ParFlow Short Course

Colorado School of Mines

CUAHSI
Universities Allied for Water Research

Integrated GroundWater Modeling Center

U.S. DEPARTMENT OF ENERGY | Office of Science

MINES

IDEAS productivity

This material and short course was supported by the National Science Foundation and Department of Energy.

Agenda

- Problem Based: Little Washita Watershed

Day 1 (Wednesday May 29th)

9:00 – 10:30	Introductions
10:30 – 12:00	Getting started with ParFlow
12:00 – 1:00	Lunch
1:00 – 2:30	ParFlow installation
2:30 – 3:30	Interacting with ParFlow
3:30 – 5:00	Hands on exercise

Day 2 (Thursday May 30th)

9:00 – 9:30	Questions and recap from Day 1
9:30 - 10:30	ParFlow manual overview
10:30 – 12:00	Domain setup and overland flow simulations
12:00 – 1:00	Lunch
1:00 – 2:00	Overland simulations and exercise continued
2:00 – 4:00	Subsurface setup and spinup exercises
4:00 – 5:00	ParFlow CLM introduction

Day 3 (Friday May 31th)

9:00 – 9:30	Questions and recap from Day 1
9:30 – 10:00	CUAHSI Overview
10:00 – 12:00	Visualization with ParaView
12:00 – 1:00	Lunch
1:00 – 4:00	ParFlow CLM exercises

Meet your instructors

Laura Condon, University of Arizona

Nick Engdahl, Washington State University

David Thompson, KitWare

Model is an ambiguous term

- What do we mean when we say *model?*

- Name some models.

There are many types of models

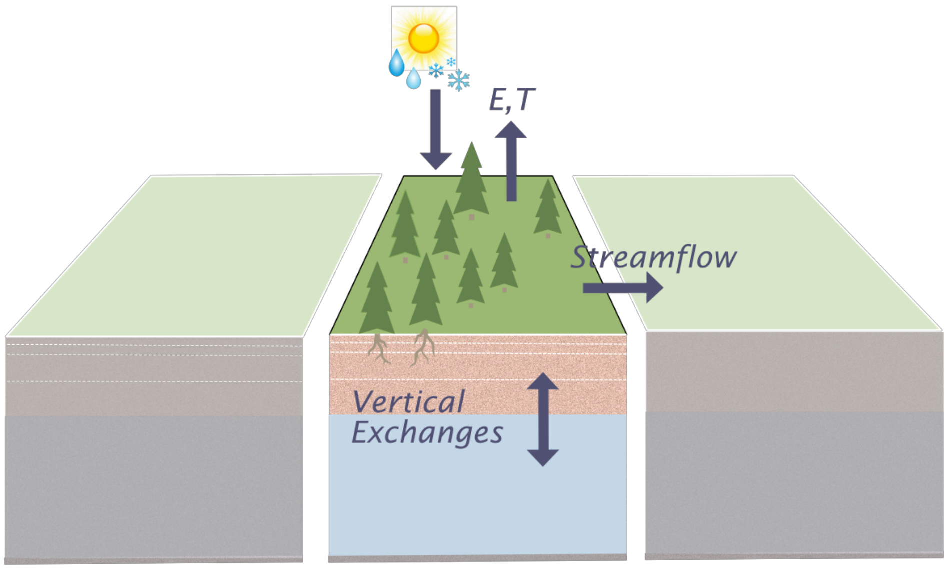
- Conceptual Model
- Physical Model
- Numerical Model

