Implicit, bound-preserving schemes for degenerate parabolic equations

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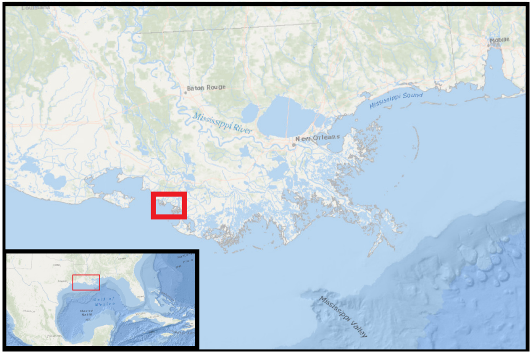
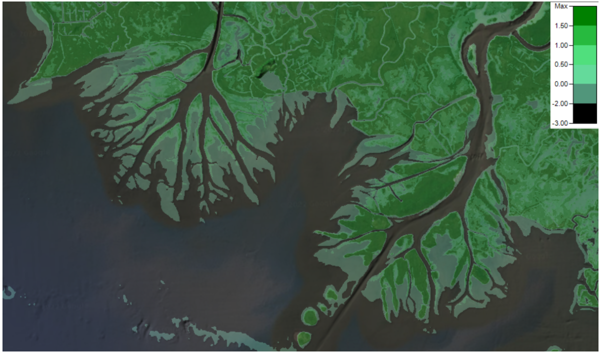
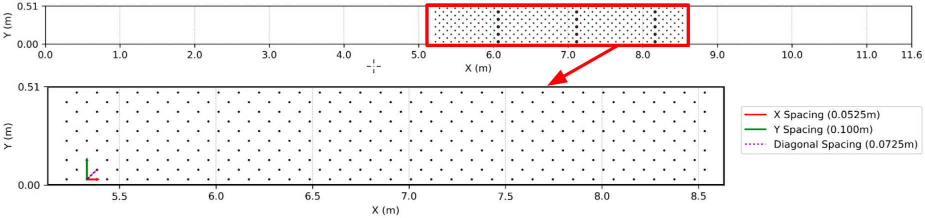
Motivation: Coastal Protection, Restoration, and Design

- Coastal ecosystems represent a “dynamic equilibrium” in biomass, sediment, water chemistry, wave & current forcing, modulated by extreme events like hurricanes, floods, wildfire, . . .
- Much work is needed to understand these dynamic systems to support conservation/restoration and design/management, with optimization of multiple objectives.

