

Land modeling challenges and the emergence of CTSM

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Main collaborators/funding



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Outline



• Background

- Remarkable scientific and technical advances in many areas supporting hydrologic modeling and prediction
- Modeling challenges
 - Processes
 - Parameters
 - Computing
- The emergence of CTSM
- Summary and research needs

Advances in remote sensing



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GRACE total water storage estimates Scanlon et al., WRR 2016





Landsat DOY 339 Planet DOY 340 Cubesats in hydrology *McCabe et al., WRR 2017*

Airborne LIDAR estimates of snow 5.8 *Lettenmaier et al., WRR 2017*

Advances in hydrologic modeling

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Clark et al., 2008; Mizukami et al., 2016

Information theory

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RESEARCH ARTICLE

10.1002/2016WR020218

This article is a companion to Goodwell and Kumar [2017], doi:10.1002/2016WR020216.

Key Points:

- A Temporal Information Partitioning Network (TIPNet) characterizes time dependencies between interacting variables
- TIPNets based on weather station data show increased complexity of interactions under heightened variability of radiation and wetness Trends in network links over a growing season reveal altered dependencies that indicate transitions in rainfall and vegetation activity

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Citation

Goodwell, A. E. and P. Kumar (2017), Temporal Information Partitioning Networks (TIPNets): A process network approach to infer ecohydrologic shifts, *Water Resour. Res.*, *53*, 5899–5919,

Temporal Information Partitioning Networks (TIPNets): A process network approach to infer ecohydrologic shifts

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Abstract In an ecohydrologic system, components of atmospheric, vegetation, and root-soil subsystems participate in forcing and feedback interactions at varying time scales and intensities. The structure of this network of complex interactions varies in terms of connectivity, strength, and time scale due to perturbations or changing conditions such as rainfall, drought, or land use. However, characterization of these interactions is difficult due to multivariate and weak dependencies in the presence of noise, nonlinearities, and limited data. We introduce a framework for Temporal Information Partitioning Networks (TIPNets), in which time-series variables are viewed as nodes, and lagged multivariate mutual information measures are links. These links are partitioned into synergistic, unique, and redundant information components, where synergy is information provided only jointly, unique information is only provided by a single source, and redundancy is overlapping information. We construct TIPNets from 1 min weather station data over several hour time windows. From a comparison of dry, wet, and rainy conditions, we find that information strengths increase when solar radiation and surface moisture are present, and surface moisture and wind variability are redundant and synergistic influences, respectively. Over a growing season, network trends reveal patterns that vary with vegetation and rainfall patterns. The framework presented here enables us to interpret process connectivity in a multivariate context, which can lead to better inference of behavioral shifts due to perturbations in ecohydrologic systems. This work contributes to more holistic characterizations of system behavior, and can benefit a wide variety of studies of complex systems.



Figure 1. Illustration of complex network behavior in an ecohydrologic system. (a) Time-dependent interactions occur between solar radiation (*Rg*), precipitation (*PPT*), leaf wetness (*LWet*) or moisture condition, wind speed (*WS*), relative humidity (*RH*), and air temperature (*Ta*). We characterize these dependencies as information transfers within a network that are associated with properties of time scale, strength, uniqueness, redundancy, and synergy. (b) Network properties that may be detected on a seasonal time scale (top) result from an accumulation of interactions that vary on much shorter time scales such as daily or subdaily (bottom).





Coupled human-hydrology interactions 🖗





Di Baldassarre et al., WRR 2015

Technological advances





High performance computing



Egohydrologist @egohydrology · Dec 5 Second law of egohydrology: ideas and can only be created but not destroyed-except *your* ideas exist solely for me to destroy.



1] 2 🖤 4 [



Egohydrologist @egohydrology · Dec 5

Third law of **egohydrology**: the conceptual entropy in any sub-field of hydrology varies inversely with my involvement in it.





Social media...

