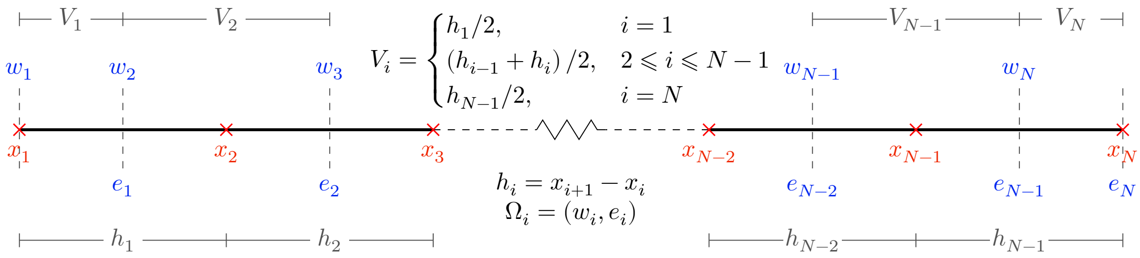

$$
\begin{aligned}
u(w_i,\, t) &= (1-\sigma)\, u_{i-1} + \sigma u_i & \partial_x u(w_i,\, t) &= (u_i - u_{i-1})/h_{i-1} & &\text{(west node)} \\
u(e_i,\, t) &= (1-\sigma)\, u_i + \sigma u_{i+1} & \partial_x u(e_i,\, t) &= (u_{i+1} - u_i)/h_i & &\text{(east node)} \\
\partial_x u(w_1,\, t) &= \partial_x u(0,\, t) & \partial_x u(e_1,\, t) &= (u_2 - u_1)/h_1 & &\text{(node 1)} \\
\partial_x u(w_N,\, t) &= (u_N - u_{N-1})/h_{N-1} & \partial_x u(e_N,\, t) &= \partial_x u(L,\, t) & &\text{(node } N\text{)}
\end{aligned}
$$

$D(u(x_i,\, t)) = D(u_i)$, $D(u(w_i,\, t)) = \frac{D(u_{i-1})+D(u_i)}{2}$, $D(u(e_i,\, t)) = \frac{D(u_i)+D(u_{i+1})}{2}$

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

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

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

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

$$\mathbf{K}_m(\mathbf{A},\, \mathbf{b}) = \operatorname{span}\left\{\mathbf{b},\ \mathbf{A}\mathbf{b},\ \mathbf{A}^2\mathbf{b},\ \ldots,\ \mathbf{A}^{m-1}\mathbf{b}\right\}$$

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 $\mathbf{Q}_m \in \mathbb{R}^{n\times m}$, $\bar{\mathbf{H}}_m \in \mathbb{R}^{m+1\times m}$. Rearrange for $\mathbf{q}_{j+1}$:

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

Arnoldi's method apply Gram-Schmidt process to $\mathcal{K}_m(\mathbf{A},\, \mathbf{b})$. For $\mathbf{q}_{j+1}$:

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

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

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 $\mathbf{x}^{(m)} \in \mathbf{x}^{(0)} + \mathcal{K}_m\left(\mathbf{A},\, \mathbf{r}^{(0)}\right)$, 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: $\mathcal{W}_m = \mathcal{K}_m\left(\mathbf{A},\, \mathbf{r}^{(0)}\right)$, **GMRES**: $\mathcal{W}_m = \mathbf{A}\mathcal{K}_m\left(\mathbf{A},\, \mathbf{r}^{(0)}\right)$.

Preconditioning (Jacobi: $\mathbf{D}$, Gauss-Seidel: $\mathbf{D} + \mathbf{L}$)

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

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

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

- $\mathbf{x}^{(m)} \in \mathbf{x}^{(0)} + \mathbf{M}^{-1}\mathcal{K}_m\left(\mathbf{A}\mathbf{M}^{-1},\, \mathbf{r}^{(0)}\right)$.
- Arnoldi method: $\left(\mathbf{A}\mathbf{M}^{-1}\right)\mathbf{Q}_m = \mathbf{Q}_{m+1}\bar{\mathbf{H}}_m$.
- 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: $\mathcal{W}_m = \mathcal{K}_m\left(\mathbf{A}\mathbf{M}^{-1},\, \mathbf{r}^{(0)}\right)$, GMRES: $\mathcal{W}_m = \left(\mathbf{A}\mathbf{M}^{-1}\right)\mathcal{K}_m\left(\mathbf{A}\mathbf{M}^{-1},\, \mathbf{r}^{(0)}\right)$.

Finite Volume Method

$$
\begin{aligned}
\frac{\partial u}{\partial t} &= -\boldsymbol{\nabla}\cdot\mathbf{q} + R,\ \mathbf{q} = \mathbf{v}u - \mathbf{D}\boldsymbol{\nabla}u \\
\frac{\mathrm{d}u_i}{\mathrm{d}t} &\approx \frac{\mathrm{d}\bar{u}_i}{\mathrm{d}t} = \frac{1}{V_i}\left(q_{w_i} - q_{e_i}\right) + \bar{R}_i \\
\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} &= \mathbf{A}\mathbf{u} + \mathbf{b}(t) \ \text{ or } \mathbf{G}(t,\, \mathbf{u}(t))
\end{aligned}
$$

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

$$
\begin{aligned}
\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathbf{G}(\mathbf{u}) &\implies \mathbf{F}\left(\mathbf{u}^{(n+1)}\right) = \mathbf{0} \\
\mathbf{F}\left(\mathbf{x}^{(k)}\right) + \mathbf{J}\left(\mathbf{x}^{(k)}\right)&\left(\mathbf{x} - \mathbf{x}^{(k)}\right) = \mathbf{0} \\
\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} &- \mathbf{J}\left(\mathbf{x}^{(k)}\right)^{-1}\mathbf{F}\left(\mathbf{x}^{(k)}\right)
\end{aligned}
$$

Newton method (quad.): update $\mathbf{J}$ every iteration
Chord (lin.): update $\mathbf{J}$ once
Shamanskii (suplin.): update $\mathbf{J}$ every m iterations

Convergence Theory

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

Cauchy if for all $\epsilon > 0$
$\exists M : \left\|\mathbf{x}^{(k)} - \mathbf{x}^{(m)}\right\| < \epsilon : \forall k, m > M$
Sequence converges ($\exists K > 0$):
Quad. $\left\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\right\| \leqslant K\left\|\mathbf{x}^{(k)} - \mathbf{x}^*\right\|^2$
Suplin. $\left\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\right\| \leqslant K\left\|\mathbf{x}^{(k)} - \mathbf{x}^*\right\|^\alpha$
Linear $\left\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\right\| \leqslant \alpha\left\|\mathbf{x}^{(k)} - \mathbf{x}^*\right\|$
order $\alpha \in (0, 1)$, factor $\sigma \in (0, 1)$, $k \gg 1$.
Lipschitz continuous $\mathbf{J} \in \operatorname{Lip}_\gamma(D)$ if
$\|\mathbf{J}(\mathbf{x}) - \mathbf{J}(\mathbf{y})\| \leqslant \gamma\|\mathbf{x} - \mathbf{y}\| : \forall \mathbf{x}, \mathbf{y} \in D$

Useful Identities

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

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

$$\mathbf{x} = \int_0^1 \mathbf{x}\, \mathrm{d}t$$

$$\left\|\int_a^b \mathbf{F}(t)\, \mathrm{d}t\right\| \leqslant \int_a^b \|\mathbf{F}(t)\|\, \mathrm{d}t.$$

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

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

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

Inexact Newton Method (≈quad.)

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