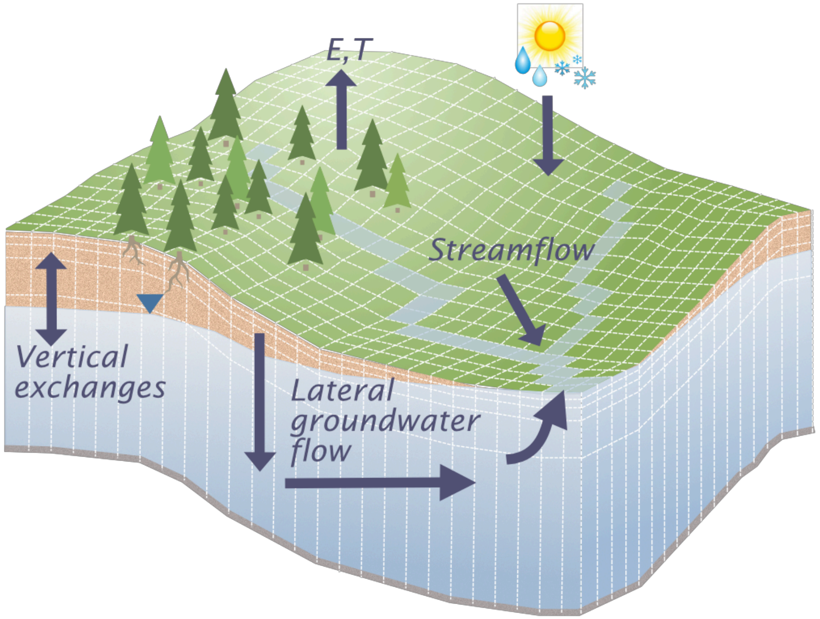
All models have many assumptions

No model is *perfect*

The process of modeling is really important

There are different approaches to modeling complex systems and it is unclear which is ideal





Traditional land surface models **simplify** processes but are **efficient**

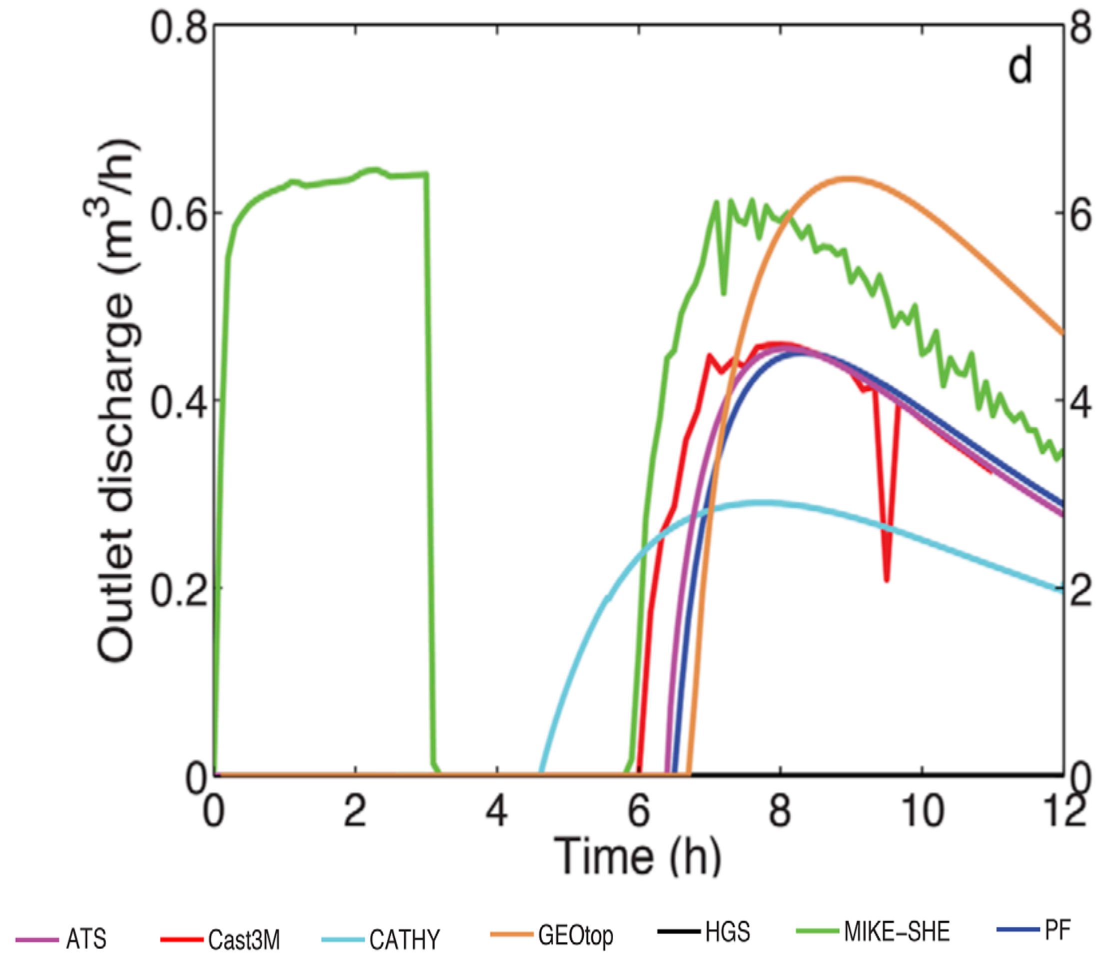
Integrated hydrologic models are **comprehensive** but **expensive**

