



Finite Differences

$$\begin{aligned}
 u(w_i, t) &= (1 - \sigma) u_{i-1} + \sigma u_i & \partial_x u(w_i, t) &= (u_i - u_{i-1}) / h_{i-1} \quad (\text{west node}) \\
 u(e_i, t) &= (1 - \sigma) u_i + \sigma u_{i+1} & \partial_x u(e_i, t) &= (u_{i+1} - u_i) / h_i \quad (\text{east node}) \\
 \partial_x u(w_1, t) &= \partial_x u(0, t) & \partial_x u(e_1, t) &= (u_2 - u_1) / h_1 \quad (\text{node 1}) \\
 \partial_x u(w_N, t) &= (u_N - u_{N-1}) / h_{N-1} & \partial_x u(e_N, t) &= \partial_x u(L, t) \quad (\text{node } N) \\
 D(u(x_i, t)) &= D(u_i), D(u(w_i, t)) = \frac{D(u_{i-1}) + D(u_i)}{2}, D(u(e_i, t)) = \frac{D(u_i) + D(u_{i+1})}{2} \\
 \text{Flow left to right } (v > 0): \sigma &= 0. \text{ Flow right to left } (v < 0): \sigma = 1.
 \end{aligned}$$

Time Discretisation (integrate between t_n and t_{n+1})

$$(\mathbf{I} - \delta t \theta_1 \mathbf{A}) \mathbf{u}^{(n+1)} = [\mathbf{I} + \delta t (1 - \theta_1) \mathbf{A}] \mathbf{u}^{(n)} + \delta t [\mathbf{b}_1 + (1 - \theta_2) \mathbf{b}_2^{(n)} + \theta_2 \mathbf{b}_2^{(n+1)}]$$

$$\text{using } \int_{t_n}^{t_{n+1}} f(t) dt \approx \delta t [(1 - \theta) f(t_n) + \theta f(t_{n+1})], \tilde{\mathbf{A}} \mathbf{u}^{(n+1)} = \tilde{\mathbf{B}} \mathbf{u}^{(n)} + \tilde{\mathbf{c}} = \tilde{\mathbf{b}}$$

FE ($\theta_1 = \theta_2 = 0$), **BE** ($\theta_1 = \theta_2 = 1$), **C-N** ($\theta_1 = \theta_2 = \frac{1}{2}$). **Dirichlet BCs** replace row of $\tilde{\mathbf{A}}$ with \mathbf{e}_1 or $\mathbf{e}_N \in \mathbb{R}^{1 \times N}$ and row of $\tilde{\mathbf{b}}$ with Dirichlet BC.

Krylov Methods $\mathbf{K}_m(\mathbf{A}, \mathbf{b}) = \text{span}\{\mathbf{b}, \mathbf{A}\mathbf{b}, \mathbf{A}^2\mathbf{b}, \dots, \mathbf{A}^{m-1}\mathbf{b}\}$

Hessenberg factorisation: $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{H}$ for $\mathbf{Q}, \mathbf{H} \in \mathbb{R}^{n \times n}$. Reduced factorisation: $\mathbf{A}\mathbf{Q}_m = \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m$ for $\mathbf{Q}_m \in \mathbb{R}^{n \times m}$, $\bar{\mathbf{H}}_m \in \mathbb{R}^{(m+1) \times m}$.

$$\mathbf{q}_{j+1} = (\mathbf{A}\mathbf{q}_j - h_{1j}\mathbf{q}_1 - h_{2j}\mathbf{q}_2 - \dots - h_{jj}\mathbf{q}_j) / h_{j+1,j} = \frac{1}{h_{j+1,j}} \left(\mathbf{A}\mathbf{q}_j - \sum_{i=1}^j h_{ij}\mathbf{q}_i \right)$$

Arnoldi's method apply Gram-Schmidt process to $\mathcal{K}_m(\mathbf{A}, \mathbf{b})$.

