Recall: Iterative solvers

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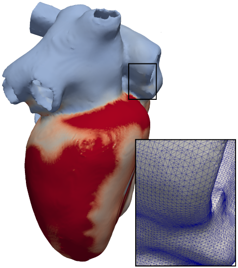
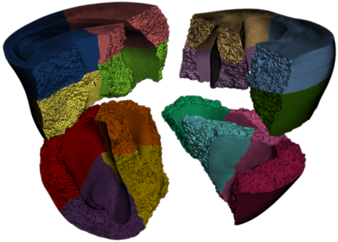
What we want to solve

We want to solve partial differential equations (PDEs)

- on parallel computers (distributed memory + shared memory)
- with $10^3 - 10^4$ CPU cores
- for $10^6 - 10^8$ discretization points.





Considered Problem Classes

$$\text{Find } u: \quad \begin{aligned} Lu(x) &= f(x) \quad \forall x \in \Omega \\ lu(x) &= g(x) \quad \forall x \in \partial\Omega \end{aligned}$$

variational $\Downarrow$ formulation

$$\text{Find} \quad u \in \mathbb{V}: \qquad a(u,v) = \langle F, v \rangle \qquad \forall v \in \mathbb{V}$$

FEM, FDM $\Downarrow$ FVM, FIT

$$\text{Solve} \qquad K_h \cdot \underline{u}_h = \underline{f}_h \qquad \underline{u}_h \in \mathbb{R}^{N_h}$$

With K_h

- symmetric, i.e., $K_h \equiv K_h^T$
- positive definite, i.e., $\langle K_h \underline{u}_h, \underline{u}_h \rangle > 0 \quad \forall \underline{u}_h \notin \ker(K_h)$

- (linear) 2[nd] order problem.
  - Poisson equation (temperature)
  - Lamé equation (deformation)
  - Maxwell's equations (magnetic field)
- Matrix K_h is sparse, positive definite (symmetric, large dimension)
- non-linear and time-dependent problems.

Richardson iteration to solve $Ku = f$

- Richardson iteration:

$$\underline{u}^{k+1} := \underline{u}^k + \tau \left(\underline{f} - K \cdot \underline{u}^k \right)$$

with $\tau_{opt} = \dfrac{2}{\lambda_{max}(K) + \lambda_{min}(K)}$.

- Preconditioned Richardson iteration:

$$\underline{u}^{k+1} := \underline{u}^k + C^{-1} \left(\underline{f} - K \cdot \underline{u}^k \right)$$

with $C \approx K$ and $C\underline{u} = \underline{f}$ can be faster solved than $K\underline{u} = \underline{f}$.

Choice $C := \frac{1}{\tau} I$ (scaled Identity) results in classical Richardson.

Richardson iteration: algorithm

Algorithm Preconditioned Richardson for $Ku = f$

Choose $u^0 = 0$; $k = 0$ ▷ initial guess
$s0 = \langle C^{-1} \cdot f, f \rangle$ ▷ initial error²
repeat
    $r := f - K \cdot u^k$ ▷ defect
    Solve $Cw = r$ ▷ correction
    $u^{k+1} := u^k + w$ ▷ update
until $\langle w, r \rangle > s0 \cdot \varepsilon^2$ ▷ relative accuracy

Basic operations:

- sparse matrix-vector product
- vector operations, inner product
- preconditioning system $Cw = r$

Jacobi iteration

Special Richardson iteration with preconditioner

$$C = \frac{1}{\omega} D$$

denoting $D := \text{diag}(K)$.

- Jacobi iteration (solver: $\omega := 1$):

$$\underline{u}^{k+1} \; := \; \underline{u}^{k} + \omega D^{-1} \left(\underline{f} - K \cdot \underline{u}^{k} \right)$$

- with the preconditioning step

$$w := \omega D^{-1} \cdot r$$

ILU iteration

Special Richardson iteration with preconditioner

$$C = L \cdot U \qquad \Longleftrightarrow \qquad L \cdot U \cdot w = r$$

resulting from an incomplete factorization $K = L \cdot U + R$, with a remainder R.

- ILU iteration:

$$\underline{u}^{k+1} := \underline{u}^k + U^{-1} L^{-1} \left(\underline{f} - K \cdot \underline{u}^k \right)$$

- with the preconditioning steps

$$\begin{aligned} \text{solve} \quad L \cdot v &= r \\ \text{solve} \quad U \cdot w &= v \end{aligned}$$

Preconditioned cg iteration to solve $Ku = f$

Choose $\underline{u}^0$

$$
\begin{aligned}
\underline{r} &:= \underline{f} - K \cdot \underline{u}^0 \\
\underline{w} &:= C^{-1} \cdot \underline{r} \\
\underline{s} &:= \underline{w} \\
\sigma &:= \sigma_{\text{old}} := \sigma_0 := (\underline{w}, \underline{r})
\end{aligned}
$$

repeat

$$
\begin{aligned}
\underline{v} &:= K \cdot \underline{s} \\
\alpha &:= \sigma / (\underline{s}, \underline{v}) \\
\underline{u} &:= \underline{u} + \alpha \cdot \underline{s} \\
\underline{r} &:= \underline{r} - \alpha \cdot \underline{v} \\
\underline{w} &:= C^{-1} \cdot \underline{r} \\
\sigma &:= (\underline{w}, \underline{r}) \\
\beta &:= \sigma / \sigma_{\mathrm{old}} \\
\sigma_{\mathrm{old}} &:= \sigma \\
\underline{s} &:= \underline{w} + \beta \cdot \underline{s}
\end{aligned}
$$

until $\sigma < \varepsilon^2 \cdot \sigma_0$

Preconditioning opportunities

Many opportunities for choosing C in $Cw = r \Longleftrightarrow w = C^{-1}r$

- $C = I$: no preconditioning, or scaled as $C = \frac{1}{\omega}I$
- $C = \frac{1}{\omega}D$: Jacobi preconditioning / diagonal scaling (one Jacobi iteration with initial guess $u^0 = 0$)
- $C = L \cdot U$: ILU-preconditioning
- Approximativ inverse as SPAI
- Additive/multiplicative Schwarz methods (ASM/MSM) incl.
  - Multilevel (ASM)
  - Multigrid (MSM)
  - Domain decomposition methods (DDM)
- Multigrid: $C^{-1} = (I_\ell - M_\ell)K^{-1}$ with

$$M_k = S_k^{post}\left(I_k - P_k(I_{k-1} - M_{k-1})K_{k-1}^{-1}R_kK_k\right)S_k^{pre}$$

or as two-grid: $M_1 = S_1^{post}\left(I_1 - P_1K_0^{-1}R_1K_1\right)S_1^{pre}$