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Hydrologic vs. atmospheric modeling

- Modeling the terrestrial water cycle depends on the (unknown) details of the landscape
- Increases in horizontal resolution often do not lead to increases in hydrologic model performance (especially at larger scales)
- Need creativity in spatial discretization of the model domain and the way that we parameterize fluxes
- Hydrologists have developed a glut of models that differ in almost every aspect of their conceptualization and implementation







The path to model improvement is not obvious...





Beyond "faith-based modeling"?

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- The choice of modeling approaches (arguably) stems from personal preferences for physics or parsimony
 - Bucket-style rainfall-runoff models
 - Assume that we know nothing
 - Process-based hydrologic models
 - Assume that we know everything

- Need a stronger scientific basis for model development/improvement
 - Treat numerical modeling as a subjective decision-making process – carefully evaluate all modeling decisions in a controlled and systematic way





The Freeze and Harlan blueprint



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BLUEPRINT FOR A PHYSICALLY-BASED, DIGITALLY-SIMULATED HYDROLOGIC RESPONSE MODEL

R. ALLAN FREEZE Inland Waters Branch, Department of Energy, M Calgary, Alberta, Canada

and

R. L. HARLAN Forestry Branch, Department of Fisheries and Forestry,

Abstract: In recent years hydrologists have subjected the hydrologic cycle to intensive study, designed to discover the arrive at physical and mathematical descriptions of the flow meaningful results are now available in the form of numeration boundary value problems for groundwater flow, unsaturate flow, and channel flow. These developments in physical tremendous advance in digital computer technology, sho necessary redirection of research in hydrologic response no sophistication that can be achieved with presently available areas for necessary future research are pinpointed.

"The ability to accurately predict beha severe test of the adequacy of knowledg subject."

CRAWFORD and L



Fig. 3. Schematic diagram of (a) Hydrologic basin and (b) Three dimensional nodal model of hydrologic basin.

Questions posed by Freeze and Harlan



- Are physically based mathematical descriptions of hydrologic processes available? Are the interrelationships between the component phenomena well enough understood? Are the developments adaptable to a simulation of the entire hydrologic cycle?
- Is it possible to measure or estimate accurately the controlling hydrologic parameters? Are the amounts of necessary input data prohibitive?
- Have the earlier computer limitations of storage capacity and speed of computation been overcome? Is the application of digital computers to this type of problem economically feasible?

Key challenges

- The choice of modeling approaches (arguably) stems from personal preferences for physics or parsimony
- Need a stronger scientific basis for model development/improvement
 - Treat numerical modeling as a subjective decision-making process *carefully evaluate all modeling decisions in a controlled and systematic way*
- Processes
 - Many models do not adequately represent dominant processes
 - The spatial gradients that drive flow occur at very small spatial scales and are not resolved by even the finest terrain grid used in largedomain hyper-resolution models
- Parameters
 - Models as mathematical marionettes
 - Vegetation and soils datasets have limited resolution and information content
- Computing
 - The rapid advances in computing are revolutionizing capabilities for simulations with large domain size, more detailed process representation, fine horizontal resolution, and large ensembles
 - The expense of complex models can sacrifice opportunities for model analysis, model improvement, and uncertainty characterization









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Two issues: Model proliferation and the shantytown syndrome



• Model proliferation: Every hydrologist has their own model, making different decisions at different points in the model development process

 The shantytown syndrome: Ad-hoc approach to model development

- Model proliferation & the shantytown syndrome make it difficult to test underlying hypotheses and identify a clear path to model improvement
- With current model structures, it is easy to incorporate new equations for a given process, but very difficult to incorporate new approaches that cut across multiple model components (multi-layer canopy example)



The interdisciplinary evolution of land models

70's

80's



10's

R. Fisher



00's

90's

Unifying models





General schematic of the terrestrial water cycle, showing dominant fluxes of water and energy

Conceptual basis:

- 1. Most modelers share a common understanding of how the dominant fluxes of water and energy affect the time evolution of model states
- 2. Differences among models relate to
 - a) the spatial discretization of the model domain;
 - b) the approaches used to parameterize individual fluxes (including model parameter values); and
 - c) the methods used to solve the governing model equations.

