Convergence Properties of Iteratively Coupled Surface-Subsurface Models

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Background: Coupled Environmental Problems

- Applications: environmental & climate science
- Problem type: coupled partial differential equations
- Research aim: understand and improve existing coupling approaches
- Today: coupled surface-subsurface flow
  - Flood prediction
  - Water management projects
  - Terrestrial water cycle modelling

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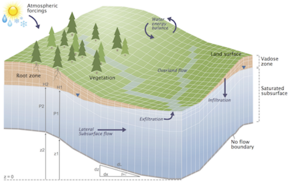
A 2D-1D Model Problem

- Subsurface flow: Richards' equation on $\Omega \subset \mathbb{R}^d$

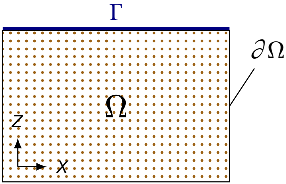
$$\begin{cases} c(\psi)\partial_t \psi + \nabla \cdot \underbrace{\left(-K(\psi)\nabla(\psi + z)\right)}_{=:\mathbf{v}(\psi)} = 0 \quad \text{on } (0,T] \times \Omega, \\ \qquad + \text{B.C., I.C.} \end{cases}$$



Source: ParFlow

- Surface flow: Shallow water equations on $\Gamma \subset \mathbb{R}^{d-1}$

$$\begin{cases} \partial_t h + \partial_x(hu) = s(t,x) + r(t,x) \qquad \text{on } (0,T] \times \Gamma, \\ \qquad + \text{equation for } u\text{, B.C., I.C.} \end{cases}$$



- Coupled via boundary conditions on Γ

$$\psi|_\Gamma = h, \quad s = \mathbf{v}(\psi)|_\Gamma \cdot \mathbf{n} \quad \text{on } (0,T] \times \Gamma.$$

Coupling Iteration

Given an initial guess $h^0(t,x)$, compute **sequentially** in each iteration $k = 1, 2, \ldots$:

$$\begin{aligned} c(\psi^k)\partial_t\psi^k + \nabla\cdot\mathbf{v}(\psi^k) = 0 \quad &\text{on } (0,T]\times\Omega, \\ \psi^k\Big|_\Gamma = h^{k-1} \quad &\text{on } [0,T]\times\Gamma, \end{aligned} \tag{1a}$$

$$\begin{aligned} \partial_t\tilde{h}^k + \partial_x(\tilde{h}^k u^k) = s^k + r \quad &\text{on } (0,T]\times\Gamma, \\ s^k = \mathbf{v}\left(\psi^k\right)\Big|_\Gamma\cdot\mathbf{n} \quad &\text{on } [0,T]\times\Gamma. \end{aligned} \tag{1b}$$

Relaxation step:

$$h^k(t,x) = \omega\tilde{h}^k + (1-\omega)h^{k-1}, \quad \omega\in(0,1]. \tag{1c}$$

Our Research Questions

Goal: Analyze this coupling iteration.

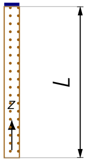
- Does it converge?
- At which rate?
- Can we accelerate convergence by picking a good ω?

Idea: Apply fully discrete analysis technique[1] for **linear** problems to this problem!

[1] Azahar Monge and Philipp Birken. "On the Convergence Rate of the Dirichlet–Neumann Iteration for Unsteady Thermal Fluid–Structure Interaction". In: *Comput. Mech.* 62.3 (Sept. 2018), pp. 525–541. DOI: 10.1007/s00466-017-1511-3.