$$\mathbf{q}_{j+1} = \frac{1}{\|\mathbf{v}_{j+1}\|} \left(\mathbf{A}\mathbf{q}_j - \sum_{i=1}^j (\mathbf{q}_i^\top \mathbf{A}\mathbf{q}_j) \mathbf{q}_i \right), \mathbf{A}\mathbf{q}_j = \sum_{i=1}^j (\mathbf{q}_i^\top \mathbf{A}\mathbf{q}_j) \mathbf{q}_i + \|\mathbf{v}_{j+1}\| \mathbf{q}_{j+1}$$

$$\bar{\mathbf{H}}_1 = \begin{bmatrix} \mathbf{q}_1^\top \mathbf{A}\mathbf{q}_1 \\ \|\mathbf{v}_2\| \end{bmatrix}, \bar{\mathbf{H}}_2 = \begin{bmatrix} \mathbf{q}_1^\top \mathbf{A}\mathbf{q}_1 & \mathbf{q}_2^\top \mathbf{A}\mathbf{q}_2 \\ \|\mathbf{v}_2\| & \|\mathbf{v}_3\| \end{bmatrix}, \dots, \bar{\mathbf{H}}_m = \begin{bmatrix} \mathbf{H}_m \\ h_{m+1,m} \mathbf{e}_m^\top \end{bmatrix}$$

Left-multiply $\bar{\mathbf{H}}_m$ by \mathbf{Q}_{m+1} to show $\mathbf{Q}_{m+1}\bar{\mathbf{H}}_m = \mathbf{Q}_m\mathbf{H}_m + h_{m+1,m}\mathbf{q}_{m+1}\mathbf{e}_m^\top$, where $\mathbf{H}_m \in \mathbb{R}^{m \times m}$. Left-multiply this result by \mathbf{Q}_m^\top to show $\mathbf{Q}_m^\top \mathbf{A}\mathbf{Q}_m = \mathbf{H}_m$.

Sparse Linear Systems

- Assume $\mathbf{x}^{(m)} \in \mathbf{x}^{(0)} + \mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$, for initial residual $\mathbf{r}^{(0)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} = \beta \mathbf{q}_1$ where \mathbf{q}_1 is taken from the Gram-Schmidt process and $\beta = \|\mathbf{r}^{(0)}\|$.
- Solution form: $\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{Q}_m \mathbf{y}_m$, solve \mathbf{y}_m using $\mathbf{r}^{(m)} = \mathbf{b} - \mathbf{A}\mathbf{x}^{(m)} \perp \mathcal{W}_m$.
- FOM: $\mathcal{W}_m = \mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$.
- GMRES: $\mathcal{W}_m = \mathbf{A}\mathcal{K}_m(\mathbf{A}, \mathbf{r}^{(0)})$.

Left preconditioning ($\mathbf{M}^{-1}\mathbf{A}\mathbf{x} = \mathbf{M}^{-1}\mathbf{b}$ where $\tilde{\mathbf{r}}^{(0)} = \mathbf{M}^{-1}\mathbf{r}^{(0)}$):

- Assume $\mathbf{x}^{(m)} \in \mathbf{x}^{(0)} + \mathcal{K}_m(\mathbf{M}^{-1}\mathbf{A}, \tilde{\mathbf{r}}^{(0)})$, with $\mathbf{q}_1 = \tilde{\mathbf{r}}^{(0)} / \beta$ for $\beta = \|\tilde{\mathbf{r}}^{(0)}\|$.
- Arnoldi decomposition: $(\mathbf{M}^{-1}\mathbf{A})\mathbf{Q}_m = \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m$.
- Solution form: $\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{Q}_m \mathbf{y}_m$, solve \mathbf{y}_m using $\tilde{\mathbf{r}}^{(m)} = \mathbf{M}^{-1}\mathbf{r}^{(m)} \perp \mathcal{W}_m$.
- FOM: $\mathcal{W}_m = \mathcal{K}_m(\mathbf{M}^{-1}\mathbf{A}, \tilde{\mathbf{r}}^{(0)})$.
- GMRES: $\mathcal{W}_m = (\mathbf{M}^{-1}\mathbf{A})\mathcal{K}_m(\mathbf{M}^{-1}\mathbf{A}, \tilde{\mathbf{r}}^{(0)})$.