The Structure for Unifying Multiple Modeling Alternatives (SUMMA):

Defines a single set of conservation equations for land biogeophysics, with the capability to use different spatial discretizations, different flux parameterizations and model parameters, & different time stepping schemes

Clark et al. (WRR 2011); Clark et al. (WRR 2015a; 2015b)

Unifying process representations



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Unifying spatial configurations





Use cases



- Large-domain extensions
 - Continental-domain simulations now feasible
 - Coupled to mizuRoute, enabling routing on multiple networks
- Model usability
 - A growing set of synthetic test cases and model use cases
 - Extensive stress testing
 - SUMMA in hydroShare

SUMMA simulation of soil water (mm)





Challenge: spatial scaling

- The spatial gradients that drive flow occur at very small spatial scales and are not resolved by even the finest terrain grid used in largedomain hyper-resolution models
 - Hot spots and hot moments
 - Small areas of the landscape and short periods of time have a disproportionate impact on large-scale fluxes

Examples

- Variable source areas
- Intermittent turbulence
- Localized rainfall/snowmelt
- Riparian transpiration
- Macropore flow
- Fill-and-spill



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Challenge: spatial scaling

 <u>Modeling challenge</u>: Develop flux parameterizations that represent the aggregate impact of sub-grid-scale heterogeneities.

- Grid-average fluxes
 - Upscaled parameter values
 - New flux parameterizations
 - Sub-grid probability distributions
 - More...
- Spatial discretization
 - Hydrologic similarity
 - Representative hillslopes
 - Separate computations for process subsets
 - More...





Example: Representative hillslopes





Courtesy Sean Swenson (NCAR)

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Challenge 2: Model parameters



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Model parameters

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- Lack of knowledge of model parameters
 - Vegetation and soils datasets do not have sufficient resolution and information content
 - Same soil type across large areas (assume no heterogeneity)
 - Often limited information on hydraulic properties necessary to simulate heterogeneous hydrologic processes
 - The rigid structure of complex models (e.g., treating uncertain parameters as physical constants) constrains capabilities to represent spatial variations in hydrologic processes
 - One solution: Stochastic hyperresolution simulation
 - Another solution: Focus squarely on relating geophysical attributes to model parameters (MPR)



Model parameters

AGU PUBLICATIONS

Water Resources Research

OPINION ARTICLES

10.1002/2014WR015820

Key Points:

- Complex process-based models have strong a priori constraints
- We provide an example demonstrating strong sensitivity of fixed parameters
- Relaxing strong a priori constraints can help improve hydrology simulations

Are we unnecessarily constraining the agility of complex process-based models?

Pablo A. Mendoza^{1,2,3}, Martyn P. Clark³, Michael Barlage³, Balaji Rajagopalan^{1,2}, Luis Samaniego⁴, Gab Abramowitz⁵, and Hoshin Gupta⁶









Model parameters

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Default parameters

 Spatial discontinuities in model parameters

VIC Soil parameters – CMIP5 default



1950-1999 annual mean runoff



 Spatial discontinuities in model simulations

Mizukami et al., WRR 2017

MPR-flex

- Modify coefficients in transfer functions that relate physical attributes (soil, veg, topography) to model parameters
- Use parameter-specific upscaling operators to represent multi-scale behavior
- Define transfer functions for new models – develop model agnostic MPR (MPR-Flex)



1950-1999 annual mean runoff



Mizukami et al., WRR 2017

- V
- No flux discontinuities
- Parameters more closely related to geophysical attributes



Transferring parameters across space What are the key challenges?

