Waveform Relaxation for Coupled Groundwater and Surface Flows

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Setting the Scene — Problems

- Applications
  - **Flood modeling (coupled groundwater-surface flows)**
  - Climate modeling (atmosphere-ocean-sea ice interaction)
  - Heat transfer (thermal FSI)
  - Bird flight (mechanical FSI)
- … more abstractly:
  - multiphysics problems
  - nonlinear PDEs, coupled through an interface
  - partitioned approach

Credit: Joshua J. Cotton (Unsplash)

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Setting the Scene — Goals & Tools

- General framework to solve coupled problems efficiently
  - Time adaptivity in each solver
  - High order in space and time
  - Parallel execution of coupled codes

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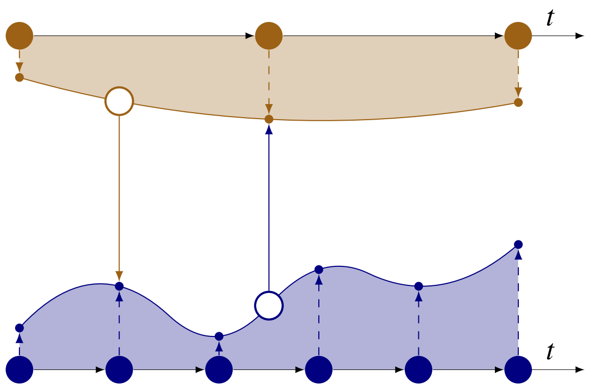
- General framework to solve coupled problems efficiently
  - **Time adaptivity** in each solver
  - **High order** in space and time
  - **Parallel** execution of coupled codes

→ Method: Waveform Relaxation (WR)



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e.g., parallel (Jacobi) WR for ODE systems:

$$\dot{\mathbf{v}}^k(t) = \mathbf{g}\left(t, \mathbf{v}^k(t), \mathbf{w}^{k-1}(t)\right), \ \mathbf{v}(0) = \mathbf{v}_0$$
$$\dot{\mathbf{w}}^k(t) = \mathbf{h}\left(t, \mathbf{v}^{k-1}(t), \mathbf{w}^k(t)\right), \ \mathbf{w}(0) = \mathbf{w}_0$$

different variants, e.g.,
Dirichlet-Neumann WR (DNWR), Neumann-Neumann WR, WACO

How fast do iterations converge & can we accelerate convergence?

Coupled Groundwater / Surface Flows

Surface: Shallow water equations (1D)

water height

$$\partial_t \begin{pmatrix} h \\ hu \end{pmatrix} + \nabla \cdot \begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \end{pmatrix} = \begin{pmatrix} S_h \\ -gh\nabla b \end{pmatrix} \qquad t \in [0,T]$$

momentum

Groundwater: Richards equation (2D)

$$c(\psi)\partial_t \psi = \nabla \cdot \underbrace{(K(\psi)\nabla(\psi + z))}_{=-\mathbf{v}(\psi)} \qquad t \in [0,T]$$

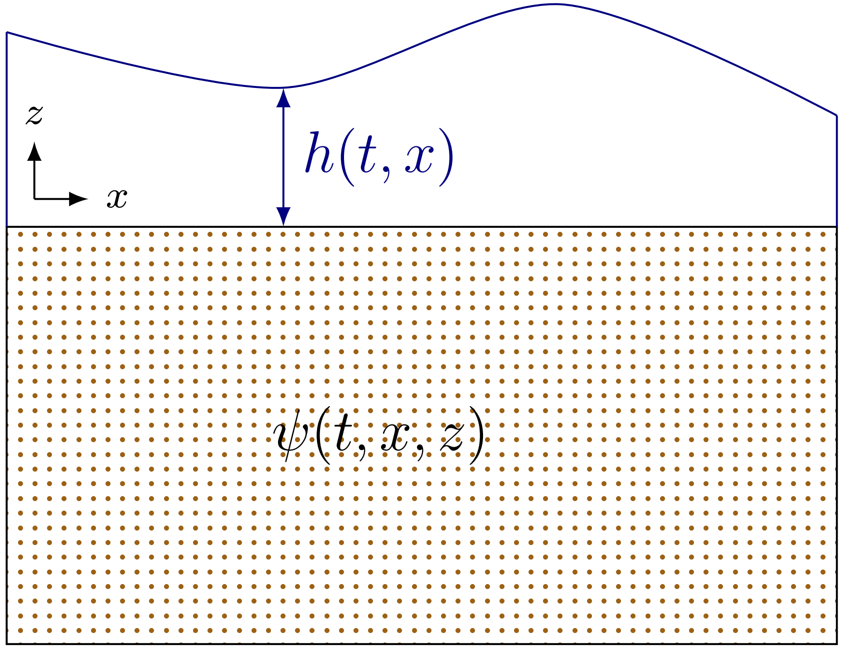
soil water potential
(suction + gravity)

