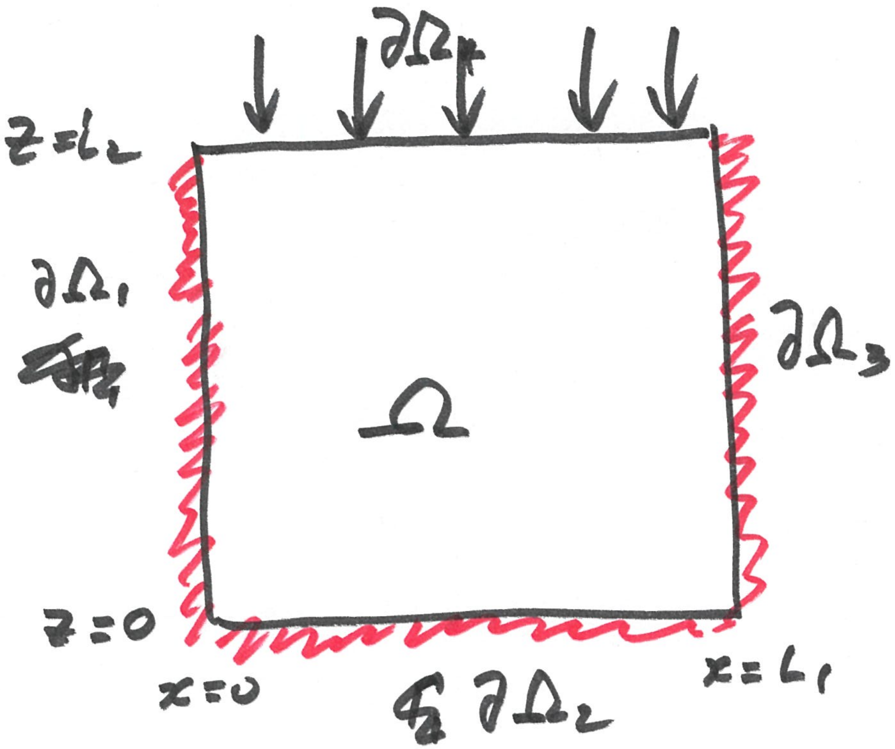


Model Verification

$$\frac{\partial \psi}{\partial t} + \underline{\nabla} \cdot \underline{q} = 0$$

on $\partial\Omega_{1,2,3}$ $\quad \underline{q} \cdot \underline{n} = 0$

on $\partial\Omega_4$ $\quad \underline{q} \cdot \underline{n} = r$

$$\int_0^{L_1}\int_0^{L_2} \frac{\partial \psi}{\partial t}\, dx\, dz + \int_0^{L_1}\int_0^{L_2} \underline{\nabla} \cdot \underline{q}\, dx\, dz = 0$$

Define $\overline{\psi(t)} = \frac{1}{L_1 L_2} \int_0^{L_1}\int_0^{L_2} \psi\, dx\, dz.$

$$\cancel{L_1 L_2} \frac{d\overline{\Psi}}{dt} + \frac{1}{L_1 L_2} \sum_{j=1}^{4} \int_{\Gamma_j} \underline{q} \cdot \underline{\hat{n}}\, d\sigma = 0.$$

TIME STEP ADAPTATION :

Initial Assumption
$\delta t = 0.1$ day.

time step process

Newton Solver

- · tolerance (Tabs, Trel)
- 10 (15) · max iterations
- · λmin .

GMRES

If we converge Newton < "5" iterations for "10" successive time steps $\delta t = \delta t \times \cancel{1.1}$ 1.2

If Newton fails

If Newton converges "well" .

$\delta t = \delta t / 2$

CHECK : MAKE SURE ALL UNITS ARE CONSISTENT.

differential equation
$$\begin{cases} \dfrac{d\overline{\Psi}}{dt} + \dfrac{1}{\cancel{L_1} L_2} r \cancel{L_1} = 0 & (r<0). \\ \overline{\Psi}(0) = \overline{\Psi}_0 . \end{cases}$$

$\sim$ constant.