- Representing landscape (vegetation, soil, climate, topography) in the models
- Which attributes have the most influence on catchment behavior (i.e. on the dominant hydrological processes)?







How well can we capture those hydrological signatures?





How well can we capture those hydrological signatures?





Which catchment attributes are most important?



22 catchment attributes as predictors

Correlation bewteen attribute and hydrological signature [-]



Most info in climate, least in soils



How do physical models compare to statistical ones?







Most info in climate, least in soils

Same difficulty in physical and statistical models



Why are simulations good/poor?



Correlation bewteen attribute and hydrological signature [-]



Most info in climate, least in soils

Same difficulty in physical and statistical models

Difficulty relates to spatial noise

Implications for model calibration, evaluation, selection

Process-based parameter estimation? 😔





Need to study process interactions across time scales

Instead of the traditional paradigm of properties define processes, study how processes define properties

How does landscape evolution define the storage and transmission properties of the landscape?

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Challenge 3: Computing

 The computational expense of complex models can sacrifice opportunities for model analysis, model improvement, and uncertainty characterization

- Solutions
 - Hydrologic similarity
 - Representative hillslopes
 - Separate computations for process subsets

••••

 Recent studies show that similarity methods have the same information content as hyperresolution models, and orders of magnitude faster





Newman et al., JHM 2014

Computing = understanding complexity

• A continuum of complexity

- Process complexity: Which processes are represented explicitly?
- <u>Spatial complexity</u>: To what extent do we explicitly represent details of the landscape, and spatial connections (flow of water) across model elements?

• Bucket-style rainfall-runoff models

- Lumping of processes, and lumping of the landscape
- Reliance on inverse methods (calibration) to estimate model parameters
 - Models as mathematical marionettes, giving the "right" answers for the wrong reasons
 - Theoretically unsatisfying

Computationally frugal

- Enables use of ensemble methods
- Enables extensive experimentation with different model parameters

- Process-based hydrologic models
 - Explicitly represent dominant hydrologic and biophysical processes; explicitly represent details of the landscape

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- Reliance on geophysical data to estimate model parameters and widespread use of spatially constant parameters obtained from limited experimental data
 - Huge challenge in relating geophysical data to model parameters
 - Common approach of treating uncertain model parameters as (hard-coded) physical constants
- Computationally expensive
 - Often restricted to a single deterministic simulation
 - Limited model analysis (and "tuning") since mode is too expensive to calibrate

Results from many catchments and models



- Large catchment sample
 - Include catchments of varying topography, climate, vegetation and soils
 - Newman et al. (2015), Addor et al. (2017)

- Large model sample
 - Existing models
 - VIC, CLM, Noah-MP, PRMS, HBV, MHM, SAC
 - Multiple hypothesis frameworks
 - FUSE and SUMMA
 - Clark et al., 2008; 2011; 2015a,b

Efforts from Nans Addor, Naoki Mizukami, Andy Newman, et al.



NSE

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The interdisciplinary challenge of land modeling



CTSM





Conceptual basis

- Modelers agree on many aspects of terrestrial system science
- Differences among models relate to
 - > Flux parameterizations
 - Spatial discretization
 - Numerical solution

SUMMA



Formulates master model template which multiple models can be derived

• Existing models (*CLM*, *Noah-MP*, *WRF-Hydro*, *etc.*) as a special case

The Community Terrestrial Systems Model (CTSM)



Unifies land models across climate, weather, water, and ecology

- Multiple configurations
- Easy to modify/use
- Centralized support

Model construction...

• Consider a very simple land model...





On top of spaghetti???

• Our very simple land model...