flux

Coupling: pressure & mass conservation

$$\psi|_{z=0} = h, \qquad S_h(t,x) = \mathbf{v}|_{z=0} \cdot \mathbf{n}$$

(cf. Dirichlet & Neumann transmission conditions)



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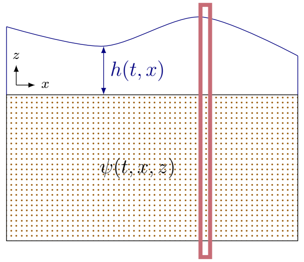
Analysis Steps — Continuous Case



A. Dimension reduction → 1D-0D + Linearization

$$c\partial_t \psi = K \partial_z^2 \psi \qquad \dot{h} = S_h$$

B. Use a coupling algorithm: sequential DNWR

1. Solve Richards equation: $c\partial_t \psi^k = K \partial_z^2 \psi^k, \quad \psi^k|_{z=0} = h^{k-1}$
2. Solve SWE: $\dot{\hat{h}}^k = S_h^k, \quad S_h^k = v(\psi)|_{z=0}^k$
3. Relaxation step: $h^k = \omega \hat{h}^k + (1-\omega) h^{k-1}$

C. Find convergence rate + optimal relaxation parameter

analysis technique from [Gander, Kwok & Mandal 2016]

$$\omega_{\text{opt}}(s) = \frac{1}{1 + \sqrt{\frac{cK}{s}} \tanh\left(\sqrt{\frac{cs}{K}} L\right)}, \quad s \in \mathbb{C}^+$$

Fully Discrete Analysis [Monge & Birken 2018]

- alternative analysis technique
  heat equation: ω_{opt} depends on mesh & discretization!
- carry out this analysis for the linearized 1D-0D system
  - space discretization: linear finite elements
  - time discretization: implicit Euler
  - analysis for one time step, same time step size
- Goal: Express as linear iteration of the form

$$\mathbf{x}^{k,n} = \Sigma(\omega)\mathbf{x}^{k-1,n} + \mathbf{b}^{n-1}$$

- Convergence if $\rho(\Sigma) < 1$,

$$\omega_{\mathrm{opt}} = \arg\min_{\omega} \rho\left(\Sigma(\omega)\right)$$

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Fully Discrete Analysis — Sequential

- Linear iteration of the form $\mathbf{x}^{k,n} = \Sigma(\omega)\mathbf{x}^{k-1,n} + \mathbf{b}^{n-1}$
- Sequential DNWR for the Richards-SWE problem:

$$\mathbf{x}^{k,n} = h^{k,n} \in \mathbb{R} \;\Rightarrow\; \rho(\Sigma(\omega)) = |\Sigma(\omega)|$$

- After discretization, we get $\Sigma(\omega) = \omega S + (1-\omega)$,

$$S = (M_{\Gamma I} + \Delta t A_{\Gamma I})\underbrace{(M_{II} + \Delta t A_{II})^{-1}}_{\text{compute explicitly (Toeplitz matrix)}}(M_{I\Gamma} + \Delta t A_{I\Gamma}) - (M_{\Gamma\Gamma} + \Delta t A_{\Gamma\Gamma})$$

