Coupled modeling of groundwater/surface water interactions: successes and challenges from recent applications



Claudio Paniconi

Institut National de la Recherche Scientifique, Centre Eau Terre Environnement (INRS-ETE) Université du Québec, Québec, Canada (claudio.paniconi@ete.inrs.ca)

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Context

Proper understanding and representation of hydrosphere interactions (between the atmosphere, land surface, soil zone, aquifers, rivers/lakes, and vegetation) is increasingly relevant to climate prediction, environmental protection, and water management



We are at a crossroads in hydrological modeling:

- models (of all flavors) are being integrated across many disciplines and over multiple scales, and they are being intercompared
- better datasets are increasingly being made available (for hypothesis testing and model validation) that provide observations (on the ground, airborne, and from space) of more processes, in more detail, and at higher accuracy
- computational boundaries are continually being pushed (cost and capabilities of systems, efficiency and robustness of algorithms), for easier and more effective data analysis and process simulation

CATHY (CATchment HYdrology) model description

Some recent studies (successes and challenges)

Extensions and evolution of the model



CATHY (CATchment HYdrology) model description

$$\sigma(S_w)\frac{\partial\psi}{\partial t} = \nabla \cdot \left[K_s K_{rw}(S_w)(\nabla\psi + \eta_z)\right] + q_s(h)$$

$$\frac{\partial Q}{\partial t} + c_k \frac{\partial Q}{\partial s} = D_h \frac{\partial^2 Q}{\partial s^2} + c_k q_L(h, \psi)$$
⁽²⁾

 σ $S_{w} \theta$ θ_{s} $S_{s} \phi$ ψ t K_{s} K_{rw} η_{z}

general storage term [1/L]: $\sigma = S_w S_s + \phi(dS_w/d\psi)$ water saturation = θ/θ_s [/] volumetric moisture content [L³/L³] saturated moisture content [L³/L³] specific storage [1/L] porosity (= θ_s if no swelling/shrinking) pressure head [L] time [T] saturated conductivity tensor [L/T] relative hydraulic conductivity [/] zero in *x* and *y* and 1 in *z* direction

Z	vertical coordinate +ve upward [L]
q_s	subsurface equation coupling term
0	(more generally, source/sink
	term) $[L^3/L^3T]$
h	ponding head (depth of water on
	surface of each cell) [L]
s	hillslope/channel link coordinate [L]
Q	discharge along s [L ³ /T]
C_k	kinematic wave celerity [L/T]
$\hat{D_h}$	hydraulic diffusivity [L ² /T]
q_L	surface equation coupling term
	(overland flow rate) [L ³ /LT]

(1) Paniconi & Wood, Water Resour. Res., 29(6), 1993 ; Paniconi & Putti, Water Resour. Res., 30(12), 1994

(2) Orlandini & Rosso, J. Hydrologic Engrg., ASCE, 1(3), 1996; Orlandini & Rosso, Water Resour. Res., 34(8), 1998

(1)+(2) Putti & Paniconi, CMWR Proceedings, 2004; Camporese, Paniconi, Putti, & Orlandini, Water Resour. Res., 46(W02512), 2010

Path-based description of surface flow across the drainage basin; several options for identifying flow directions, for separating channel cells from hillslope cells (same governing equation), and for representing stream channel hydraulic geometry.

The coupling term for the model is computed as the balance between atmospheric forcing (rainfall and potential evaporation) and the amount of water that can actually infiltrate or exfiltrate the soil. This threshold-based boundary condition switching partitions potential fluxes into actual fluxes and changes in surface storage.





Various functional forms for $S_w(\psi)$ and $K_{rw}(\psi)$

Heterogeneities (K_{sx} , K_{sy} , K_{sz} , S_s , ϕ) by "zone" and by layer

DEM-based (uniform) grid or user-defined (nonuniform) surface grid input

3D grid automatically generated with variable layer thicknesses and different base ("bedrock") shapes

Finite element spatial integrator (Galerkin scheme, tetrahedral elements, linear basis functions)

Weighted finite difference discretization in time

Time-varying boundary conditions: Neumann, Dirichlet, source/sink terms, seepage faces, and atmospheric fluxes

Adaptive time stepping; Newton and Picard linearization; selection of CG-type linear solvers; etc









Overland (hillslope rills) and channel flow along s

DEM pre-analysis for definition of cell drainage directions, catchment drainage network and outlet, etc

"Constant critical support area": overland flow \forall cells with upstream drainage area $A < A^*$; else channel flow (2 other threshold-based options also implemented)

Leopold & Maddock scaling relationships; Muskingum-Cunge solution scheme (explicit and sequential); etc

"Lake boundary-following" procedure to pre-treat lakes

Storage and attenuation effects of lakes and other topographic depressions are accounted for by transferring with infinite celerity all the water drained by the "buffer" cells to the "reservoir" cell; level pool routing calculates the outflow from this cell:

$$\frac{\partial V}{\partial t} = I(t) - O(h^*)$$









Surface runoff propagated through a network of rivulets and channels automatically extracted from the DEM.