$$\frac{d\overline{\Psi}}{dt} = -\frac{r}{L_2}$$

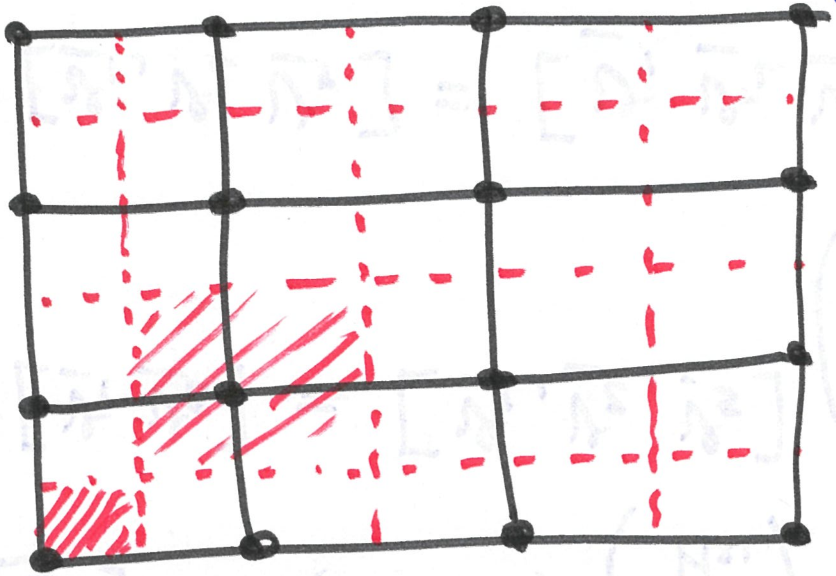
Integration gives

$$\overline{\Psi}(t) = At + c \quad , \quad A = -\frac{r}{L_2}$$

using the I.C. we have

$$\overline{\Psi}(t) = At + \overline{\Psi}_0 .$$

$$\overline{\psi}(t) = \frac{1}{L_1 L_2} \int_0^{L_1}\int_0^{L_2} \psi(x,z,t)\, dx\, dz \simeq \frac{1}{L_1 L_2} \sum_{i=1}^{N} \Delta V_i\, \psi_i .$$



$$\underbrace{J(\underline{x}^{(k)})\,\underline{\delta x}^{(k)} = -\underline{F}(x^{(k)})}.$$

Krylov subspace Method.

$$A\underline{x} = \underline{b} \qquad \underline{A} \in R^{n\times n} \quad \left(\begin{matrix}\text{large,}\\ \text{sparse}\end{matrix}\right).$$

$\underline{x}^{(0)}$ good estimate of solution,

Q: How can we obtain a good approximate solution of the linear system.

× characteristic polynomial.

$$c(A) = \underline{0}_{n\times n} \leftarrow \text{Cayley \& Hamilton}$$

$$p(A) =: A^{-1}, \quad A^{-1} = c_0 I + c_1 A + \cdots + c_{n-1} A^{n-1}$$

$$\underline{x} = A^{-1}\underline{b} = c_0\underline{b} + c_1 A\underline{b} + \cdots + c_{n-1} A^{n-1}\underline{b}$$

$\underline{x} \in \mathrm{span}\{\underline{b}, A\underline{b}, \ldots, A^{m-1}\underline{b}\}$

$K(\cancel{\underline{b}}, A, \underline{b}) \leftarrow$ Krylov subspace.

$c(t) = \det(tI - A)$.

$= \prod_{i=1}^{n} (t - \lambda_i)$

Projection Methods:

- **Search space**

$\underline{x}_m \in \underline{x}^{(0)} + K_m(A, \overset{\underline{r}^{(0)}}{\cancel{\underline{b}}})$.

- **Constraint space**.

$\underline{r}_m = b - A\underline{x}_m \perp AK_m(A, \underline{r}^{(0)})$.

$K_m(A, \underline{r}^{(0)}) = \mathrm{span}\{\underline{r}^{(0)}, A\underline{r}^{(0)}, \ldots, A^{m-1}\underline{r}^{(0)}\}$

$AK_m(A, \underline{r}^{(0)}) = \mathrm{span}\{A\underline{r}^{(0)}, A^2\underline{r}^{(0)}, \ldots, A^m\underline{r}^{(0)}\}$.