Conservation equations

$$\frac{dS_1}{dt} = p - q_{sx} - e - q_{12}$$
$$\frac{dS_2}{dt} = q_{12} - q_b$$

Common numerical implementation

$$S_{1}^{n+1,*} = S_{1}^{n} + p\Delta t$$

$$S_{1}^{n+1,**} = S_{1}^{n+1,*} + q_{sx}\Delta t$$

$$S_{1}^{n+1,***} = S_{1}^{n+1,**} + e\Delta t$$

$$S_1^{n+1} = S_1^{n+1,***} + q_{12}\Delta t$$

Non-standard! Physics are intertwined with numerics

Can't capitalize on decades of progress in applied math



More standard implementations



• The model state equations can be written as

$$\frac{\mathrm{d}\mathbf{S}}{\mathrm{d}t} = \mathbf{g}(\mathbf{S},t)$$

 The <u>exact solution</u> of the average flux over the interval tⁿ (start of the time step) to tⁿ⁺¹ (end of the time step) is

$$\overline{\mathbf{g}}^{n \to n+1} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} (\mathbf{g}(\mathbf{S},\varsigma),\varsigma) \mathbf{d}\varsigma$$

• Given an estimate of the average flux, the model state variables can be updated as

$$\mathbf{S}(t^{n+1}) = \mathbf{S}(t^n) + \Delta t \overline{\mathbf{g}}^{n \to n+1}$$

- The exact solution is computationally expensive, so approximations to the exact solution are used
- The approximation controls the stability, accuracy, smoothness, and efficiency of the solution

A controlled approach to model development

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Laugh tests for land models

Constant precip for three hours at top of a 1-m snowpack

Analytical solution



CTSM is public





Plans for the next-generation land model

- Ecosystem vulnerability and impacts on carbon cycle and ecosystem services
- Sources of predictability from land processes
- Impacts of land use and land-use change on climate, carbon, water, and extremes
- Water and food security in context of climate change, climate variability, and extreme weather



Lateral fluxes of water



Water and land management

Ecosystem Demography / Multi-layer canopy



Key opportunities

- Land modeling applications in climate, weather, water, and ecology
 - Hydrologic prediction across scales / hydrologic ensemble methods
 - Interdisciplinary advances (e.g., the union of hillslope hydrology and FATES)
 - ESM concepts for short-term prediction problems (e.g., impact of vegetation phenology on meteorological prediction, estimating fuel loads for fire)

Integrate land modeling expertise

- Land-atmosphere interactions, hydrologic prediction, water and land management, data assimilation, model analysis
- Monthly NCAR-wide science discussions
- Simplify incorporating new capabilities in land models
 - Modular structure and separating physics from numerics reduces the in-person cost of modifying CLM, a cost borne by NCAR scientists and software engineers and university collaborators







Benefits of a unified land model

- Improve understanding of differences among models (debate about processes)
 - Model inter-comparison experiments flawed because too many differences among participating models
- Improve understanding of model limitations
 - Most models not constructed to enable a controlled and systematic approach to model development and improvement
- Improve characterization of model uncertainty
 - Explicitly characterize uncertainty in individual modeling decisions
 - Enables shift from small-ensemble to large-ensemble framework
- Unite disparate (disciplinary) modeling efforts
 - Without a unified modeling framework the community cannot effectively work together, learn from each other, and accelerate model development
- Reduce duplication of effort







Benefits of the proposed model structure

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- Simplifies sharing of code and concepts across different model development groups
 - Separating physics from numerics (the "structural core") and modularity at the flux level accelerates the process of adding/testing new capabilities
- Enables users to include/exclude specific processes
 - Model can be tailored to suit multiple applications
 - Model simplification opens up new possibilities for teaching and research
- Simplifies data assimilation efforts
 - Formalizes the input-state-output relationships, meaning land model construction matches data assimilation methods
- Reduces development costs
 - Modular structure and separating physics from numerics reduces the in-person cost of modifying CLM, a cost borne by NCAR scientists and software engineers and university collaborators





CTSM challenges

- Parallel development
 - Existing models currently used across multiple projects
 - Initially the effort is diffuse (e.g., individuals developing code for both Noah-MP and CTSM)
 - Need to accelerate early applications for different model use cases
 - Rapid prototyping in SUMMA