Computational hydrology is hard but is our best way to relax assumptions

- we solve systems of **nonlinear PDEs**
- we use and develop **robust** and efficient **parallel solution techniques**
- **real problems** with land surface processes are very **hard to solve**

For some problems, this may make the difference between getting the right answers for the right reasons and not

Simulation results from the *superslab* test case show disagreement between conceptual approaches



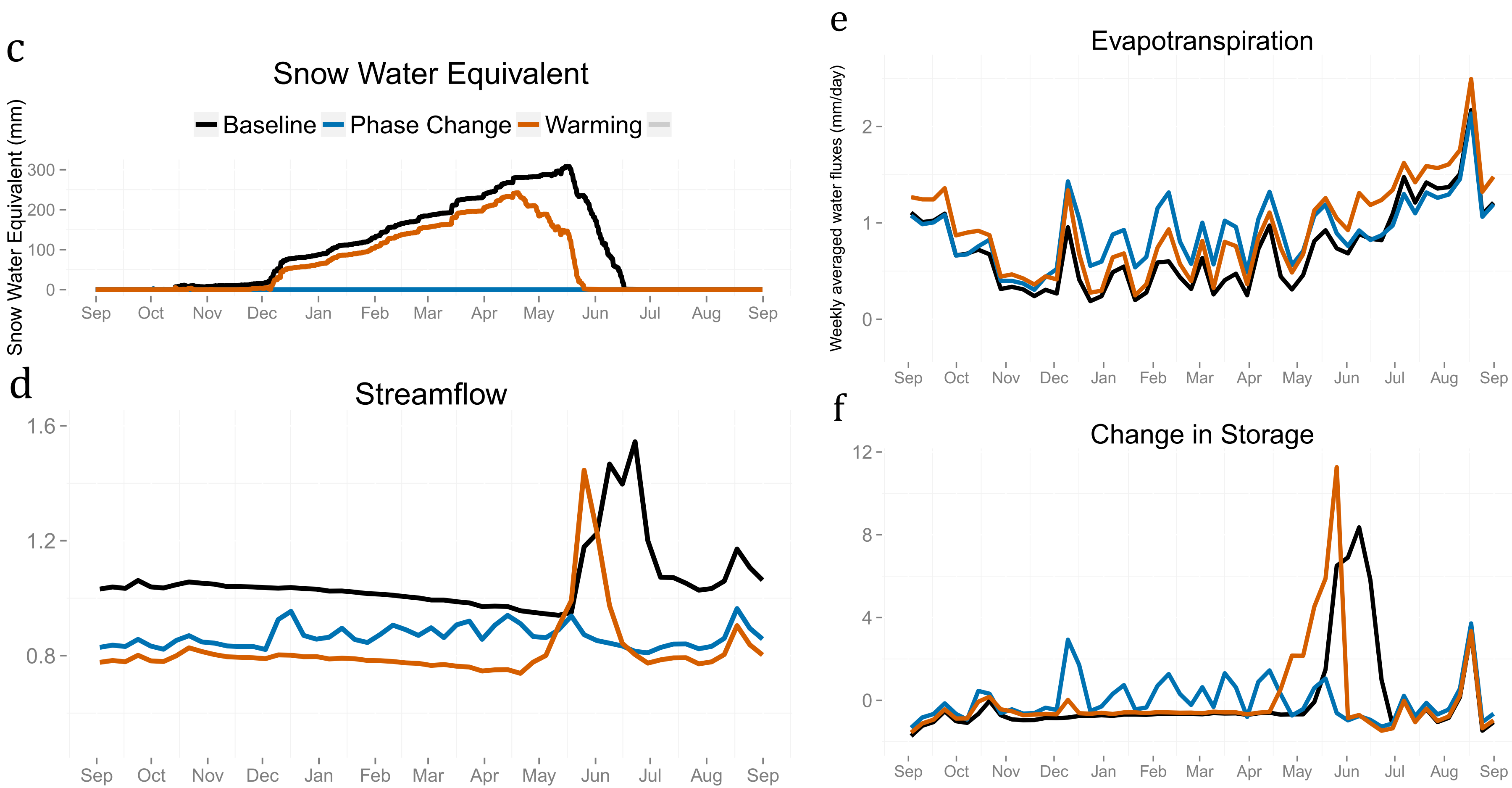