Simplifying the Model Problem

1. Reduce dimension: Vertical processes matter most
2. Linearize: Assume $c(\psi) = c > 0$, $K(\psi) = K > 0$



Given $h^0(t)$, compute sequentially for $k = 1, 2, \ldots$:

$$
\begin{aligned}
c\frac{\partial \psi^k}{\partial t} - K\frac{\partial^2}{\partial z^2}\psi^k &= 0 \quad \text{on } (0,T] \times \Omega \\
\psi^k\Big|_{z=L} &= h^{k-1} \quad \text{on } [0,T]
\end{aligned}
\tag{2a}
$$

$$
\frac{d\tilde{h}^k}{dt} = -K\,\partial_z\left(\psi^k + z\right)\Big|_{z=L} \quad \text{on } (0,T] \tag{2b}
$$

Relaxation step:

$$
h^k(t) = \omega\tilde{h}^k(t) + (1-\omega)h^{k-1}(t) \tag{2c}
$$

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Discretization in Space & Time

- Consider coupled system without coupling iteration
- Space: Linear finite elements for subsurface flow
- Time: Implicit Euler (IE) method in both solvers $\Rightarrow \vec{\psi}^n \in \mathbb{R}^{M-1}, h^n \in \mathbb{R}$

$$\begin{bmatrix} B_1 & B_2 \\ {B_2}^T & B_3 + 1 \end{bmatrix} \begin{pmatrix} \vec{\psi}^n \\ h^n \end{pmatrix} = - \begin{bmatrix} M_1 & M_2 \\ {M_2}^T & M_3 + 1 \end{bmatrix} \begin{pmatrix} \vec{\psi}^{n-1} \\ h^{n-1} \end{pmatrix} + \begin{pmatrix} 0 \\ -\Delta t K \end{pmatrix}$$

- $B_i := M_i + \Delta t A_i$ mass + stiffness matrices
- Coupling iteration: splitting of this system!

Fully Discrete Coupling Iteration

Given $h^{n,0}$, compute sequentially for $k = 1, 2, \dots$:

$$B_1 \vec{\psi}^{n,k} = -B_2 h^{n,k-1} + M_1 \vec{\psi}^{n-1} + M_2 h^{n-1} \tag{3a}$$

$$\tilde{h}^{n,k} = -B_2{}^T \vec{\psi}^{n,k} - B_3 h^{n,k-1} + M_2 \vec{\psi}^{n-1} + (M_3 + 1) h^{n-1} - \Delta t K \tag{3b}$$

Relaxation step:

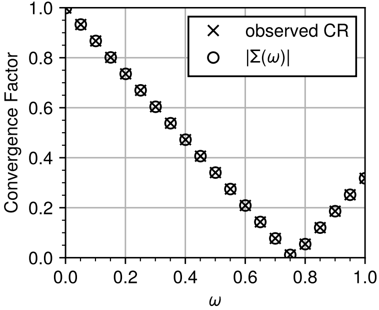
$$h^{n,k} = \omega \tilde{h}^{n,k} + (1-\omega) h^{n,k-1} \tag{3c}$$

Discrete Analysis

Idea 1: Express everything in terms of h (scalar!), giving a matrix $S \in \mathbb{R}^{1\times 1}$

$$h^{n,k} = \underbrace{(\omega S + (1-\omega))}_{=:\Sigma(\omega)} h^{n,k-1} + \xi^{n-1}.$$

Convergence governed by $|\Sigma(\omega)|$: ("Fundamental Thm. of Numerical Linear Algebra!" — P. Birken)



Explicit Value for S

Idea 2: Compute S explicitly, using knowledge about the discretization matrices. (B_1 sym. tridiag. Toeplitz!)[2]

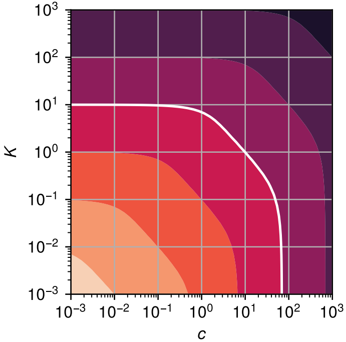
$$S := {B_2}^T {B_1}^{-1} B_2 - B_3 = b^2 \alpha - \frac{a}{2}$$