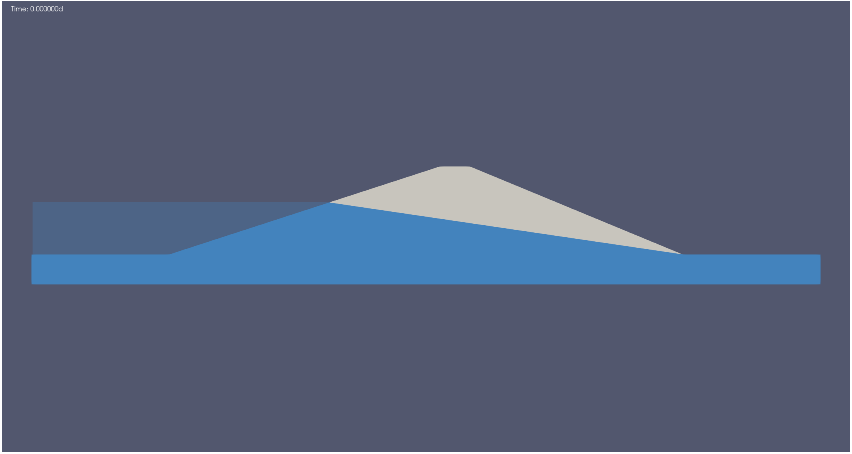




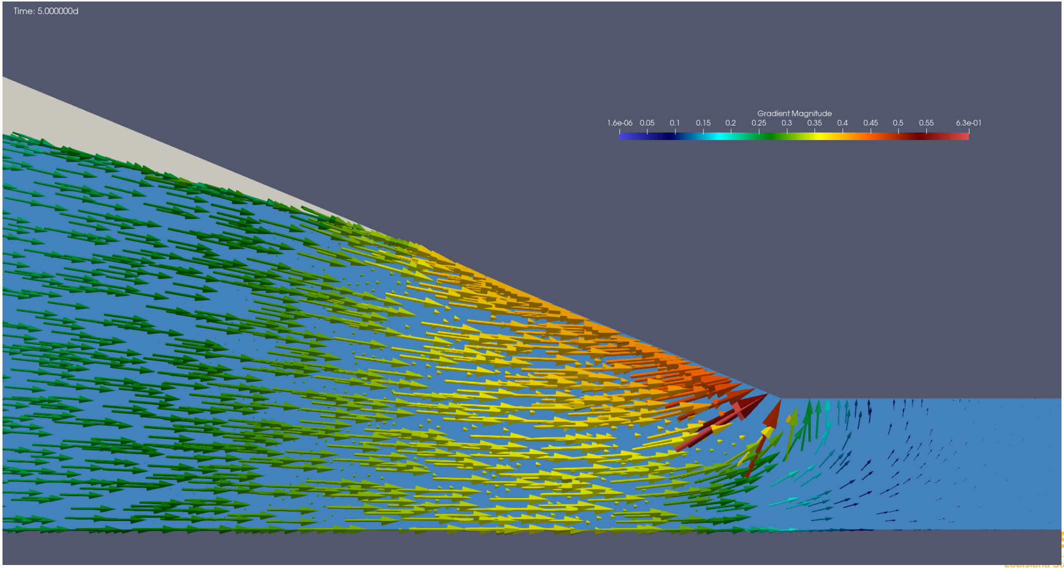
Example: Multiscale Modeling of Vegetation



Example: Flood Risks and Stormwater



Example: Flood Risks and Stormwater, Cont'd



Background: Two-Phase Flow In Porous Media

$$\frac{\partial(\omega s_w \rho_w)}{\partial t} + \nabla \cdot (\rho_w \mathbf{v}_w) = 0 \quad (0.1)$$

$$\frac{\partial(\omega s_n \rho_n)}{\partial t} + \nabla \cdot (\rho_n \mathbf{v}_n) = 0 \quad (0.2)$$

$$\mathbf{v}_w = -\bar{\boldsymbol{K}}\bar{\boldsymbol{k}}_{rw}(\nabla\psi_w + \nabla z) \quad (0.3)$$

$$\mathbf{v}_n = -\bar{\boldsymbol{K}}_i\bar{\boldsymbol{k}}_{rn}(\nabla\psi_n + \nabla z) \quad (0.4)$$

$$s_n = 1 - s_w \quad (0.5)$$

$$p_n - p_w = p_c(\mathbf{x}, s_w) \quad (0.6)$$

$$\bar{\boldsymbol{k}}_{r\alpha} = \bar{\boldsymbol{k}}_{r\alpha}(\mathbf{x}, s_w) \quad (0.7)$$

$$\bar{\boldsymbol{K}}_i = \bar{\boldsymbol{K}}_i(\mathbf{x}) \quad (0.8)$$

Background: Fractional Flow Form, [Chavent & Jaffré (1986)]

$$\frac{\partial \omega s_w}{\partial t} + \nabla \cdot \mathbf{q}_w = 0 \tag{0.9}$$

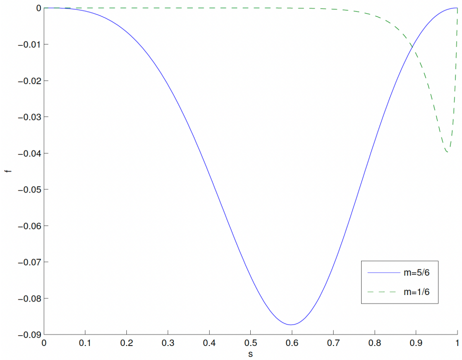
$$\mathbf{q}_w = f_w \mathbf{q}_t + \bar{\boldsymbol{K}} \lambda_w f_n \nabla \psi_c + \bar{\boldsymbol{K}} \lambda_w f_n \left(b\rho_n - \rho_w \right) \nabla z \tag{0.10}$$