- **Result:**

$$\rho(\Sigma(\omega)) = 1 - \omega + \omega\left(b^2\alpha - \frac{a}{2}\right)$$

wherein

$$a = \frac{2}{3}c\Delta z + 2\frac{K\Delta t}{\Delta z} \qquad b = \frac{1}{6}c\Delta z - \frac{K\Delta t}{\Delta z} \qquad \alpha = \Delta z \sum_{j=1}^{M-1} \frac{\sin^2(j\pi\Delta z)}{a - 2b\cos(j\pi\Delta z)}$$

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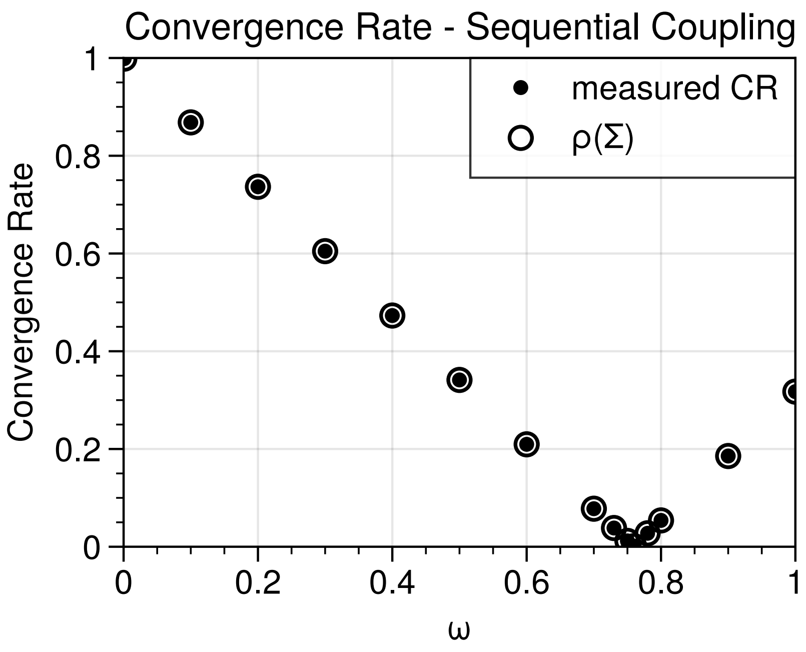
Verification of Analysis

$$K = c = L = 1, \Delta t = \frac{1}{10}, \Delta z = \frac{1}{500}$$

Test code, 1D-0D implementation in Python
using DUNE (dune-project.org) and preCICE (precice.org)



→ What about parallel coupling?

github.com/valentinaschueller/richards-swe-coupling

Parallel DNWR (I)

1a. Solve Richards equation: $c\partial_t \psi^k = K\partial_z^2 \psi^k, \quad \psi^k|_{z=0} = h^{k-1}$