with

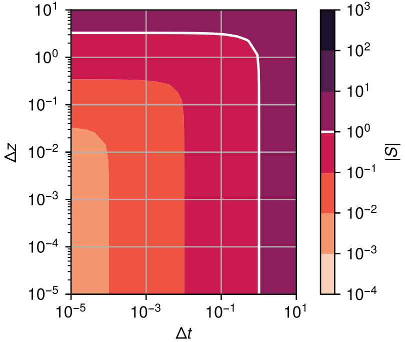
$$a := \frac{2}{3} c\Delta z + \frac{2K\Delta t}{\Delta z}, \quad b := \frac{1}{6} c\Delta z - \frac{K\Delta t}{\Delta z}, \quad \alpha := \frac{\Delta z}{L} \sum_{j=1}^{M-1} \frac{\sin^2\left(\frac{j\pi\Delta z}{L}\right)}{\frac{a}{2} - b\cos\left(\frac{j\pi\Delta z}{L}\right)}.$$

[2] Azahar Monge and Philipp Birken. "On the Convergence Rate of the Dirichlet–Neumann Iteration for Unsteady Thermal Fluid–Structure Interaction". In: *Comput. Mech.* 62.3 (Sept. 2018), pp. 525–541. DOI: 10.1007/s00466-017-1511-3.

$|S|$ for different parameter choices



Varying c, K, fixed $\Delta z = 1/20$, $\Delta t = 10^{-1}$.



Fixed $c = K = 1$, varying grid sizes.

Fast, slow, and no convergence possible; smaller $\Delta t, \Delta z, c, K$ give faster convergence.

$\rightarrow$ Does this hold in the nonlinear, 2D-1D case?

Numerical Results

Notes on the Implementation

- Implicit Euler in time, Linear FE & FV in space
- Python bindings of DUNE (subsolvers) + preCICE (coupling)[3]
- Termination criterion based on residual:

$$\mathrm{res}^{n,k} := \left\| \tilde{h}^{n,k} - h^{n,k-1} \right\|_2 < \mathrm{TOL} = 10^{-8}$$

- Experimental convergence factor:

$$\mathrm{CR} = \frac{1}{K-2} \sum_{k=2}^{K-1} \frac{\mathrm{res}^{n,k}}{\mathrm{res}^{n,k-1}}$$

- Expected convergence factor: $S(\Delta t, \Delta z, \overline{c(\psi^n)}, \overline{K(\psi^n)})$

[3] Code available at: `https://gitlab.maths.lu.se/nuan/projects/coupled-hydrology`

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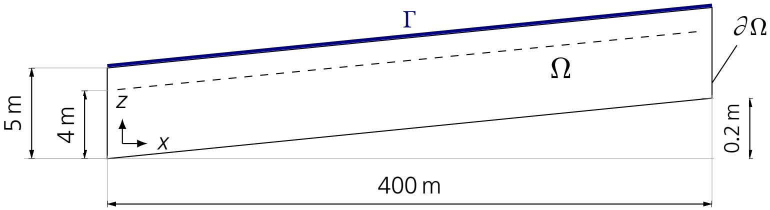
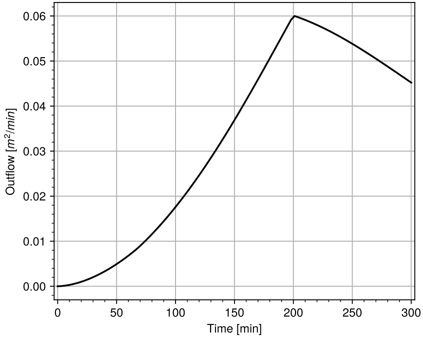
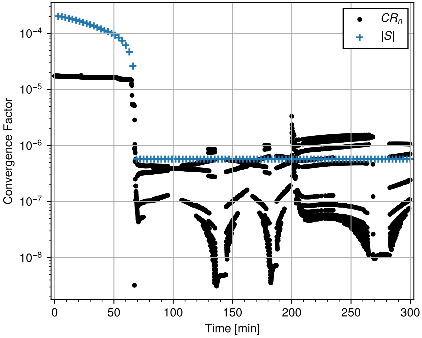
Case 1: Coupled Hillslope



- Large-scale experiment based on [2]
- Uniform rainfall rate, cut off after 200 min → outflow at left boundary!
- Soil: homogeneous silt loam

Case 1: Results





→ $|S|$ captures convergence factor decrease due to changing c, K!
Nonlinear effects not captured.