$\underline{x}_m = \underline{x}^{(0)} + V_m \underline{y}_m$? ; $V_m = [\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_m]$

where $\underline{v}_i$'s form a basis for the Krylov subspace :

$\underline{v}_1 = \dfrac{\underline{r}^{(0)}}{\beta_0}$, $\beta_0 = \|\underline{r}^{(0)}\|$

$$K_m(A, \underline{r}^{(0)}) = \text{span}\{\underline{r}^{(0)}, A\underline{r}^{(0)}, \ldots, A^{m-1}\underline{r}^{(0)}\}$$

(ARNOLDI'S method) $= \text{span}\{\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_m\}$

ARNOLDI'S RELATION

$$\boxed{A V_m = V_{m+1} \bar{H}_m}$$

$V_{m+1} \underline{e}_1 = \underline{v}_1 = \dfrac{\underline{r}^{(0)}}{\beta_0}$

$\therefore \underline{r}^{(0)} = \beta_0 V_{m+1} \underline{e}_1$

Residual:

$$\begin{aligned} \underline{r}_m &= \underline{b} - A\underline{x}_m \\ &= \underline{b} - A(\underline{x}^{(0)} + V_m \underline{y}_m) \\ &= \underline{r}^{(0)} - A V_m \underline{y}_m = \underline{r}^{(0)} - V_{m+1} \bar{H}_m \underline{y}_m . \\ &= \beta_0 V_{m+1} \underline{e}_1 - V_{m+1} \bar{H}_m \underline{y}_m . \end{aligned}$$

Arnoldi's Method

- This means that $\mathbf{V}_m^T\mathbf{V}_m = \mathbf{I}_m$ and $\mathbf{V}_{m+1}^T\mathbf{V}_{m+1} = \mathbf{I}_{m+1}$, where $\mathbf{I}$ is the identity matrix. Note also that $\mathbf{V}_m^T\mathbf{A}\mathbf{V}_m = \mathbf{H}_m$.
- The rectangular matrix $\overline{\mathbf{H}}_m \in \mathbb{R}^{(m+1)\times m}$ is an upper Hessenberg matrix:

$$\overline{\mathbf{H}}_m = \begin{array}{c} H_m \\ \left[\begin{array}{ccccc} h_{1,1} & h_{1,2} & \cdots & h_{1,m-1} & h_{1,m} \\ h_{2,1} & h_{2,2} & \cdots & h_{2,m-1} & h_{2,m} \\ & h_{3,2} & \cdots & h_{3,m-1} & h_{3,m} \\ & & \ddots & \vdots & \vdots \\ & & & h_{m,m-1} & h_{m,m} \\ 0 & 0 & \cdot & - \; 0 & h_{m+1,m} \end{array}\right] \\ \longleftarrow m \text{ columns.} \longrightarrow \end{array} \begin{array}{l} m+1 \\ \text{rows} \\ \\ h_{m+1,m}\,\underline{e}_m^T. \end{array}$$

$$\underline{r}_m = V_{m+1}\left\{\beta_0 \underline{e}_1 - \overline{H}_m \underline{y}_m\right\}$$ — what is this vector?

$$V_{m+1} = \left[\underline{v}_1, \underline{v}_2, \ldots, \underline{v}_m, \underline{v}_{m+1}\right].$$

<u>Constraint</u> : $\underline{r}_m \perp AK_m$

$\therefore$ $\underline{r}_m$ must be orthogonal to all basis vectors for AK_m.

i.e., $\underline{r}_m^T (AV_m) = \underline{0}$ X.

$$\left[V_{m+1}\left\{\beta_0 \underline{e}_1 - \overline{H}_m \underline{y}_m\right\}\right]^T \left(V_{m+1}\overline{H}_m\right) = 0$$

or $$\left\{\beta_0 \underline{e}_1 - \overline{H}_m \underline{y}_m\right\}^T \underbrace{\left(V_{m+1}^T V_{m+1}\right)}_{I} \overline{H}_m = 0$$

$$\beta_0 \underline{e}_1^T - \underline{y}_m^T \overline{H}_m^T \overline{H}_m = \underline{0}$$