Spatial (term I) and temporal (term II) variations of flow characteristics of the drainage network (stream channel geometry W and conductance coefficient k_s) derived from application of downstream (according to upstream drainage area) and at-a-station (according to flow discharge) fluvial relationships:



* From L. B. Leopold and T. Maddock Jr. (1953), "The hydraulic geometry of stream channels and some physiographic implications", U. S. Geological Survey, Professional Paper no. 252

Coupling, time stepping, and iteration

"Pond_head_min" threshold parameter accounts for microtopography

Coupled system solved sequentially^{*}: surface first, for Q^{k+1} and h^{k+1} ; then subsurface, for ψ^{k+1} ; finally overland flow rates q_L^{k+1} are back-calculated from subsurface solution [*sequential solution procedure but with iterative BC switching during subsurface resolution to resolve the coupling]

Nested time stepping: one or more surface solver time steps for each subsurface time step (based on Courant and Peclet criteria for the explicit surface routing scheme; also reflects typically faster surface dynamics compared to subsurface)

Interaction between cell-based surface grid and nodebased subsurface grid includes input option for coarsening of latter grid. Allows us to exploit slower subsurface dynamics and looser grid constraints (implicit scheme), and can lower CPU and storage costs of 3D module





Boundary condition-based coupling (surface BC switching procedure)



Some recent studies (successes and challenges)

Recharge estimation (impact of heterogeneity

Hydrograph separation (model coupling approaches)

Bedrock leakage (and the importance of boundary conditions)

Seepage faces (more on BCs)

Predicting near-surface soil moisture (a "too-wet" bias?)

Storage-discharge hysteresis (and other nonlinear phenomena

Rill flow vs sheet flow (model intercomparison exercises)

Simulation of multiple response variables (flow only, integrated measures)

Simulation of multiple response variables (add transport, distributed measures)

Grid scale variance (problem or fact of life?)

Nonlinear solver performance (numerical issues)

Recharge estimation (impact of heterogeneity): Thomas Brook catchment, Annapolis Valley, Nova Scotia



What is the role of mechanisms such as reinfiltration or fill-and-spill?

Gauthier et al.: Hydrol. Earth Syst. Sci., 2009

Hydrograph separation (model coupling approaches): Havelock hillslope, southwestern Quebec



Bedrock leakage (and the importance of BCs): idealized hillslopes / sloping unconfined aquifers



Broda et al.: J. Hydrol., 2011

Seepage faces (more on BCs): idealized hillslopes, Landscape Evolution Observatory (LEO)



Predicting near-surface soil moisture (a "too-wet" bias?): des Anglais river basin, southwestern Quebec





CATHY can reproduce hysteresis and thresholding behavior observed in the relationship between the subsurface storage and discharge responses of a small catchment. No ad hoc parameterization is needed.

Is there any link to or contribution from unsaturated zone hysteresis?

Nature and role of nonlinear phenomena in atmosphere– land surface–soil–aquifer interactions and feedbacks are poorly understood.

Simulated (top) and observed (bottom) responses in shallow, deep, and intermediate observation wells for 7-8 August 2009 (left) and 16-18 August 2009 (right) rainfall events.

Rill flow vs sheet flow (model intercomparison exercises): benchmark problems





Benchmarking is a complicated business even for synthetic test cases ... Why and how do different models (even based on the same equations) perform differently? And what to do about it??

Evolution of the point of intersection between the water table and the land surface for the sloping plane test case. The outlet face is at x = 400 m. ParFlow: solid line; CATHY: dashed-dotted (sheet flow) and dashed (rill flow).

Simulation of multiple response variables (flow only, integrated measures): Biosphere 2 LEO



"Perfect knowledge" of the bottom BC ... how much does this

Niu et al.: Hydrol. Earth Syst. Sci., 2014



All three variables on previous slide are integrated measures of the hillslope response. How does the model perform when we examine distributed responses? And what happens when we include solute transport? ...







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Grid scale variance (problem or fact of life?): des Anglais river basin, southwestern Quebec



Nonlinear solver performance (numerical issues): synthetic test case with dynamic ponding



Iterative schemes (Picard, Newton, nested Newton, ...), mass conservation (including data assimilation considerations), accuracy of velocity calculations (especially important for gw recharge and for solute transport), etc – all still ongoing research topics!



Adaptive time stepping behavior for Picard (top) and Newton (bottom) at four different vertical discretizations (10, 50, 250, and 500 layers for black, green, red, and blue curves, respectively).