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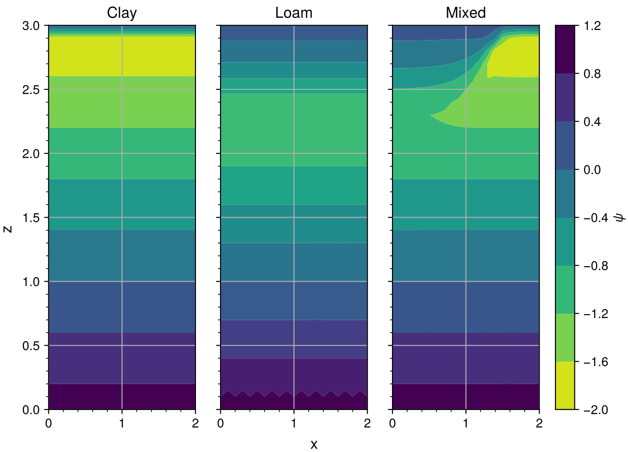
Case 2: Coupled Drainage Trench

- Small-scale experiment based on [3]
- Flat water surface, filled at rate $10\,\mathrm{cm\,h^{-1}}$ for $2\,\mathrm{h}$



Soil water potential ψ after $3\,\mathrm{h}$.

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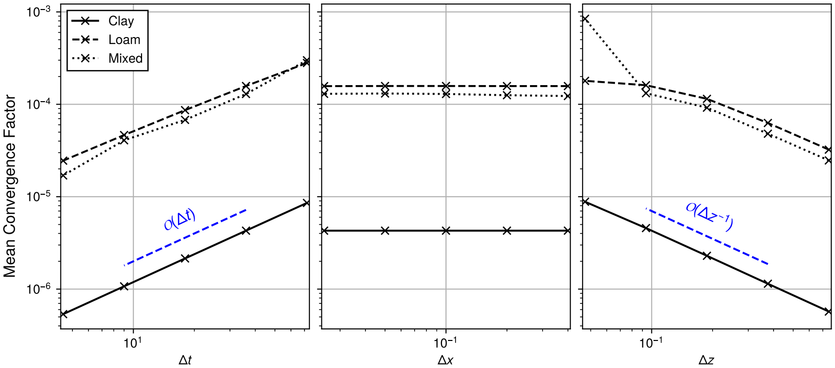
Case 2: Observed Grid Dependence



→ No dependence on Δx; Qualitative differences for $\Delta z, \Delta t$ dependence!

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Summary

- Partitioned, iteratively coupled surface-subsurface flow model
- Richards' equation + shallow water equations
- Linear, 1D-0D analysis for a highly nonlinear, 2D-1D problem
- Merits: we can explain fast convergence, dynamic behavior due to changing c, K
- Limits:
  - nonlinear effects not captured
  - qualitative & quantitative differences between analysis and experiments
- In practice, iterations converge quickly; no acceleration necessary!

Full paper on arXiV![4]

[4] V. S., Philipp Birken, and Andreas Dedner. *Convergence Properties of Iteratively Coupled Surface-Subsurface Models*. Submitted. arXiv: 2408.12582.

Thank You!

References

[1] Azahar Monge and Philipp Birken. “On the Convergence Rate of the Dirichlet–Neumann Iteration for Unsteady Thermal Fluid–Structure Interaction”. In: *Comput. Mech.* 62.3 (Sept. 2018), pp. 525–541. DOI: 10.1007/s00466-017-1511-3.

[2] Reed M. Maxwell et al. “Surface-Subsurface Model Intercomparison: A First Set of Benchmark Results to Diagnose Integrated Hydrology and Feedbacks”. In: *Water Resour. Res.* 50.2 (2014), pp. 1531–1549. ISSN: 1944-7973. DOI: 10.1002/2013WR013725.