$\underline{r}_m \perp A K_m$ ✓

The basis vectors are

$$A [\underline{v}_1 \vdots \underline{v}_2 \vdots \ldots \vdots \underline{v}_m]$$

$$= [A\underline{v}_1 \vdots A\underline{v}_2 \ldots \vdots A\underline{v}_m] = A V_m$$

$$= V_{m+1} \overline{H}_m .$$

$$(V_{m+1} \overline{H}_m)^T \underline{r}_m = \underline{0}$$

$$(V_{m+1} \overline{H}_m)^T V_{m+1} \{ \beta_0 \underline{e}_1 - \overline{H}_m \underline{y}_m \} = \underline{0}$$

$$\overline{H}_m^T \underbrace{(V_{m+1}^T V_{m+1})}_{I_{m+1}} \{ \beta_0 \underline{e}_1 - \overline{H}_m \underline{y}_m \} = \underline{0}$$

$$\therefore \quad \beta_0 \overline{H}_m^T \underline{e}_1 - \overline{H}_m^T \overline{H}_m \underline{y}_m = \underline{0}$$

or

$$\boxed{\overline{H}_m^T \overline{H}_m \underline{y}_m = \beta_0 \overline{H}_m^T \underline{e}_1}$$

solve for $\underline{y}_m$.

Solving the normal equations:

$$\overline{H}_m^T H_m y_m = \beta_0 \overline{H}_m^T \underline{e}_1$$

This is the solution of least squares problem:

$$\boxed{\min_{y \in \mathbb{R}^m} \| \beta_0 \underline{e}_1 - \overline{H}_m y \|_2}$$

Another way to do this is using S.V.D. (Singular Value Decomposition).

$$y_m = \arg\min_{y \in \mathbb{R}^m} \| \beta_0 \underline{e}_1 - \overline{H}_m y \|_2$$

$$\underset{(m+1 \times m)}{\overline{H}_m} = \underset{(m+1 \times m+1)}{Q_{m+1}} \underset{(m+1 \times m)}{\Sigma_m} \underset{m \times m}{(P_m)^T}, \quad \Sigma_m = \begin{pmatrix} S_m \\ \cdots \\ 0 \cdots 0 \end{pmatrix}, \quad S_m = \begin{pmatrix} \sigma_1 \sigma_2 \cdots \sigma_m \end{pmatrix}$$

$$y_m = \overline{H}_m^+ (\beta_0 \underline{e}_1) = \sum_{i=1}^{m} \left[\frac{(q_i^T \beta_0 \underline{e}_1)}{\sigma_i} \right] p_i$$

$$\|\underline{v}_m\|_2^2 = (V_{m+1}\underline{z})^T (V_{m+1}\underline{z})$$

$$= \underline{z}\, \underbrace{V_{m+1}^T V_{m+1}} \underline{z} = \|\underline{z}\|^2$$

$$V_{m+1} = \left(\underline{v}_1 \,\vdots\, \underline{v}_2 \,\vdots\, \cdots \,\vdots\, \underline{v}_{m+1} \right)$$

$$V_{m+1}^T = \begin{pmatrix} \underline{v}_1^T \\ \underline{v}_2^T \\ \vdots \\ \underline{v}_{m+1}^T \end{pmatrix}$$

$$\begin{array}{cccc} 1 & 0 & \cdots & 0 \end{array}$$

$$V_{m+1}^T V_{m+1} = \begin{pmatrix} \underline{v}_1^T\underline{v}_1 & \underline{v}_1^T\underline{v}_2 & \cdots & \underline{v}_1^T\underline{v}_{m+1} \\ \underline{v}_2^T\underline{v}_1 & \underline{v}_2^T\underline{v}_2 & \cdots & \underline{v}_2^T\underline{v}_{m+1} \\ \vdots & 1 & & \vdots \\ \vdots & & & 1 \\ & & & \underline{v}_{m+1}^T\underline{v}_{m+1} \end{pmatrix}$$

$$I_{m+1}$$

ALGORITHM:

- $\underline{x}^{(0)}$ initial estimate of solution.
- Compute $\underline{r}^{(0)} = \underline{b} - A\underline{x}^{(0)}$.
- Use ARNOLDI to generate O.N.B. for $\mathcal{K}_m(A, \underline{r}^{(0)}) = \operatorname{span}\{\underline{r}^{(0)}, A\underline{r}^{(0)}, \dots, A^{m-1}\underline{r}^{(0)}\}$

$$= \operatorname{span}\{\underline{v}_1, \underline{v}_2, \dots, \underline{v}_m\}$$

- Use GRAM-SCHMIDT process to generate $\underline{v}_i$'s:

$$\boxed{AV_m = V_{m+1}\overline{H}_m}$$

(for free out of Gram-Schmidt!)

- Solve least squares problem

$$\underline{y}_m = \underset{\underline{y}\in\mathbb{R}^m}{\operatorname{argmin}} \|\beta_0 \underline{e}_1 - \overline{H}_m \underline{y}\|_2, \quad \beta_0 = \|\underline{r}^{(0)}\|_2$$

$\underline{e}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbb{R}^{m+1}$

using S.V.D.

