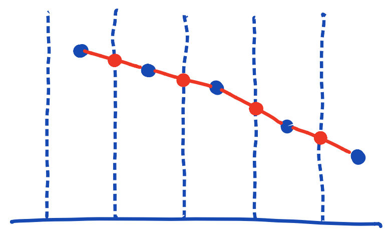
Numerical solution for steady unconfined flow

1) Residual

Consider the discretization of steady unconfined flow:

continuous: $-\nabla \cdot [h \nabla h] = f_s$

discrete: $-\underline{\underline{D}} * [\,?\,\underline{\underline{G}} * \underline{h}] = \underline{f}_s$



Interpolate $\underline{h}$ to the interfaces:

$\underline{\underline{H}} = \{\underline{\underline{M}}\,\underline{h}\}_f$ is Nf by Nf matrix with $\underline{\underline{M}}\,\underline{h}$ on diagonal

here $\underline{\underline{M}}$ is the Nf by N matrix that computes the arith. ave. of cell centered values on faces.

$$\Rightarrow \quad \boxed{-\underline{\underline{D}} * \{\underline{\underline{M}}\,\underline{h}\}_f * \underline{\underline{G}} * \underline{h} = \underline{f}_s}$$

Note: We cannot form the "system matrix" $\underline{\underline{L}}$!

$\Rightarrow$ not a linear system of algebraic equations

$\Rightarrow$ need to solve it with Newton-Raphson method.

Main challenge is forming the N by N Jacobian matrix !

I) Residual vector

The residual is the system of N non-linear algebraic equations we want to find the roots of. It is given by

$$\boxed{\underline{r}(h) = \underline{\underline{D}}\left[\{\underline{\underline{M}}\,\underline{h}\}\,\underline{\underline{G}}\,\underline{h}\right] + f_s}$$

We seek $\underline{h}$ such that $\underline{r}(\underline{h}) = \underline{0}$.

Linearizing the discrete residual

As before the linearization is:

$$\begin{aligned} L_{\bar{h}}\underline{r} &= \underline{r}(\bar{\underline{h}}) + \nabla_{\underline{h}}\underline{r}\,\underline{\Delta h} \\ &= \underline{r}(\bar{\underline{h}}) + \epsilon\,\nabla_{\underline{h}}\underline{r}\,\hat{h} \\ &= \underline{r}(\bar{\underline{h}}) + \epsilon\,D_{\hat{h}}\,\underline{r}(\bar{h}) \end{aligned}$$

$$\underline{\Delta h} = \epsilon\,\hat{\underline{h}}$$

$$D_{\hat{h}}\underline{r}(\bar{\underline{h}}) = \nabla_{\underline{h}}\underline{r}\,\hat{\underline{h}}$$

Here $D_{\hat{h}}\,\underline{r}(\bar{h})$ is the directional derivative of $\underline{r}$ at $\bar{\underline{h}}$ in direction $\hat{\underline{h}}$, which is defined as

$$\boxed{D_{\hat{h}}\,\underline{r}(\bar{\underline{h}}) = \frac{d}{d\varepsilon}\,\underline{r}(\bar{\underline{h}} + \epsilon\,\hat{\underline{h}})\Big|_{\varepsilon=0}}$$

Simple example: Scalar-valued vector function

$$f(\underline{x}) = x + y^2 \qquad \nabla f = \begin{pmatrix} 1 \\ 2y \end{pmatrix}$$

Given some direction $\hat{\underline{x}} = \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix}$ and location $\bar{\underline{x}} = \begin{pmatrix} \bar{x} \\ \bar{y} \end{pmatrix}$ we have

a) $$D_{\hat{\underline{x}}} f(\bar{\underline{x}}) = \nabla f \big|_{\bar{x}} \hat{x} = (1 \quad 2\bar{y}) \begin{pmatrix} \hat{x} \\ \hat{y} \end{pmatrix} = \underline{\hat{x} + 2\bar{y}\hat{y}}$$

b) $$D_{\hat{\underline{x}}} f(\bar{\underline{x}}) = \frac{d}{d\epsilon} f(\bar{x} + \epsilon \hat{x}) \Big|_{\epsilon=0} = \frac{d}{d\epsilon} (\bar{x} + \epsilon \hat{x}) + (\bar{y} + \epsilon \hat{y})^2 \Big|_{\epsilon=0}$$

$$= \hat{x} + 2(\bar{y} + \epsilon \hat{y})\, \hat{y} \Big|_{\epsilon=0} = \underline{\hat{x} + 2\bar{y}\hat{y}}$$

