\Omega_{m-2}\cdots\Omega_1 \in \mathbb{R}^{m\times m}$,

$\tilde{R}_m := Q_{m-1}H_m$: upper triangular,

$\tilde{g}_m := Q_{m-1}(\beta e_1) = \bar{g}_{m-1} = [\,\gamma_1\ \gamma_2\ \ \cdots\ \ \gamma_m\,]^T$.

$$
\begin{aligned}
& H_m y = \beta e_1 \\
\Leftrightarrow\ \ & Q_{m-1}H_m y = Q_{m-1}\beta e_1 \\
\Leftrightarrow\ \ & \tilde{R}_m y = \tilde{g}_m\ .
\end{aligned}
$$

H_m : regular $\Leftrightarrow [\tilde{R}_m]_{k\,k} \neq 0 (1 \leq k \leq m) \Rightarrow y = \tilde{R}_m^{-1}\tilde{g}_m$.

Relation between GMRES and FOM in case of $\exists y_m^{\text{FOM}}$

$\rho_m^{\text{GMRES}} := ||b - Ax_m^{\text{GMRES}}|| = |\gamma_{m+1}|, \quad \rho_m^{\text{GMRES}} = |s_m|\rho_{m-1}^{\text{GMRES}}$.

$\rho_m^{\text{FOM}} := ||b - Ax_m^{\text{FOM}}|| = ||r_0 - AV_m y_m^{\text{FOM}}|| = h_{m+1\,m}|(e_m, y_m^{\text{FOM}})|$,

$\rho_m^{\text{FOM}} = h_{m+1\,m}\left|\frac{\gamma_m}{h_{m\,m}^{(m)}}\right| = \frac{h_{m+1\,m}}{|h_{m\,m}^{(m)}|}|\gamma_m| = \frac{|s_m|}{|c_m|}\rho_{m-1}^{\text{GMRES}} = \frac{1}{|c_m|}\rho_m^{\text{GMRES}}$.

Remark : $x_{m-1}^{\text{GMERS}} = x_m^{\text{GMERS}}$ (stagnation) $\Leftrightarrow H_m$ is singular.

Treatment of essential boundary conditions (1/3)

solution of homogeneous Dirichlet problem:

$u_h = \sum_{\beta\in\Lambda_Y} [\vec{u}]_\beta \varphi_\beta \in V_h \Leftrightarrow G\vec{u} = \vec{0}$.

matrix for the constraint: $G \in \mathbb{R}^{N_D\times N}$, $G^T = [\,\{\vec{e}_\beta\}_{\beta\in\Lambda_D}\,]$.

$\vec{V} := \{\vec{u}\in\mathbb{R}^N\,;\, G\vec{u}=\vec{0}\}$.

homogeneous Dirichlet problem:

Find $\vec{u}\in\vec{V}$ such that $(A\vec{u},\vec{v}) = (\vec{f},\vec{v})\ \ \forall\vec{v}\in\vec{V}$.

an alternative to solver with re-indexing unknowns:

Lagrange multiplier $\vec{\lambda}\in\mathbb{R}^{N_D}$:

$$\begin{bmatrix} A & G^T \\ G & 0 \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{\lambda} \end{bmatrix} = \begin{bmatrix} \vec{f} \\ \vec{0} \end{bmatrix} \quad .$$

matrix size is enlarged to $(N+N_D)\times(N+N_D)$.

$\begin{bmatrix} A & G^T \\ G & 0 \end{bmatrix}$ is regular. $\rightarrow$ factorization with pivoting.

solution of homogeneous Dirichlet problem:

$u_h = \sum_{\beta\in\Lambda_Y} [\vec{u}]_\beta \varphi_\beta \in V_h \Leftrightarrow G\vec{u} = \vec{0}$.

matrix for the constraint: $G \in \mathbb{R}^{N_D\times N}$, $G^T = [\,\{\vec{e}_\beta\}_{\beta\in\Lambda_D}\,]$.

$\vec{V} := \{\vec{u} \in \mathbb{R}^N \,;\, G\vec{u} = \vec{0}\}$.

homogeneous Dirichlet problem:

Find $\vec{u} \in \vec{V}$ such that $(A\vec{u}, \vec{v}) = (\vec{f}, \vec{v}) \;\; \forall \vec{v} \in \vec{V}$.

orthogonal projection: $P \,:\, \mathbb{R}^N \to \vec{V}$,

$P\vec{u} = \vec{u} - \sum_{\beta\in\Lambda_D} (\vec{u}, \vec{e}_\beta)\vec{e}_\beta$.

homogeneous Dirichlet problem:

Find $\vec{u} \in \vec{V}$ such that $PAP^T\vec{u} = P\vec{f}$.

precoditioned CG for the linear system with matrix PAP.

solution of inhomogeneous Dirichlet problem:

$u_h = \sum_{\beta\in\Lambda_Y} [\vec{u}]_\beta \varphi_\beta \in V_h(g) \Leftrightarrow G\vec{u} = \vec{g}$.

inhomogeneous Dirichlet problem:

Find $\vec{u} \in \vec{V}(g)$ such that $(A\vec{u}, \vec{v}) = (\vec{f}, \vec{v}) \;\; \forall \vec{v} \in \vec{V}$.

Lagrange multiplier $\vec{\lambda} \in \mathbb{R}^{N_D}$:

$$\begin{bmatrix} A & G^T \\ G & 0 \end{bmatrix} \begin{bmatrix} \vec{u} \\ \vec{\lambda} \end{bmatrix} = \begin{bmatrix} \vec{f} \\ \vec{g} \end{bmatrix} .$$

orthogonal projection: $P \, : \, \mathbb{R}^N \to \vec{V}$,

Find $\vec{u}_0 \in \vec{V}$ such that

$PAP(\vec{u}_0 + \vec{u}_g) = P\vec{f} \;\Leftrightarrow\; PAP\vec{u}_0 = P\vec{f} - PAP\vec{u}_g$,

where $\vec{u}_g$ satisfying $G\vec{u}_g = \vec{g}$, (e.g.,$[\vec{u}_g]_\beta = 0 \; (\, \beta \notin \Lambda_D \,)$)

$\mathcal{A}$, Q : symmetric, positive on $R(\mathcal{A}) = R(Q)$. $P : \mathbb{R}^N \to R(\mathcal{A})$.

Algorithm (p-CG with orthogonal projection):

$$x_0 \in R(\mathcal{A}) \,,$$

$$r_0 := P(b - \mathcal{A}x_0) \,,$$

$$p_0 := Qr_0 \,,$$

do $n = 0, 1, \ldots,$ until $||r_n|| < \varepsilon$

$$\alpha_n := (Qr_n, r_n)/(\mathcal{A}\, p_n, p_n) \,,$$

$$x_{n+1} := P(x_n + \alpha_n p_n) \,,$$

$$r_{n+1} := P(r_n - \alpha_n \mathcal{A} p_n) \,,$$

$$\beta_n := (Qr_{n+1}, r_{n+1})/(Qr_n, r_n) \,,$$

$$p_{n+1} := P(Qr_{n+1} + \beta_n p_n) \,,$$

enddo.

$Q = P\widetilde{\mathcal{A}}^{-1}P$, $\widetilde{\mathcal{A}}$: an incomplete LDL^T factorization.

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