1b. Solve SWE: $\dot{\hat{h}}^k = S_h^k, \quad S_h^k = v(\psi)|_{z=0}^{k-1}$

2. Relaxation step: $h^k = \omega \hat{h}^k + (1-\omega)h^{k-1}$

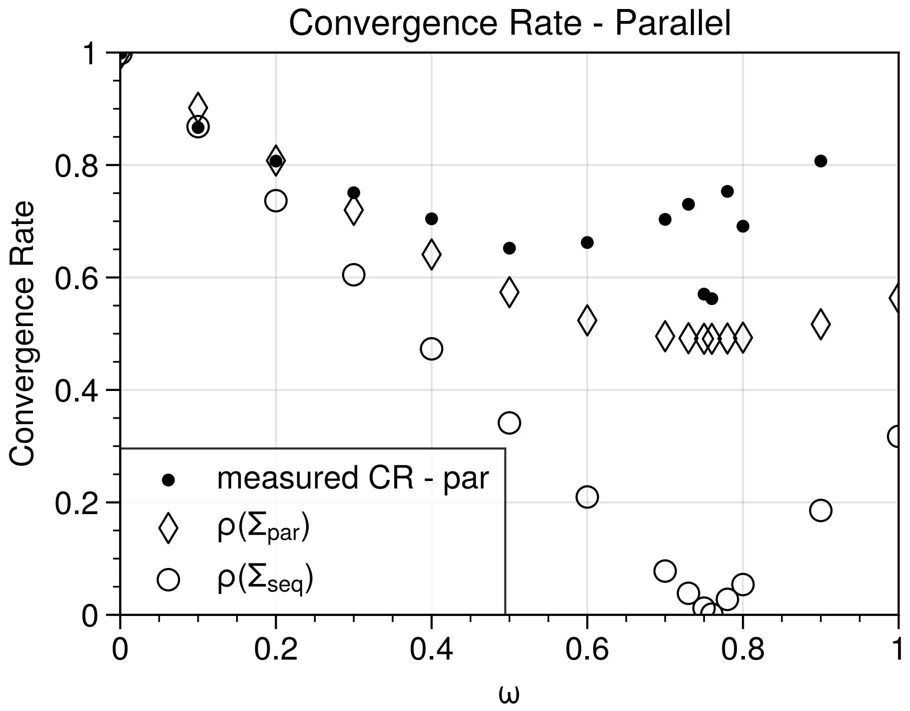
$$v(\psi)|_{z=0}^k = \omega \hat{v}(\psi)|_{z=0}^k + (1-\omega)v(\psi)|_{z=0}^k$$

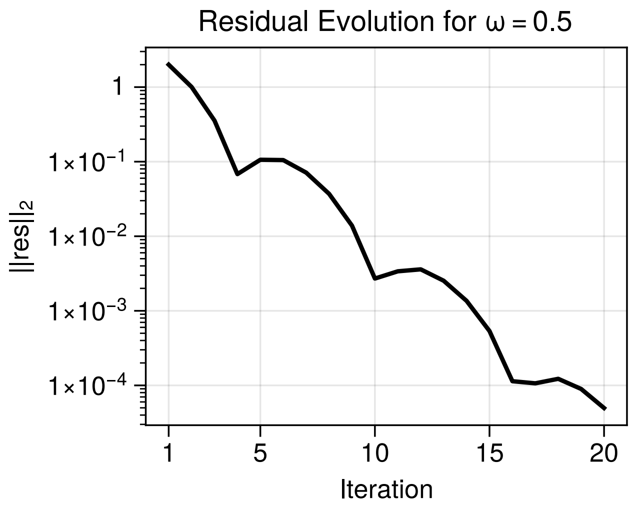
- Analyze with $\mathbf{x}^{k,n} = (h^{k,n}, v^{k,n})^T \Rightarrow \Sigma(\omega) \in \mathbb{R}^{2\times 2}$ [Meisrimel & Birken, 2022]
- **Result:** This does not work in the continuous setting!

$$\rho(\Sigma_{\text{par}}) = \sqrt{1 - 2\omega - \omega^2\left(b^2\alpha - \frac{a}{2} - 1\right)} \qquad \omega_{\text{opt}}^{\text{par}} = \frac{1}{1 - b^2\alpha + \frac{a}{2}} = \omega_{\text{opt}}^{\text{seq}}$$

Parallel DNWR (II)