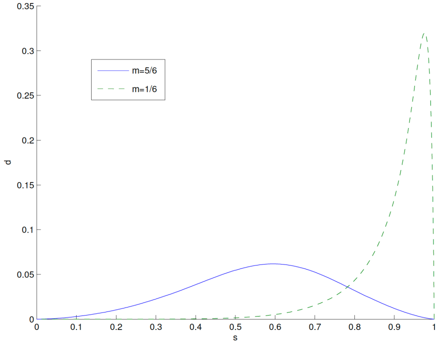
$$\nabla \cdot \mathbf{q}_t = 0 \tag{0.11}$$

$$\mathbf{q}_t = -\bar{\boldsymbol{K}} \lambda_t \left(\nabla \psi_t + \rho_t \nabla z \right) \tag{0.12}$$

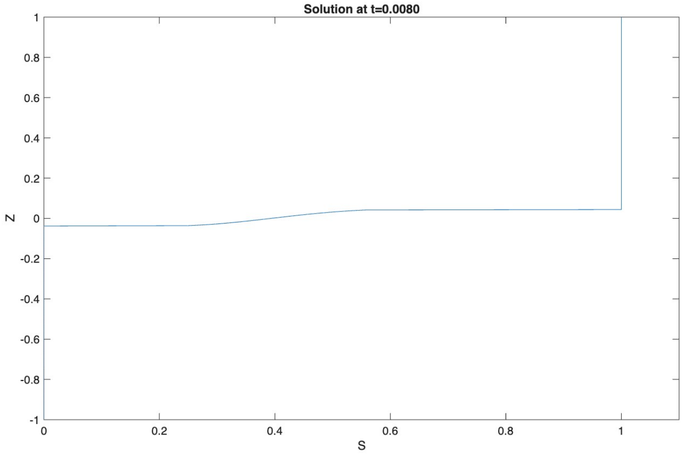
Background: Type Change, [Kees (2004)]

$$\frac{\partial s_w}{\partial t} + \nabla \cdot [f(s) - d(s)\nabla s] = 0$$

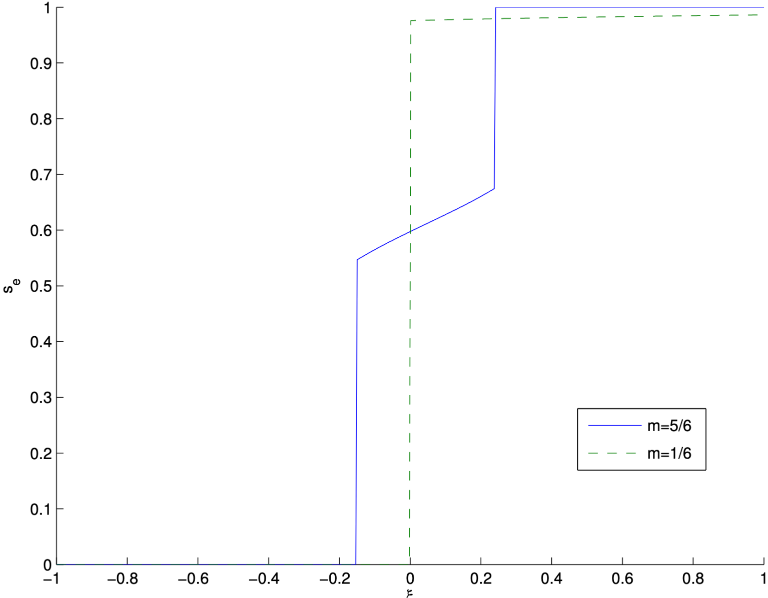




Riemann Solution



Riemann Solution: Fast Air Wave



Background: Light, inviscid non-wetting phase limit

$$\frac{\partial s_w}{\partial t} + \nabla \cdot [f(s) - d(s)\nabla s] = 0$$

$$d = -\frac{k_i}{\omega\mu_w}\frac{k_{rw}k_{rn}}{\frac{\mu_n}{\mu_w}k_{rw} + k_{rn}}\frac{dp_c}{ds} \approx -\frac{k_i k_{rw}}{\omega\mu_w}\frac{dp_c}{ds} \quad (0.13)$$

$$f = \frac{k_i\mu_n}{\omega\mu_w}\frac{k_{rw}}{\frac{\mu_n}{\mu_w}k_{rw} + k_{rn}}q_t + \frac{k_i}{\omega\mu_w}\frac{k_{rw}k_{rn}}{\frac{\mu_n}{\mu_w}k_{rw} + k_{rn}}(1 - \frac{\rho_n}{\rho_w})\rho_w g \quad (0.14)$$