- Approximate solution: $\underline{x}_m = \underline{x}_0^{(0)} + V_m \underline{y}_m$.
- Residual: $\underline{r}_m = V_{m+1}\{\beta_0 \underline{e}_1 - \overline{H}_m \underline{y}_m\}$ (No matrix multiplying by A!).

Classical Gram–Schmidt

Arnoldi's Method - CGS

$\mathbf{V}(:,1) = \mathbf{r}^{(0)}/\|\mathbf{r}^{(0)}\|_2$
For $m = 1, 2, \ldots$
    $\mathbf{V}(:,m+1) = \mathbf{A}\mathbf{V}(:,m)$
    For $j = 1, \ldots, m$
        $\mathbf{H}(j,m) = \mathbf{V}(:,j)^T\mathbf{A}\mathbf{V}(:,m)$
        $\mathbf{V}(:,m+1) = \mathbf{V}(:,m+1) - \mathbf{H}(j,m)\mathbf{V}(:,j)$
    End
    $\mathbf{H}(m+1,m) = \|\mathbf{V}(:,m+1)\|_2$
    If $\mathbf{H}(m+1,m) \neq 0$
        $\mathbf{V}(:,m+1) = \mathbf{V}(:,m+1)/\mathbf{H}(m+1,m)$
    End
End

Modified Gram–Schmidt

Arnoldi's Method - MGS

$\mathbf{V}(:,1) = \mathbf{r}^{(0)}/\|\mathbf{r}^{(0)}\|_2$

For $m = 1, 2, \ldots$

  $\mathbf{V}(:,m+1) = \mathbf{A}\mathbf{V}(:,m)$

  For $j = 1, \ldots, m$

    $\mathbf{H}(j,m) = \mathbf{V}(:,j)^T\mathbf{V}(:,m+1)$

    $\mathbf{V}(:,m+1) = \mathbf{V}(:,m+1) - \mathbf{H}(j,m)\mathbf{V}(:,j)$

  End

  $\mathbf{H}(m+1,m) = \|\mathbf{V}(:,m+1)\|_2$

  If $\mathbf{H}(m+1,m) \neq 0$

    $\mathbf{V}(:,m+1) = \mathbf{V}(:,m+1)/\mathbf{H}(m+1,m)$

  End

End

```
function [x,m] = GMRESver01(A,b,x0,tol,MaxKrylov)
%Calculates the General Minimal Residual Method (GMRES) for a given matrix
%A and solution vector b.
%Input: Matrix A, vector b
%output: solution vector x and number of loops m

%Initialise
N = size(A,1);
H = zeros(MaxKrylov+1,MaxKrylov);
V = zeros(N,MaxKrylov+1);

r = b - A*x0;
beta = norm(r,2);
V(:,1) = r/beta;

for m = 1:MaxKrylov

    %Arnoldi (Modified Gram-Schmidt)
    V(:,m+1) = A*V(:,m);
    for j = 1:m
        H(j,m) = V(:,j)'*V(:,m+1);
        V(:,m+1) = V(:,m+1) - H(j,m)*V(:,j);
    end
    H(m+1,m) = norm(V(:,m+1),2);

    % Check for breakdown
    if abs(H(m+1,m)) < 1e-14
        fprintf('Invariant Krylov Subspace detected at m=%g\n',m);
        y = (H(1:m,1:m)'*H(1:m,1:m)) \ ([beta; zeros(m-1,1)]); % Invariant space
detected
        break;
    else
        V(:,m+1) = V(:,m+1)/H(m+1,m);
    end
    % Solve small m dimensional least squares problem for y
    rhs= [beta; zeros(m,1)];          βe₁
SVD y = (H(1:m+1,1:m)'*H(1:m+1,1:m)) \ rhs;

    % determine residual norm (remember this is a least squares problem)
    rnorm = norm(rhs-H(1:m+1,1:m)*y);

    if diagnostics, fprintf('m=%g ||r_m||=%g tol=%g\n',m,rnorm,beta*tol); end

    % check if converged and if so, break out of Arnoldi look to compute
    % approximate solution
    if rnorm <= beta*tol, break; end

end

%% Compute approximate solution
x = x0 + V(:,1:m)*y;

end
```