Modularity/coupling

- Support contributions at multiple levels of granularity (e.g., FATES)
- Community standards for model construction, to simplify sharing code/concepts across model development groups
- Simplify coupling/ease of use across multiple communities

Funding

Support the interdisciplinary challenge of land modeling



SUMMA simulation of soil water (mm)



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Modeling opinions

- We need better frameworks to evaluate the myriad of decisions made during model development (multiple hypothesis frameworks + information theory + ...)
- We need to treat parameter estimation as a model development problem
- Processes
 - We really need to focus on the scaling problem use a mix of explicit discretization and implicit parameterizations to improve simulations of large-scale fluxes
- Parameters
 - We really need to incorporate stronger hydrologic theory when evaluating model parameters it's a physics problem
 - Process parameterizations and model parameters are highly interrelated and should be considered together
- Computing
 - We should not let the allure of computing advances constrain our capabilities for model analysis (let's not get ahead of our skis)
 - Always make room for model analysis









Modeling strategy



- A three-pronged modeling strategy
 - **Processes**: Isolate and evaluate competing modeling approaches.
 - **Parameters**: Improve the agility of process-based models, and focus squarely on relating geophysical attributes to model parameters
 - **Computing**: Take advantage of hydrologic similarity methods to reduce redundancies in hydrologic models and enable extensive analysis. Explore accuracy-efficiency tradeoffs in numerical solutions.
- Modeling strategy explicitly characterizes model uncertainty, as well as uncertainty in model input/response data
 - Probabilistic QPE
 - Ensembles of alternative model configurations
 - Seek to characterize and reduce uncertainties
- Overall goal: Improve the physical realism of models at any scale through better informed choices about the physics.

Continental-domain modeling



Advance large-domain simulations



Specific research needs

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- 1. Unify process-based land modeling
 - Inter-component coupling (make use of legacy models)
 - Intra-component coupling (advance model construction)
- 2. Advance community hydrologic modeling (rather than a single model)
 - Provide accessible and extensible modeling tools
 - Provide key research datasets and model test cases
 - Increase the effectiveness and efficiency in sharing data and model source code (simplify the sharing of data and source code developed by different groups)
- 3. Include/improve missing/poorly represented processes in land models
 - Glaciers, permafrost dynamics, water quality, stream temperature, river ice, etc.
 - Groundwater, humans as an endogenous component of the Earth System
- 4. Systematically explore the benefits of competing modeling approaches
 - Scrutinize models using data from research watersheds
 - Evaluate information gains/losses using models of varying complexity
- 5. Construct variable-complexity models
 - Capabilities to simplify process complexity and spatial complexity
 - Advance applications that require "agile" models
 - Evaluate accuracy-efficiency tradeoffs

Specific research needs (cont.)



- 6. Develop better continental-domain forcing data
 - Probabilistic approach to combine NWP models, radar, and station data
 - Meaningful multi-scale structure and inter-variable relationships
- 7. Advance research on process-oriented approaches to estimate spatial fields of model parameters *parameter estimation as a physics problem*
 - Estimate spatial variations in storage/transmission properties of the landscape
 - New data sources on geophysical attributes, new approaches to link geophysical attributes to model parameters, and new diagnostics to infer model parameters
- 8. Advance methods for model analysis, especially for complex models.
 - Currently very little insight into process/parameter dominance and process/parameter interactions in very complex models
 - Information is desperately needed to inform parameter estimation strategies
- 9. Advance methods to characterize and quantify uncertainty
 - Epistemic and aleatory uncertainty
 - Ensure conclusions are not contaminated by over-confidence
- 10.Obtain better data on hydrologic processes.
 - Motivate and design new field experiments to advance understanding of the terrestrial component of the water cycle across scales and locations.
 - A more productive dialog between experimentalists and modelers



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