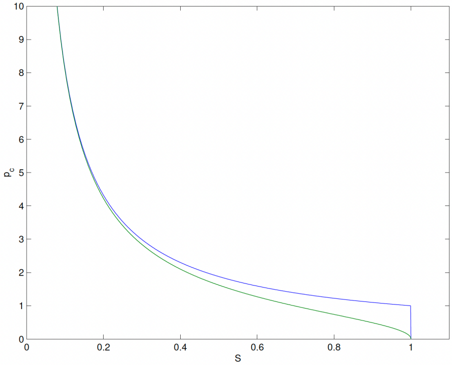
$$\approx \frac{k_i k_{rw}}{\omega\mu_w}\rho_w g \quad (0.15)$$

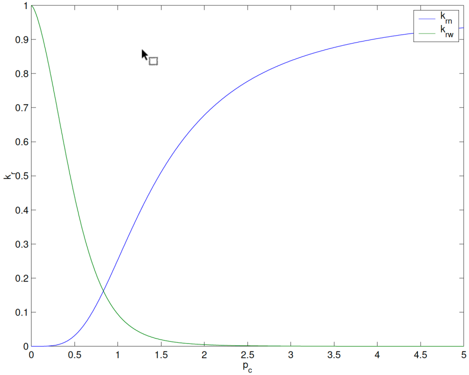
Background: Richards Equation, [Richards (1931)]

Approximating the capillary head by $\psi_w \approx \frac{p_a - p_w}{\rho_w g} = \psi_c$, we get

$$\frac{\partial \omega s_w}{\partial t} + \nabla \cdot \left[-\frac{k_i \rho_w g}{\mu_w} k_{rw} \left(\nabla \psi_w + \nabla z \right) \right] = 0$$

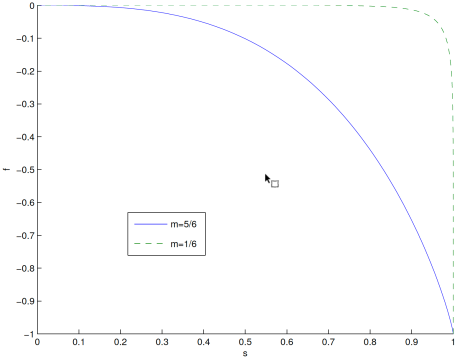
nonlinearities $k_{rw}(s_w)$ and $s_w(\psi_w)$, total head $\phi_w = \psi_w + z$

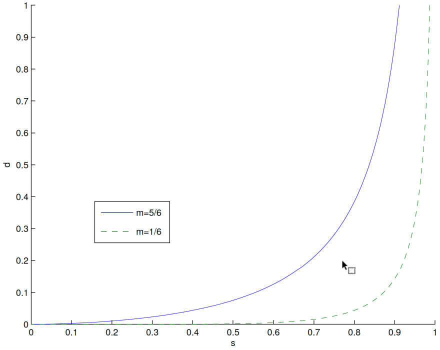




Background: What happened to the air wave?

$$\frac{\partial s_w}{\partial t} + \nabla \cdot [f(s) - d(s)\nabla s] = 0$$





(Group) Finite Element Method [Kuzmin and Hajduk **2024**]

$$\int_\Omega \frac{\sum_j m_j w_j - \sum_j m_j^n w_j}{\Delta t} w_i dV + \int_\Omega K k_r \sum_j \phi_j \nabla w_j \cdot \nabla w_i dV = 0 \qquad \forall i$$

or

$$M_{ij}^C \frac{m_j - m_j^n}{\Delta t} + a_{ij}\phi_j = 0$$

or

$$M_{ij}^L \frac{m_j - m_j^n}{\Delta t} = \sum_{j \neq i} f_{ij}^H = M_{ij}^C (\dot{m}_i - \dot{m}_j) - a_{ij}\left(\phi_i - \phi_j\right)$$

with

$$M_{ii}^L = \sum_j M_{ij}^C \qquad \dot{m}_i = -(M^C)^{-1} a_{ij}\phi_j$$

Low Order Predictor, [Forsyth and Kropinski (**1997**) and Ait Hammou Oulhaj, Cancès, and Chainais–Hillairet (**2018**)]