Right preconditioning ($\mathbf{A}\mathbf{M}^{-1}\tilde{\mathbf{x}} = \mathbf{b}$ where $\mathbf{M}\tilde{\mathbf{x}} = \mathbf{x}$):

- Assume $\mathbf{x}^{(m)} \in \mathbf{x}^{(0)} + \mathbf{M}^{-1}\mathcal{K}_m(\mathbf{A}\mathbf{M}^{-1}, \mathbf{r}^{(0)})$.
- Arnoldi decomposition: $(\mathbf{A}\mathbf{M}^{-1})\mathbf{Q}_m = \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m$.
- Solution form: $\mathbf{x}^{(m)} = \mathbf{x}^{(0)} + \mathbf{M}^{-1}\mathbf{Q}_m \mathbf{y}_m$, solve \mathbf{y}_m using $\mathbf{r}^{(m)} \perp \mathcal{W}_m$.
- FOM: $\mathcal{W}_m = \mathcal{K}_m(\mathbf{A}\mathbf{M}^{-1}, \mathbf{r}^{(0)})$.
- GMRES: $\mathcal{W}_m = (\mathbf{A}\mathbf{M}^{-1})\mathcal{K}_m(\mathbf{A}\mathbf{M}^{-1}, \mathbf{r}^{(0)})$.

No/right preconditioning GMRES solution minimises $\|\mathbf{r}^{(m)}\|$ over the affine space:

$$\mathbf{y}_m = \arg \min_{\mathbf{y}} \|\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m \mathbf{y}\| \implies \mathbf{y}_m = \beta \bar{\mathbf{H}}_m^\dagger \mathbf{e}_1$$

Finite Volume Method

$$\frac{\partial u}{\partial t} + \underbrace{\nabla \cdot (\mathbf{v}u)}_{\text{advection}} = \underbrace{\nabla \cdot (\mathbf{D} \nabla u)}_{\text{diffusion}} + \underbrace{R}_{\text{reaction}}$$

$$\partial_t u = -\nabla \cdot \mathbf{q} + R, \mathbf{q} = \mathbf{v}u - \mathbf{D} \nabla u$$

$$\frac{du_i}{dt} \approx \frac{d\bar{u}_i}{dt} = \frac{1}{V_i} (q_{w_i} - q_{e_i}) + \bar{R}_i$$

$$\frac{d\mathbf{u}}{dt} = \mathbf{A}\mathbf{u} + \mathbf{b}(t) \text{ or } \mathbf{G}(t, \mathbf{u}(t))$$

Newton Methods ($\mathbf{u}^{(n+1)} := \mathbf{x}^{(k)}$)

$$\frac{d\mathbf{u}}{dt} = \mathbf{G}(\mathbf{u}) \implies \mathbf{F}(\mathbf{u}^{(n+1)}) = \mathbf{0}$$

$$\mathbf{F}(\mathbf{x}^{(k)}) + \mathbf{J}(\mathbf{x}^{(k)}) (\mathbf{x} - \mathbf{x}^{(k)}) = \mathbf{0}$$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - \mathbf{J}(\mathbf{x}^{(k)})^{-1} \mathbf{F}(\mathbf{x}^{(k)})$$

Newton (quad.): $m = 1$

Shamanskii (suplin.): m

Chord (lin.): $m = \infty$

Convergence Theory

$$\lim_{k \rightarrow \infty} \|\mathbf{x}^{(k)} - \mathbf{x}^*\| = 0 \implies \{\mathbf{x}^{(k)}\}_{k=0}^\infty \rightarrow \mathbf{x}^*$$

Cauchy if for all $\epsilon > 0$

$$\exists M : \|\mathbf{x}^{(k)} - \mathbf{x}^{(m)}\| < \epsilon : \forall k, m > M$$

Sequence converges ($\exists K > 0$):

$$\text{Quad. } \|\mathbf{x}^{(k+1)} - \mathbf{x}^*\| \leq K \|\mathbf{x}^{(k)} - \mathbf{x}^*\|^2$$

$$\text{Suplin. } \|\mathbf{x}^{(k+1)} - \mathbf{x}^*\| \leq K \|\mathbf{x}^{(k)} - \mathbf{x}^*\|^\alpha$$

Linear $\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\| \leq \alpha \|\mathbf{x}^{(k)} - \mathbf{x}^*\|$ order $\alpha \in (0, 1)$, factor $\sigma \in (0, 1)$, $k \gg 1$.