$$K = c = L = 1, \Delta t = \frac{1}{10}, \Delta z = \frac{1}{500}$$



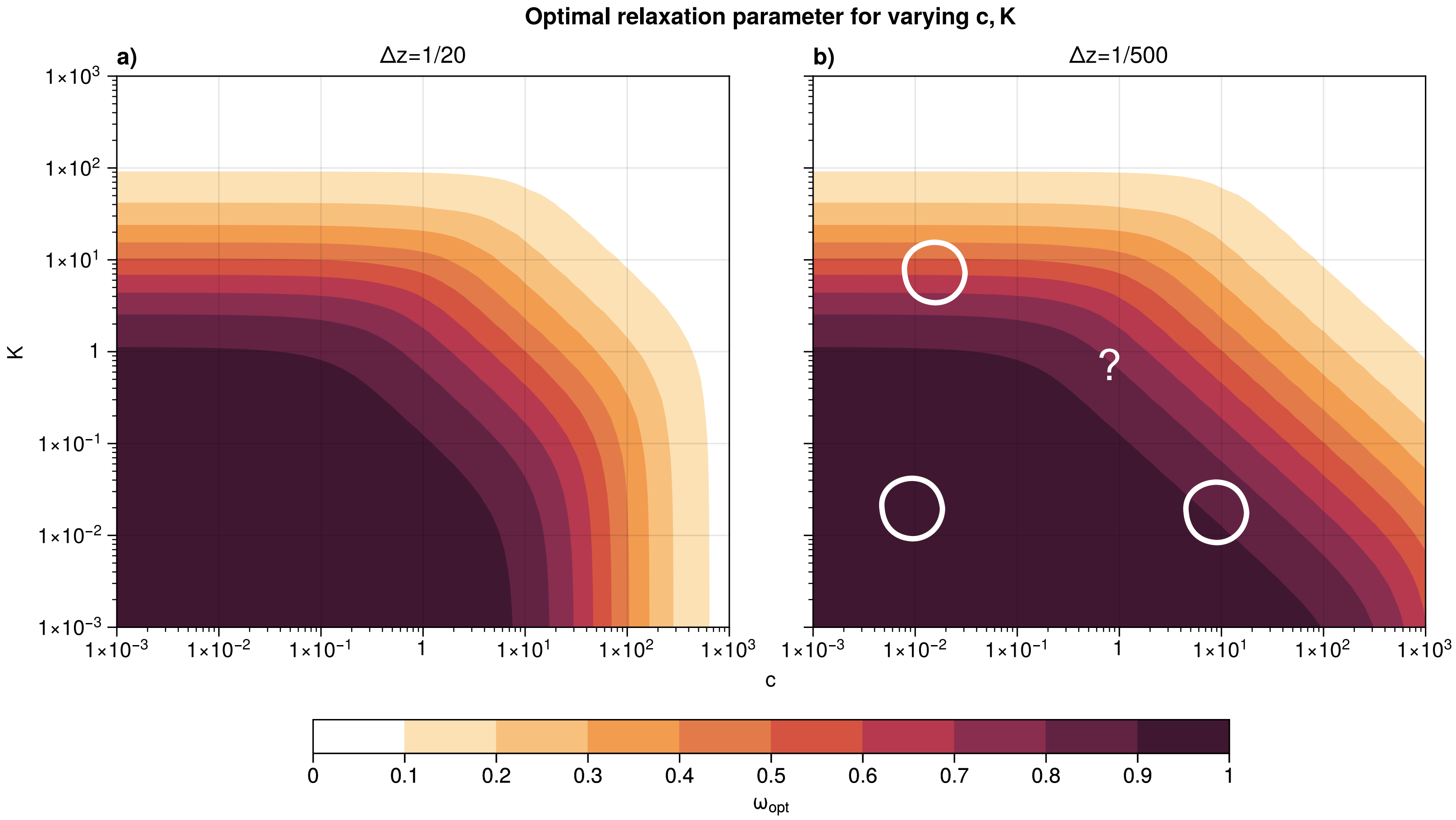


Takeaways:

- Is time-parallelism worth it in this form? Not really!
- Results still relevant for, e.g., WACO (WR + MPI one-sided communication) [Meisrimel & Birken, 2022]

Sequential Analysis: Material Properties

using our sequential analysis results for one time step: $\Delta t = \frac{1}{10}, L = 1$



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To the Real World: Fully Nonlinear Example