- Row sum mass lumping: $M^C \approx M^L$
- Upwind k_r:

$$k_{rij} = \begin{cases} k_r(m_i) & \tilde{a}_{ij}(\phi_i - \phi_j) > 0 \\ k_r(m_j) & \tilde{a}_{ij}(\phi_i - \phi_j) \leq 0 \end{cases} \qquad \tilde{a}_{ij} = \int_\Omega \bar{\boldsymbol{K}} \nabla w_j \cdot \nabla w_i dV$$

- Monotonicity for ϕ and therefore $m(\phi)$ since m is a monotone function of ϕ.

$$M^L \frac{m(\phi_i) - m_i^n}{\Delta t} = \sum_{j \neq i} f_{ij}^L = k_{rij} \tilde{a}_{ij} \left(\phi_i - \phi_j\right)$$

- We enable weak enforcement of Dirichlet conditions with a Nitsche term and also check for loss of coercivity due to anisotropic K or poor quality mesh.

FCT Scheme [Boris & Book 73]

- We can write the Galerkin (high-order) form as

$$M^L \frac{m(\phi_i) - m_i^n}{\Delta t} = \sum_{j \neq i} \left(f_{ij}^L + f_{ij}^A \right)$$

where

$$f_{ij}^A = M_{ij}^C (\dot{m}_i - \dot{m}_j) + f_{ij}^H - f_{ij}^L$$

- Solve the low order scheme for ψ^L (and m^L) using Newton's method.
- Apply Zalesak's limiter to f^A to obtain bound-preserving m^H:

$$M^L \frac{m^H - m_i^n}{\Delta t} = \sum_{j \neq i} \left(f_{ij}^L + f_{ij}^{A*} \right)$$

- Since $m(\psi)$ in invertible for $-\infty < \psi < 0$, invert at unsat nodes to get ψ^H

FCT Variants

- The exact antidiffusive fluxes make the scheme nonlinear and are not easy to compute exactly:

$$f_{ij}^{A} = M_{ij}^{C}(\dot{m}_i - \dot{m}_j) + f_{ij}^{H} - f_{ij}^{L}$$

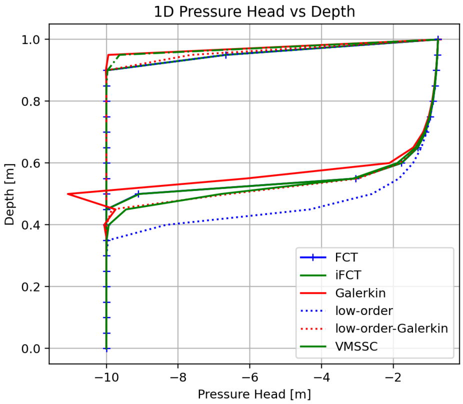
- Nodal time derivative approximations:

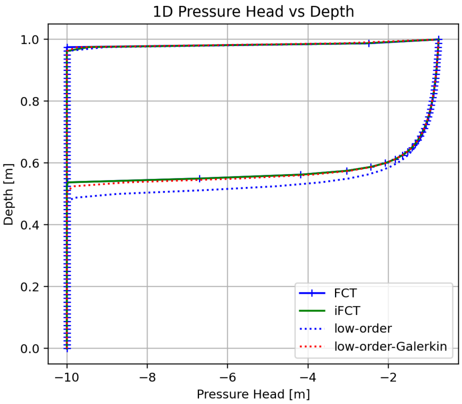
$$\dot{m}_i \approx f_{ij}^{H}/M_{ii}^{L} \tag{0.16}$$

$$\dot{m}_i \approx M^{L,-1}\left(I + (M^{L} - M^{C})M^{L,-1}\right) f_{ij}^{H} \tag{0.17}$$