The linearization of f is then:

$$L_{\bar{\underline{x}}} f(\hat{\underline{x}}) = f(\bar{\underline{x}}) + D_{\hat{\underline{x}}} f(\bar{\underline{x}}) = \bar{x} + \bar{y}^2 + \hat{x} + 2\bar{y}\hat{y}$$

Directional derivative of the residual

To linearize our discrete system we need the directional derivative of a vector-valued vector function.

$$\boxed{D_{\hat{\underline{h}}} \underline{r}(\bar{\underline{h}}) = \frac{d}{d\epsilon} \underline{r}(\bar{\underline{h}} + \epsilon \hat{\underline{h}}) \Big|_{\epsilon=0}}$$

$$\underline{r}(\underline{h}) = \underline{\underline{D}} * \left[\{ \underline{\underline{M}} * \underline{h} \}_f * \underline{\underline{G}} * \underline{h} \right] - \underline{f}_s$$

$$\frac{d}{d\epsilon}\underline{r}(\bar{\underline{h}}+\epsilon\hat{\underline{h}})\Big|_{\epsilon=0} = \frac{d}{d\epsilon}\,\underline{\underline{D}}*\left[\{\underline{\underline{M}}*(\bar{\underline{h}}+\epsilon\hat{\underline{h}})\}_f * \underline{\underline{G}}*(\bar{\underline{h}}+\epsilon\hat{\underline{h}})\right] - \cancelto{0}{f_s}\Big|_{\epsilon=0}$$

$$= \frac{d}{d\epsilon}\,\underline{\underline{D}}*\left[\{\underline{\underline{M}}\bar{\underline{h}}+\epsilon\underline{\underline{M}}\hat{\underline{h}}\}_f\,(\underline{\underline{G}}\bar{\underline{h}}+\epsilon\,\underline{\underline{G}}\hat{\underline{h}})\right]_{\epsilon=0}$$

$$= \frac{d}{d\epsilon}\,\underline{\underline{D}}*\left[\left(\{\underline{\underline{M}}\bar{\underline{h}}\}_f+\epsilon\,\{\underline{\underline{M}}\hat{\underline{h}}\}_f\right)\left(\underline{\underline{G}}\bar{\underline{h}}+\epsilon\,\underline{\underline{G}}\hat{\underline{h}}\right)\right]_{\epsilon=0}$$

$$= \frac{d}{d\epsilon}\,\underline{\underline{D}}*\left[\cancelto{0}{\{\underline{\underline{M}}\bar{\underline{h}}\}_f\underline{\underline{G}}\bar{\underline{h}}}+\epsilon\{\underline{\underline{M}}\bar{\underline{h}}\}\underline{\underline{G}}\hat{\underline{h}}+\epsilon\{\underline{\underline{M}}\hat{\underline{h}}\}_f\underline{\underline{G}}\bar{\underline{h}}+\epsilon^2\{\underline{\underline{M}}\hat{\underline{h}}\}_f\underline{\underline{G}}\hat{\underline{h}}\right]_{\epsilon=0}$$

now we differentiate

$$= \underline{\underline{D}}*\left[\{\underline{\underline{M}}\bar{\underline{h}}\}_f\underline{\underline{G}}\hat{\underline{h}}+\{\underline{\underline{M}}\hat{\underline{h}}\}_f\underline{\underline{G}}\bar{\underline{h}}+2\epsilon\{\underline{\underline{M}}\hat{\underline{h}}\}_f\underline{\underline{G}}\hat{\underline{h}}\right]_{\epsilon=0}$$

and evaluate at $\epsilon=0$

$$= \underline{\underline{D}}\left[\{\underline{\underline{M}}\bar{\underline{h}}\}_f\underline{\underline{G}}\hat{\underline{h}}+\{\underline{\underline{M}}\hat{\underline{h}}\}_f\underline{\underline{G}}\bar{\underline{h}}\right] \stackrel{?}{=} \underline{\underline{J}}(\bar{\underline{h}})\,\hat{\underline{h}}$$