Kollet et al *WRR* 2017

Models can be useful tools to provide insight

- Controlled **numerical experiments** elucidate process interactions under change
- A single perturbation (e.g. temperature increase) can be tracked through the **entire nonlinear system**
- **Connections** we see in simulations can provide **insight** and guide **observations**

Models are useful in ways that the real world isn't

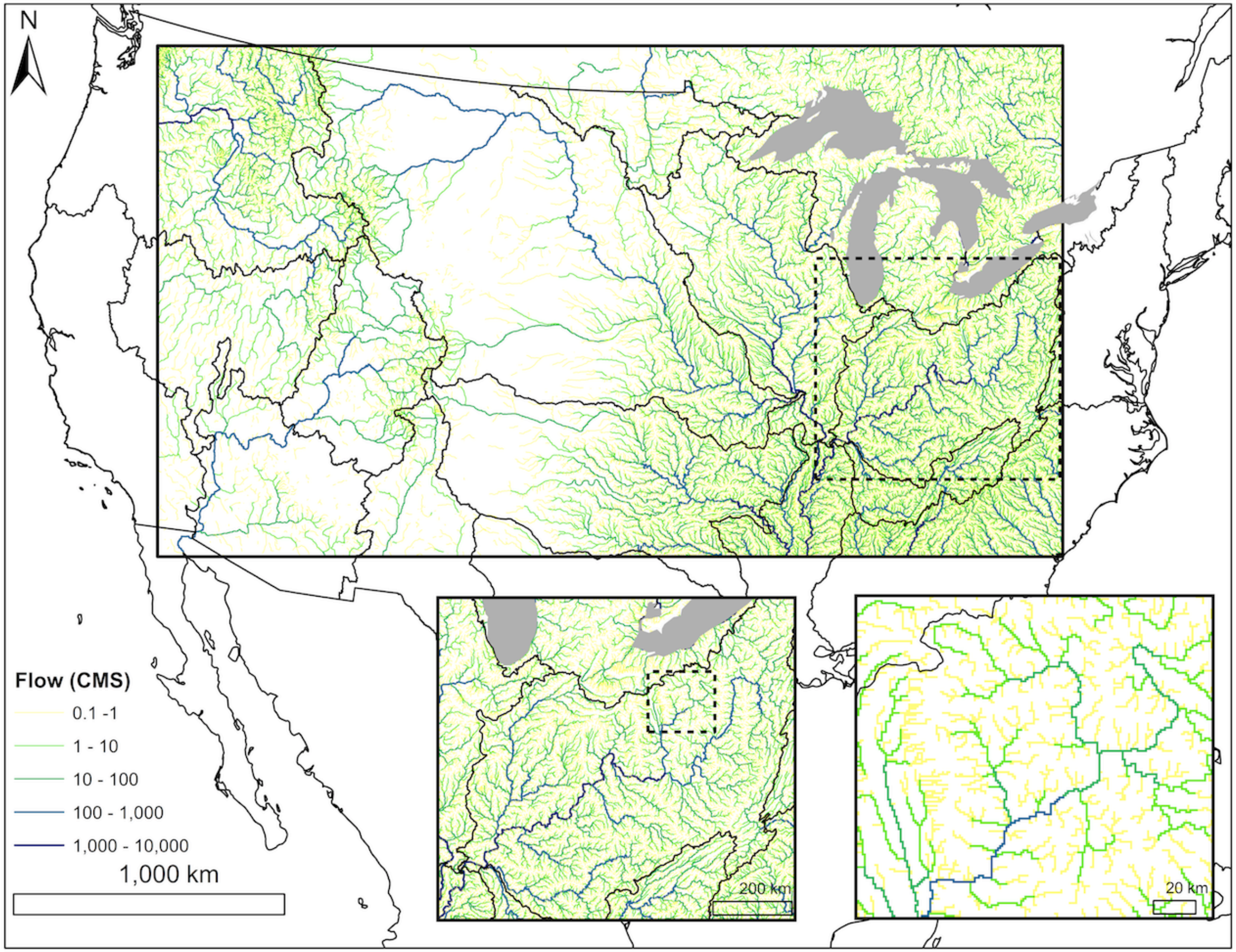
In a hypothetical battle between increased ET and phase change, ET wins