Lipschitz continuous $\mathbf{J} \in \text{Lip}_\gamma(D)$ if

$$\|\mathbf{J}(\mathbf{x}) - \mathbf{J}(\mathbf{y})\| \leq \gamma \|\mathbf{x} - \mathbf{y}\| : \forall \mathbf{x}, \mathbf{y} \in D$$

Useful Identities

$$\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|, \|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\|$$

$$\|\mathbf{A} + \mathbf{B}\| \leq \|\mathbf{A}\| + \|\mathbf{B}\|, \|\mathbf{A}\mathbf{x}\| \leq \|\mathbf{A}\| \|\mathbf{x}\|$$

$$\mathbf{x} = \int_0^1 \mathbf{x} dt$$

$$\left\| \int_a^b \mathbf{F}(t) dt \right\| \leq \int_a^b \|\mathbf{F}(t)\| dt.$$

$$\mathbf{F}(\mathbf{x} + \mathbf{h}) - \mathbf{F}(\mathbf{x}) = \int_0^1 \mathbf{J}(\mathbf{x} + t\mathbf{h}) \mathbf{h} dt$$

$$\int_a^b \frac{\partial}{\partial t} \mathbf{F}(t) dt = \mathbf{F}(b) - \mathbf{F}(a)$$

$$\frac{d}{dx} \left(\int_a^b f(x, t) dt \right) = \int_a^b \frac{\partial f(x, t)}{\partial x} dt$$

Inexact Newton Method ($\approx \text{quad.}$)

$$\tilde{\mathbf{J}}(\mathbf{x}) \mathbf{e}_j = (\mathbf{F}(\mathbf{x} + \varepsilon \mathbf{e}_j) - \mathbf{F}(\mathbf{x})) / \varepsilon$$

FOM Solution and Residual Norm Derivations

No preconditioning

$$\begin{aligned}
\mathbf{Q}_m^\top \mathbf{r}^{(m)} &= \mathbf{0} \\
\mathbf{Q}_m^\top (\mathbf{b} - \mathbf{A}\mathbf{x}^{(m)}) &= \mathbf{0} \\
\mathbf{Q}_m^\top (\mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{Q}_m\mathbf{y}_m) &= \mathbf{0} \\
\mathbf{Q}_m^\top (\mathbf{r}^{(0)} - \mathbf{A}\mathbf{Q}_m\mathbf{y}_m) &= \mathbf{0} \\
\mathbf{Q}_m^\top \mathbf{r}^{(0)} - (\mathbf{Q}_m^\top \mathbf{A}\mathbf{Q}_m) \mathbf{y}_m &= \mathbf{0} \\
\beta \mathbf{Q}_m^\top \mathbf{q}_1 - \mathbf{H}_m \mathbf{y}_m &= \mathbf{0} \\
\mathbf{H}_m \mathbf{y}_m &= \beta \mathbf{e}_1
\end{aligned}$$

$$\begin{aligned}
\|\mathbf{r}^{(m)}\| &= \|\mathbf{b} - \mathbf{A}\mathbf{x}^{(m)}\| \\
&= \|\mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{Q}_m\mathbf{y}_m\| \\
&= \|\mathbf{r}^{(0)} - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m\| \\
&= \|\mathbf{Q}_m\mathbf{Q}_m^\top \mathbf{r}^{(0)} - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m\| \\
&= \|\beta \mathbf{Q}_m\mathbf{Q}_m^\top \mathbf{q}_1 - (\mathbf{Q}_m\mathbf{H}_m + h_{m+1,m}\mathbf{q}_{m+1}\mathbf{e}_m^\top) \mathbf{y}_m\| \\
&= \|\beta \mathbf{Q}_m\mathbf{e}_1 - \mathbf{Q}_m\mathbf{H}_m\mathbf{y}_m - h_{m+1,m}\mathbf{q}_{m+1}\mathbf{e}_m^\top \mathbf{y}_m\| \\
&= \|\beta \mathbf{Q}_m\mathbf{e}_1 - \beta \mathbf{Q}_m\mathbf{H}_m\mathbf{H}_m^{-1}\mathbf{e}_1 - h_{m+1,m}\mathbf{q}_{m+1}\mathbf{e}_m^\top \mathbf{y}_m\| \\
&= h_{m+1,m}\|\mathbf{q}_{m+1}\mathbf{e}_m^\top \mathbf{y}_m\| = h_{m+1,m}|\mathbf{e}_m^\top \mathbf{y}_m|
\end{aligned}$$

Left preconditioning

Same solution \mathbf{y}_m , with appropriate substitutions.