[3] Florian List and Florin A. Radu. “A Study on Iterative Methods for Solving Richards’ Equation”. In: *Comput Geosci* 20.2 (Apr. 2016), pp. 341–353. ISSN: 1573-1499. DOI: 10.1007/s10596-016-9566-3.

[4] V. S., Philipp Birken, and Andreas Dedner. *Convergence Properties of Iteratively Coupled Surface-Subsurface Models*. Submitted. arXiv: 2408.12582.

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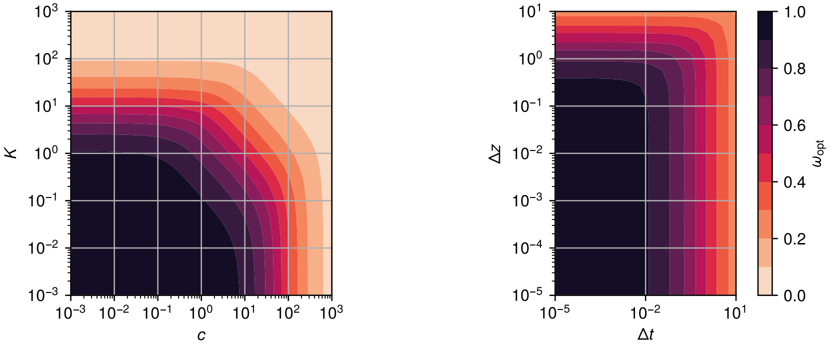
Appendix

Exploring 1D-0D Results



Varying c, K, fixed $\Delta z = 1/20$, $\Delta t = 10^{-1}$.

Fixed $c = K = 1$, varying grid sizes.

$\omega_{\text{opt}} = 1/(1-S)$ for different parameter choices.

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Constitutive Equations: van Genuchten Model

$$c(\psi) = \begin{cases} \alpha(\theta_S - \theta_R)(n_G - 1)(\alpha|\psi|)^{n_G - 1}(1 + (\alpha|\psi|)^{n_G})^{(1/n_G - 2)}, & \psi \leq 0, \\ 0, & \psi > 0. \end{cases}$$

$$K(\psi) = \begin{cases} K_S\sqrt{\theta(\psi)}\left[1 - \left(1 - \theta(\psi)^{\frac{n_G}{n_G - 1}}\right)^{\frac{n_G - 1}{n_G}}\right]^2, & \psi \leq 0, \\ K_S, & \psi > 0. \end{cases}$$

Material Parameters

Parameter		Unit	Beit-Netofa Clay	Silt Loam	Sandy Loam
Alpha	α	m^{-1}	0.152	0.423	100.0
Pore-size distributions	n_G	-	1.17	2.06	2.0
Residual water content	θ_R	-	0.0	0.131	0.2
Saturated water content	θ_S	-	0.446	0.396	1.0
Sat. hydraulic conductivity	K_s	m/s	9.49×10^{-9}	5.74×10^{-7}	$1.16 \times 10^{\{-5,-6,-7\}}$
Max. hydraulic capacity	c	m^{-1}	7.45×10^{-3}	0.0449	30.6

The van Genuchten parameters used in the nonlinear numerical experiments. The last two rows state maxima for K and c for all ψ according to the van Genuchten model.

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Simulation Parameters: Hillslope

Parameter		Unit	Sandy Loam	Silt Loam
Time step size	Δt	s	60	1
Horizontal mesh size	Δx	m	80	80
Vertical mesh size	Δz	m	0.2	0.2
Manning's coefficient	n_M	$m^{1/3}$min	3.31×10^{-3}	3.31×10^{-3}
Bed slope	S_f	%	0.05	0.05
Rainfall rate	r	m/min	3.30×10^{-4}	3.30×10^{-4}, 3.30×10^{-5}

Simulation parameters for the coupled hillslope experiments.

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