This is linear in $\hat{\underline{h}}$ but how do we pull $\hat{\underline{h}}$ out of second term?

$$\{\underline{\underline{M}}\hat{\underline{h}}\}_f\,\underline{\underline{G}}\bar{\underline{h}} = \underbrace{(\underline{\underline{M}}\hat{\underline{h}})}_{\text{vector}}.*\underbrace{(\underline{\underline{G}}\bar{\underline{h}})}_{\text{vector}} = (\underline{\underline{G}}\bar{\underline{h}}).*(\underline{\underline{M}}\hat{\underline{h}}) = \{\underline{\underline{G}}\bar{\underline{h}}\}\,\underline{\underline{M}}\,\hat{\underline{h}}$$

$$D_{\hat{\underline{h}}}\underline{r}(\bar{\underline{h}}) = \underline{\underline{D}}\left[\{\underline{\underline{M}}\bar{\underline{h}}\}_f\underline{\underline{G}}\hat{\underline{h}}+\{\underline{\underline{G}}\bar{\underline{h}}\}_f\underline{\underline{M}}\hat{\underline{h}}\right]$$

$$= \underbrace{\underline{\underline{D}}\left[\{\underline{\underline{M}}\bar{\underline{h}}\}_f\underline{\underline{G}}+\{\underline{\underline{G}}\bar{\underline{h}}\}_f\underline{\underline{M}}\right]}_{\underline{\underline{J}}(\bar{\underline{h}})}\hat{\underline{h}}$$

Hence the Jacobian for steady unconfined flow is

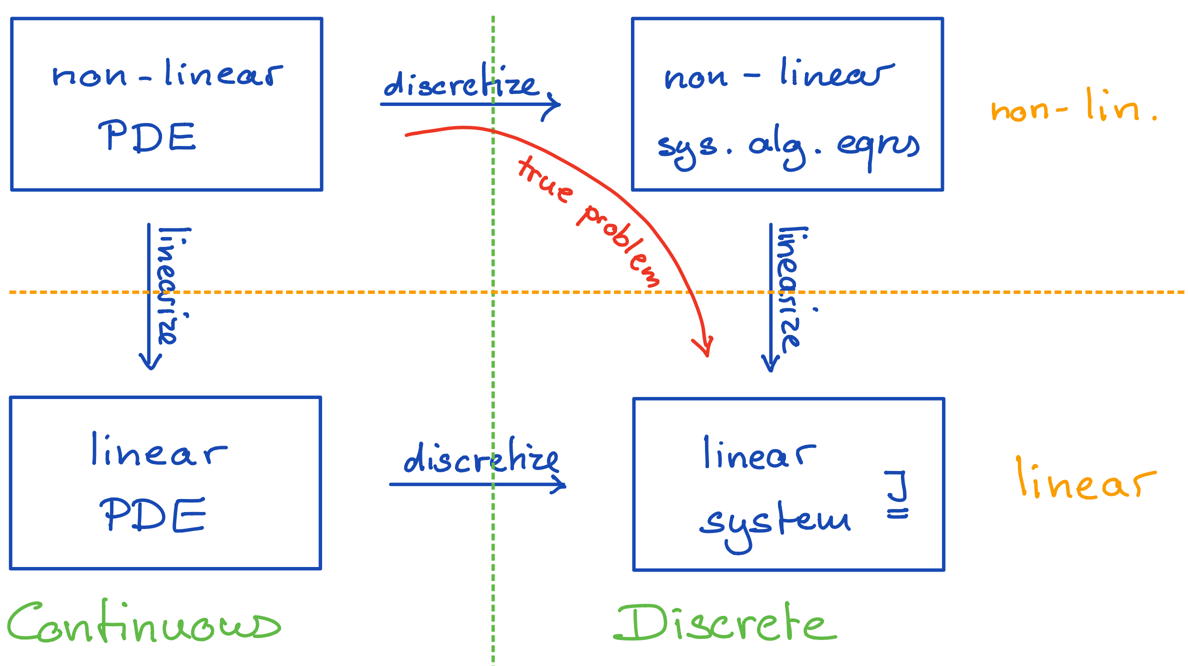
$$\boxed{\underline{\underline{J}}(\bar{\underline{h}}) = \underline{\underline{D}}\left[\{\underline{\underline{M}}\,\bar{\underline{h}}\}_f\,\underline{\underline{G}} + \{\underline{\underline{G}}\,\bar{\underline{h}}\}_f\,\underline{\underline{M}}\right]}$$

where $\{\underline{v}\}_f$ is an N_f by N_f diagonal matrix with $\underline{v}$ on the diagonal