- Previously: results for *linearized*, *1D-0D* system, one time step
- How does this translate to a *2D-1D nonlinear* case? → test code:
  - DUNE + preCICE
  - SWE solver: Finite Volume method, local Lax-Friedrichs-flux
  - Richards solver: linear FEM + Newton iterations
  - support for various materials (e.g., loam, gravel, clay)
  - same time step size + both solvers use implicit Euler
- In principle “easy” to make the code more complex:
  - higher order FEM
  - DG instead of FVM
  - other time integration methods
  - support for multirate/time-adaptive setups

gitlab.maths.lu.se/robertk/coupling

Nonlinear Simulation Example, 2D-1D

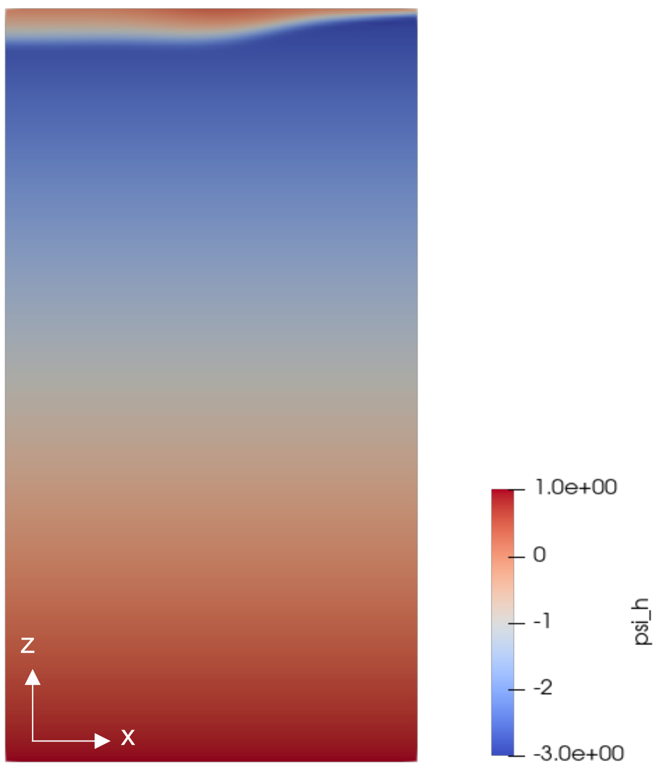
mixed soils (loam and clay) + lake at rest — output of Richards solver:

$$c(\psi)\partial_t\psi = \nabla \cdot \underbrace{(K(\psi)\nabla(\psi + z))}_{=-\mathbf{v}(\psi)}$$

$$c(\psi > 0) = 0$$

→ the Richards equation degenerates to an elliptic equation in saturated regions

This happens at the interface!



Conclusions

- WR as a tool for robust coupled simulations which make use of time adaptivity — time-parallel WR possible
- fully discrete analysis for Richards-SWE coupling
  - can give different results than continuous analysis
  - allows us to study acceleration of parallel DNWR
  - parallel DNWR has the same optimal relaxation parameter but slower convergence than sequential DNWR
- next steps: link linear & nonlinear simulations → how much can the linear analysis serve as a reliable estimator?

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Thank You!

Questions?

References

M. J. Gander, F. Kwok, and B. C. Mandal, “Dirichlet-Neumann and Neumann-Neumann Waveform Relaxation for the Wave Equation,” in *DDM XXII*, T. Dickopf, M. J. Gander, L. Halpern, R. Krause, and L. F. Pavarino, Eds., in Lecture Notes in Computational Science and Engineering. Cham: Springer International Publishing, 2016, pp. 501–509. doi: 10.1007/978-3-319-18827-0_51.

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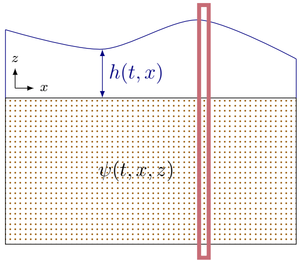
A. Monge and P. Birken, “On the convergence rate of the Dirichlet–Neumann iteration for unsteady thermal fluid–structure interaction,” *Comput. Mech.*, vol. 62, no. 3, pp. 525–541, Sep. 2018, doi: 10.1007/s00466-017-1511-3.