Foster et al *ERL* 2016

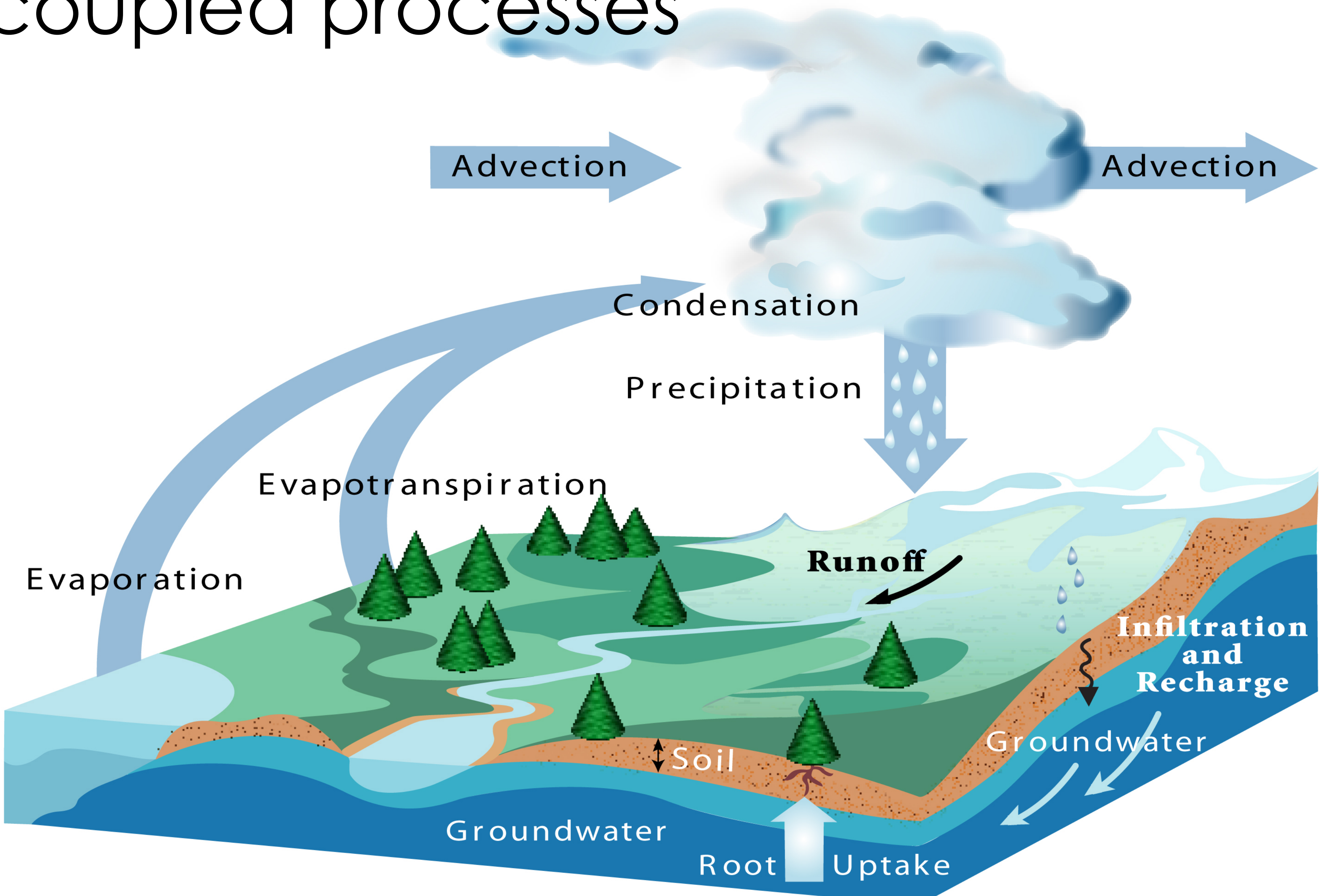
Many things pretend not to be models but really are