$\underline{\underline{M}}$ is an N_f by N matrix that averages from cell centers to cell faces

Given $\underline{r}$ and $\underline{\underline{J}}$ and setting $\bar{\underline{h}} = \underline{h}^k$ and $\hat{\underline{h}} = \underline{dh}^k$ we have the Newton update:

$$\underline{dh}^k = -\underline{\underline{J}}(\underline{h}^k)^{-1}\,\underline{r}(\underline{h}^k), \qquad \underline{h}^{k+1} = \underline{h}^k + \underline{dh}^k$$



Path 2: Linearize then discretize

$r(h) = \nabla \cdot [h \nabla h] + 1$

Note: Here we are linearizing a function r that takes another function h as an input!

$r(h)$ is a non-linear functional or operator.

Instead of derivatives we call the change of the functional r at $\bar{h}$ in direction $\delta h = \epsilon \hat{h}$ its functional derivative

$$\boxed{D_{\hat{h}} r(\bar{h}) = \frac{d}{d\epsilon} r(\bar{h} + \epsilon \hat{h}) \Big|_{\epsilon=0} \approx \frac{r(\bar{h}+\epsilon\hat{h}) - r(\bar{h})}{\epsilon}}$$

Note:
- This is also called first variation in the Calculus of Variations.
- Gateaux derivative

  Continuum equivalent to the directional derivative

The linearization of the functional is then

$$\boxed{L_{\bar{h}} r(\hat{h}) = r(\bar{h}) + \epsilon D_{\hat{h}} r(\bar{h})}$$

Linearizing the the eqn for unconfined flow

$r(h) = \nabla\cdot[h\,\nabla h] + 1$ ($\bar{h}$ is known $\hat{h}$ need to be found)

$$\frac{d}{d\epsilon} r(\bar{h}+\epsilon\hat{h})\Big|_{\epsilon=0} = \frac{d}{d\epsilon}\left\langle \nabla\cdot\left[(\bar{h}+\epsilon\hat{h})\,\nabla(\bar{h}+\epsilon\hat{h})\right] + \cancelto{0}{1} \right\rangle\Big|_{\epsilon=0}$$

$$= \frac{d}{d\epsilon}\left\langle \nabla\cdot\left[\cancelto{0}{\bar{h}\nabla\bar{h}} + \epsilon\,\bar{h}\nabla\hat{h} + \epsilon\,\hat{h}\nabla\bar{h} + \epsilon^2\,\hat{h}\nabla\hat{h}\right\rangle\Big|_{\epsilon=0}$$

$$= \nabla\cdot\left[\bar{h}\nabla\hat{h} + \hat{h}\nabla\bar{h} + 2\cancelto{0}{\epsilon}\,\hat{h}\nabla\hat{h}\right]_{\epsilon=0}$$

$$= \nabla\cdot\left[\bar{h}\nabla\hat{h} + \hat{h}\nabla\bar{h}\right] \qquad \text{linear in } \hat{h}$$

$$= \underbrace{\nabla\cdot\left[\bar{h}\nabla + \nabla\bar{h}\right]}_{\text{linearized differential operator } \mathcal{L}}\hat{h} = \mathcal{L}\,\hat{h}$$

Discretize $\mathcal{L}$ to obtain $\underline{\underline{J}}$ matrix

$$\mathcal{L} = \nabla\cdot\left[\bar{h}\,\nabla + \nabla\bar{h}\right]$$

$$\underline{\underline{J}} = \underline{\underline{D}}\left[\{\underline{\bar{h}}\}_f\,\underline{\underline{G}} + \{\underline{\underline{G}}\,\underline{\bar{h}}\}\right] \qquad \text{as before}$$

$\Rightarrow$ both paths give the same form of the Jacobian matrix.

If the two ways feel so similar as to be redundant, that is only due to our operator based implementation which hides the complexities of the discretization.