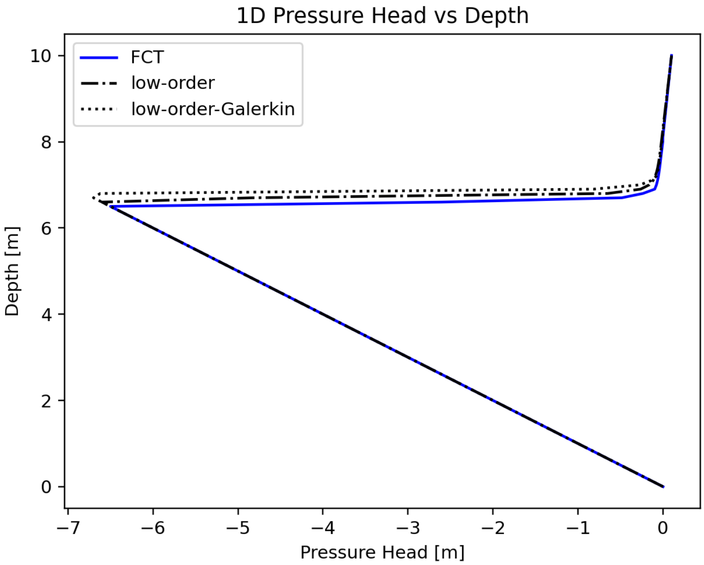
- Evaluate f_{ij}^{H} at converged iterate of ψ^{L} (FCT)
- Apply f^{A} to each Newton iterate ("iFCT") or apply to final iterate ("FCT")

Celia Test Problem, [Celia, Bouloutas, and Zarba (1990)]





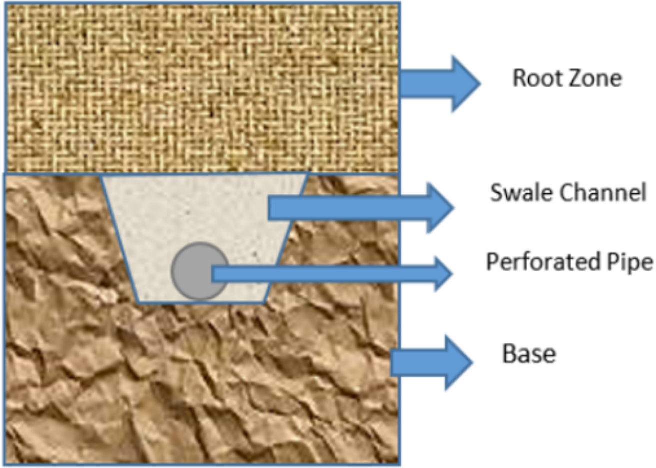
Sand Problem



Seepage Face Boundaries (Signiorini Condition)

- We often need to model an air-exposed boundary where water leaves the porous media (a seepage face) or more generally where surface flow may take place once saturation is reached.
- The situation can be described by a Signiorini condition on Γ_s where $q = -Kk_r \nabla \phi \cdot n$:
$$\psi q = 0 \qquad \psi \leq 0 \qquad q \geq 0$$
- We implement by checking the conditions and dynamically switching between $\psi = 0$ (Dirichlet) and $q = 0$ (Nuemann).

Bioswale



Ongoing

- Investigate stability of explicit mass correction
- Investigate robustness of mass inversion
- Enable arbitrary order Bernstein and nonuniform nodal bases.
- Enable VSVO BDF for higher-order in time.
- Investigate stabilization for high order flux (we have VMS and EV built).
- Explore Kuzmin's monolithic limiting

(FLC)BDF [Gear, Petzold, Jackson & Sacks-Davis]

Predictor:

$$\omega^p_{k,n+1}(t_{n-i}) = m_{n-i} \quad i = 0, 1, \ldots, k$$

Corrector:

$$\omega^c_{k,n+1}(t_{n+1} - ih) = \omega^p_{k,n+1}(t_{n+1} - ih) \quad i = 0, 1, \ldots, k$$

"Backward Euler" derivative approximation:

$$\frac{d\omega^c_{k,n+1}}{dt} = \alpha m_{n+1} - \alpha\omega^p_{k,n+1} - \frac{d\omega^p_{k,n+1}}{dt} = \alpha m_{n+1} + \beta$$

with

$$\alpha = \frac{1}{h_{n+1}} \sum_{j}^{k} \frac{1}{j}$$

Ideas: (1) Bernstein for the corrector (2) FCT for β (Kuzmin, Luna, Ketchison 22).

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