$$\begin{aligned}
\|\mathbf{r}^{(m)}\| &= \|\mathbf{M}\tilde{\mathbf{r}}^{(m)}\| \\
&= \|\mathbf{M}\mathbf{M}^{-1}(\mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{Q}_m\mathbf{y}_m)\| \\
&= \|\mathbf{M}(\mathbf{M}^{-1}\mathbf{r}^{(0)} - (\mathbf{M}^{-1}\mathbf{A})\mathbf{Q}_m\mathbf{y}_m)\| \\
&= \|\mathbf{M}(\tilde{\mathbf{r}}^{(0)} - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m)\| \\
&= h_{m+1,m}\|\mathbf{M}\mathbf{q}_{m+1}\mathbf{e}_m^\top \mathbf{y}_m\|
\end{aligned}$$

Right preconditioning

Same solution \mathbf{y}_m and residual norm, with appropriate substitutions.

GMRES Solution and Residual Norm Derivations

No preconditioning

$$\begin{aligned}
(\mathbf{A}\mathbf{Q}_m)^\top \mathbf{r}^{(m)} &= \mathbf{0} \\
(\mathbf{A}\mathbf{Q}_m)^\top (\mathbf{b} - \mathbf{A}\mathbf{x}^{(m)}) &= \mathbf{0} \\
(\mathbf{A}\mathbf{Q}_m)^\top (\mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{Q}_m\mathbf{y}_m) &= \mathbf{0} \\
(\mathbf{Q}_{m+1}\bar{\mathbf{H}}_m)^\top (\mathbf{r}^{(0)} - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m) &= \mathbf{0} \\
\bar{\mathbf{H}}_m^\top \mathbf{Q}_{m+1}^\top (\beta \mathbf{q}_1 - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m) &= \mathbf{0} \\
\beta \bar{\mathbf{H}}_m^\top \mathbf{Q}_{m+1}^\top \mathbf{q}_1 - \bar{\mathbf{H}}_m^\top \bar{\mathbf{H}}_m\mathbf{y}_m &= \mathbf{0} \\
\bar{\mathbf{H}}_m^\top \bar{\mathbf{H}}_m\mathbf{y}_m &= \beta \bar{\mathbf{H}}_m^\top \mathbf{e}_1
\end{aligned}$$

$$\begin{aligned}
\|\mathbf{r}^{(m)}\| &= \|\mathbf{b} - \mathbf{A}\mathbf{x}^{(m)}\| \\
&= \|\mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{Q}_m\mathbf{y}_m\| \\
&= \|\mathbf{r}^{(0)} - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m\| \\
&= \|\mathbf{Q}_{m+1}\mathbf{Q}_{m+1}^\top \mathbf{r}^{(0)} - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m\| \\
&= \|\beta \mathbf{Q}_{m+1}\mathbf{Q}_{m+1}^\top \mathbf{q}_1 - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m\| \\
&= \|\beta \mathbf{Q}_{m+1}\mathbf{e}_1 - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m\| \\
&= \|\mathbf{Q}_{m+1}(\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y}_m)\| = \|\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y}_m\|
\end{aligned}$$

Left preconditioning

Same solution \mathbf{y}_m , with appropriate substitutions.

$$\begin{aligned}
\|\mathbf{r}^{(m)}\| &= \|\mathbf{M}\tilde{\mathbf{r}}^{(m)}\| \\
&= \|\mathbf{M}\mathbf{M}^{-1}(\mathbf{b} - \mathbf{A}(\mathbf{x}^{(0)} + \mathbf{Q}_m\mathbf{y}_m))\| \\
&= \|\mathbf{M}\mathbf{M}^{-1}(\mathbf{b} - \mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{Q}_m\mathbf{y}_m)\| \\
&= \|\mathbf{M}(\mathbf{M}^{-1}\mathbf{r}^{(0)} - (\mathbf{M}^{-1}\mathbf{A})\mathbf{Q}_m\mathbf{y}_m)\| \\
&= \|\mathbf{M}(\tilde{\mathbf{r}}^{(0)} - \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m\mathbf{y}_m)\| \\
&= \|\mathbf{M}\mathbf{Q}_{m+1}(\beta \mathbf{e}_1 - \bar{\mathbf{H}}_m\mathbf{y}_m)\|
\end{aligned}$$

Right preconditioning

Same solution \mathbf{y}_m and residual norm, with appropriate substitutions.