Appendix

Dimension Reduction



$$\partial_t \begin{pmatrix} h \\ hu \end{pmatrix} + \nabla \cdot \begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \end{pmatrix} = \begin{pmatrix} S_h \\ -gh\nabla b \end{pmatrix} \quad \longrightarrow \quad \dot{h} = S_h$$

$$c(\psi)\partial_t\psi = \nabla \cdot \underbrace{(K(\psi)\nabla(\psi + z))}_{=-\mathbf{v}(\psi)} \quad \longrightarrow \quad c(\psi)\partial_t\psi = \partial_z \underbrace{(K(\psi)(\partial_z\psi + 1))}_{=-v(\psi)}$$

Fully Discrete Analysis — Matrices

$$M_{II} = \frac{c\Delta z}{6}\begin{bmatrix} 2 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 1 & 4 \end{bmatrix} \in \mathbb{R}^{M\times M}$$

$$A_{II} = \frac{K}{\Delta z}\begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \in \mathbb{R}^{M\times M}$$

$$M_{I\Gamma} = \frac{c\Delta z}{6}\begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}, A_{I\Gamma} = \frac{K}{\Delta z}\begin{bmatrix} 0 \\ \vdots \\ 0 \\ -1 \end{bmatrix} \in \mathbb{R}^{M}$$

$$M_{\Gamma} = \begin{bmatrix} M_{\Gamma I} & M_{\Gamma\Gamma} \end{bmatrix} = \frac{c\Delta z}{6}\begin{bmatrix} 0 & \cdots & 0 & 1 & 2 \end{bmatrix} \in \mathbb{R}^{1\times(M+1)}$$

$$A_{\Gamma} = \begin{bmatrix} A_{\Gamma I} & A_{\Gamma\Gamma} \end{bmatrix} = \frac{K}{\Delta z}\begin{bmatrix} 0 & \cdots & 0 & -1 & 1 \end{bmatrix} \in \mathbb{R}^{1\times(M+1)}$$

Fully Discrete Coupling Algorithm

1. Solve Richards equation $\rightarrow$ **find** $\boldsymbol{\psi}_I^{n,k}$

$$\begin{aligned}(M_{II} + \Delta t A_{II})\,\boldsymbol{\psi}_I^{n,k} &= -(M_{I\Gamma} + \Delta t A_{I\Gamma})\psi_\Gamma^{n,k-1} \\ &\quad + M_{II}\boldsymbol{\psi}_I^{n-1} + M_{I\Gamma}\psi_\Gamma^{n-1} + \Delta t \boldsymbol{f}_I \\ \boldsymbol{\psi}_I^{0,k} &= \boldsymbol{g}\end{aligned}$$

2. Solve shallow water equation $\rightarrow$ **find** $\tilde{\psi}_\Gamma^{n,k}$

$$\begin{aligned}\tilde{\psi}_\Gamma^{n,k} &= -\,(M_{\Gamma I} + \Delta t A_{\Gamma I})\boldsymbol{\psi}_I^{n,k} - (M_{\Gamma\Gamma} + \Delta t A_{\Gamma\Gamma})\psi_\Gamma^{n,k-1} \\ &\quad + M_{\Gamma I}\boldsymbol{\psi}_I^{n-1} + (1 + M_{\Gamma\Gamma})\psi_\Gamma^{n-1} - \Delta t K \\ \tilde{\psi}_\Gamma^{0,k} &= \eta.\end{aligned}$$

here $\tilde{\psi}_\Gamma^{n,k} = \hat{h}^{n,k}$

3. Relaxation step $\rightarrow$ **find** $\psi_\Gamma^{n,k}$

$$\psi_\Gamma^{n,k} = \omega\tilde{\psi}_\Gamma^{n,k} + (1-\omega)\psi_\Gamma^{n,k-1}$$

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