

## Non-Linear Microproblem

$$\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D} \nabla c) - \frac{\partial f(c)}{\partial t}$$

Applying chain rule to  $\frac{\partial f}{\partial t}$  yields

$$\frac{\partial c}{\partial t} = \nabla \cdot (\mathbf{D} \nabla c) - \frac{\partial f(c)}{\partial c} \frac{\partial c}{\partial t}.$$

Discretizing the time derivative by means of an implicit Euler scheme leads to

$$c^{n+1} - \Delta t \nabla \cdot (\mathbf{D} \nabla c^{n+1}) + \frac{\partial f(c^{n+1})}{\partial c^{n+1}} (c^{n+1} - c^n) - c^n = 0.$$

Integrating over domain  $\Omega$  and multiplying test function  $v$  results in

$$F := \int_{\Omega} c^{n+1} v + \Delta t \nabla v^T \mathbf{D} \nabla c^{n+1} + \frac{\partial f(c^{n+1})}{\partial c^{n+1}} (c^{n+1} - c^n) v - c^n v = 0.$$

Using the following definitions

$$c = \sum_j^n \phi_j c_j$$

$$v = \phi_j \quad \text{since } \forall v \in V_h$$

$$f := \frac{Q_m K_n c}{1 + K_n c}$$

$$\frac{\partial f(c)}{\partial c} = f'(c) = \frac{Q_m K_n}{(1 + K_n c)^2} = Q_m K_n (1 + K_n c)^{-2}$$

$$\frac{\partial^2 f(c)}{\partial c^2} = f''(c) = -2 Q_m K_n^2 (1 + K_n c)^{-3}$$

we obtain the nonlinear problem with Jacobian

$$J_{ij} := \frac{\partial F_i}{\partial c_j} = \int_{\Omega} \phi_i \phi_j + \Delta t \nabla \phi_j^T \mathbf{D} \nabla \phi_i + \tag{1}$$

$$f'(c^-) \phi_i \phi_j + f''(c^-) c^- \phi_i \phi_j - f''(c^-) c^n \phi_i \phi_j \tag{2}$$

with  $c^-$  being the most recent Newton approximation.

$$\mathbf{J} \Delta \mathbf{c} = -\mathbf{F}(\mathbf{c}^-)$$

$$\mathbf{c} = \mathbf{c}^- + \omega \Delta \mathbf{c}$$

$$\mathbf{c}^- \leftarrow \mathbf{c}$$