Extensions and evolution of the model (flow and transport; other processes)

Flow (water quantity and distribution)

Surface

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{c}_k \frac{\partial \mathbf{Q}}{\partial \mathbf{s}} = \mathbf{D}_h \frac{\partial^2 \mathbf{Q}}{\partial \mathbf{s}^2} + \mathbf{c}_k \mathbf{q}_s$$

Subsurface

$$\sigma(\mathbf{S}_{w})\frac{\partial \psi}{\partial t} = \nabla \cdot \left[\mathbf{K}_{s}\mathbf{K}_{r}(\mathbf{S}_{w})(\nabla \psi + \eta_{z})\right] + \mathbf{q}_{ss}$$

Transport (water quality and interactions with other substances)

Surface

$$\frac{\partial \mathbf{Q}_m}{\partial t} + \mathbf{C}_t \frac{\partial \mathbf{Q}_m}{\partial \mathbf{s}} = \mathbf{D}_c \frac{\partial^2 \mathbf{Q}_m}{\partial \mathbf{s}^2} + \mathbf{C}_t \mathbf{q}_{ts}$$

Subsurface

$$\frac{\partial \theta c}{\partial t} = \nabla \cdot \left[-qc + D\nabla c \right] + q_{tss}$$

Weill et al.: Adv. Water Resour., 2011

Coupling scheme (sequential; iterative BC switching provides updated information)



Atmospheric forcing land surface models

hydrostatic and nonhydrostatic LAM

Water "quantity"

surface flow saturated flow unsaturated flow multiphase flow preferential flow root water uptake

"Coupled" models

surface-subsurface reaction-transport-mechanics erosion & sediment transport DSS & cost-benefit analysis saltwater & brines vegetation & crops water-solute-heat

Water "quality"

advection-dispersion transport linear sorption and decay reaction kinetics (non-LEA) multi-component and -species biodegradation redox, precipitation/dissolution

Evolution of the model

face hydrologic processes Water Resour, Res., 29, 1993 solution of multidimensional variably saturated flow problems. Water Resour. Res., 30, 1994 ariable density, transport_{8, 1995} (an early coupled model) dra. SIAM J. Sci. Comput., 19, 1998 stributed modeling of catchi Vnt dynamics. Water Resour, Res., 34, 1998 ndent flow and miscible salt transport. Seawater Intrusion in Coastal Aquifers, chap. 10, Kluwer Academic, 1999 Surface/Subsurface flow Shestopalov, Bublias, Bohuslavsky, Kastel GOUD : Modeling groundwater-surface water interactions in the Chernobyl exclusion zone. Environ. Geol., 42, 2002 ation-based distributed hydrological model. Adv, Water Resour., 26, 2003 for density driven flow sim<mark>v</mark>ations in porous media. **J. Comp. Phys.**, 208, 2005 Advanced numerics Res., 42 nent-Finite Volume approach for the solution of der<mark>s</mark>ity dependent flow in porous media. **J. Comput, Appl, Math.,** 185, 2006 Int. J. Numer, Meth. Fluids. Surface-subsurface modeling with pamproved grid-based DEMg, and assimilation of multisource observation data. Water Resour. Res., 46, 2010 ions in grid-based digital elevation models. Water Resour, Res., 39, 2003 determination of nond similation for a process-based, atchment scale model of surface and subsurface flow. Water Resour, Res., 45, 2009 vation data. Water Resour, Res., 45, 2009 Data assimilation nulating surface water-groundwater interactions. Adv. Water Resour., 33, 2010 -subsurface hydrological model. Adv. Water Resour., 34, 2011 Surf/subsurf-&_flow/ Water Resour. Res., 47. 2011 coupling odel. Adv. Water Resour., 47, 2012 Comparison of two modeling approaches for groundwater-surface water interactions. Hydrol, Process., 27, 2013 nulations and field observations, Adv. Water Resour., 59, 2013 Ecohydrological modeling (LSM coupling, vegetation, energy Ecohydrol, 7, 2014 balance, CO2, nutrient cycles) eg, CATHY-NoahMP for soil moisture in a 3D so -plant model. Adv. Water Resour., 66 Maxwell, Putti, Meverhoff, Delfs, Ferguson, Ivanov, Kim, Kolletz, Kollet, Kumar, Lopez, Niu, Panico VPark, Phanikumar, Shen, Sudicky, Sulis; Surface-subsurface model intercomparison; A first set of benchmark results to diagnose integrated hydrology and feedbacks. Water Resour. Res., 50, Detailed experiments a geophysical inversion a parameter estimation at, 514, 2014 sensitivity & uncertainty analysis, model intercomparison, experiment at the Biosphere 2 Landscape biogeochemistry & soil weathering, sediment transport & erosion,

soil freezing & snowmelt, preferential flow, unstructured grids, RCM/NWP coupling (CATHY-NoahMP-WRF?), ...

Mario Putti, Annamaria Mazzia, Matteo Camporese, Gabriele Manoli, Sara Bonetti – *University of Padua, Italy*

Stefano Orlandini, Giovanni Moretti, Marcello Fiorentini – University of Modena and Reggio Emilia, Italy

Mauro Sulis – now at University of Bonn, Germany

Sylvain Weill – now at University of Strasbourg, France

Guo-Yue Niu – University of Arizona, USA

Cécile Dagés – INRA-Montpellier, France

Damiano Pasetto, Carlotta Scudeler – INRS-ETE and University of Padua

many others (sensitivity tests, case studies, ...)