The ParFlow Hydrologic Model: A *brief overview*



Reed Maxwell, *Colorado School of Mines*

Terrestrial hydrologic cycle: many coupled processes



The concept for integrated hydrologic models was envisioned almost a half-century ago

Journal of Hydrology **9** (1969) 237-258; © *North-Holland Publishing Co., Amsterdam*

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

R. ALLAN FREEZE
Inland Waters Branch, Department of Energy, Mines and Resources,
Calgary, Alberta, Canada

and

R. L. HARLAN
Forestry Branch, Department of Fisheries and Forestry, Calgary, Alberta, Canada

Abstract: In recent years hydrologists have subjected the various subsystems of the hydrologic cycle to intensive study, designed to discover the mechanisms of flow and to

Traditional watershed models are *situation based* and involve multiple *decision points*

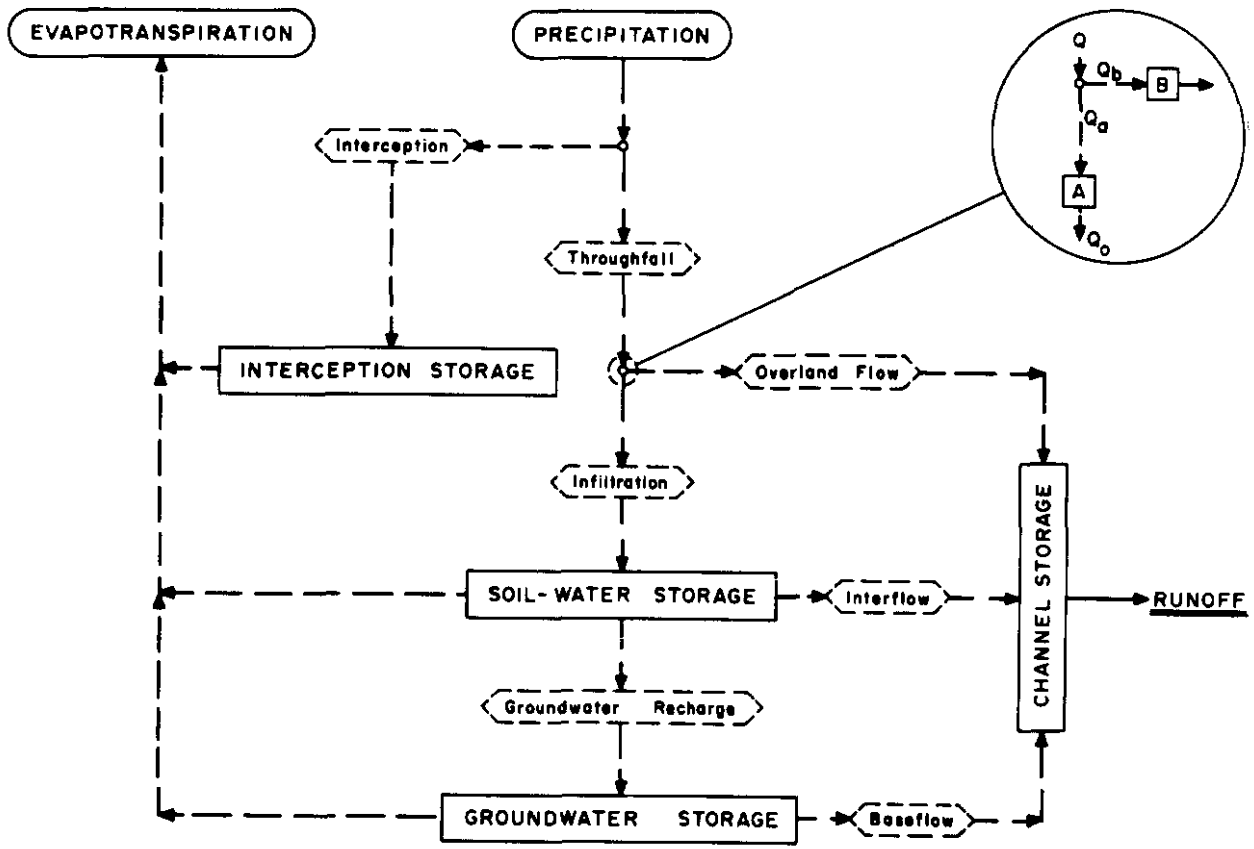
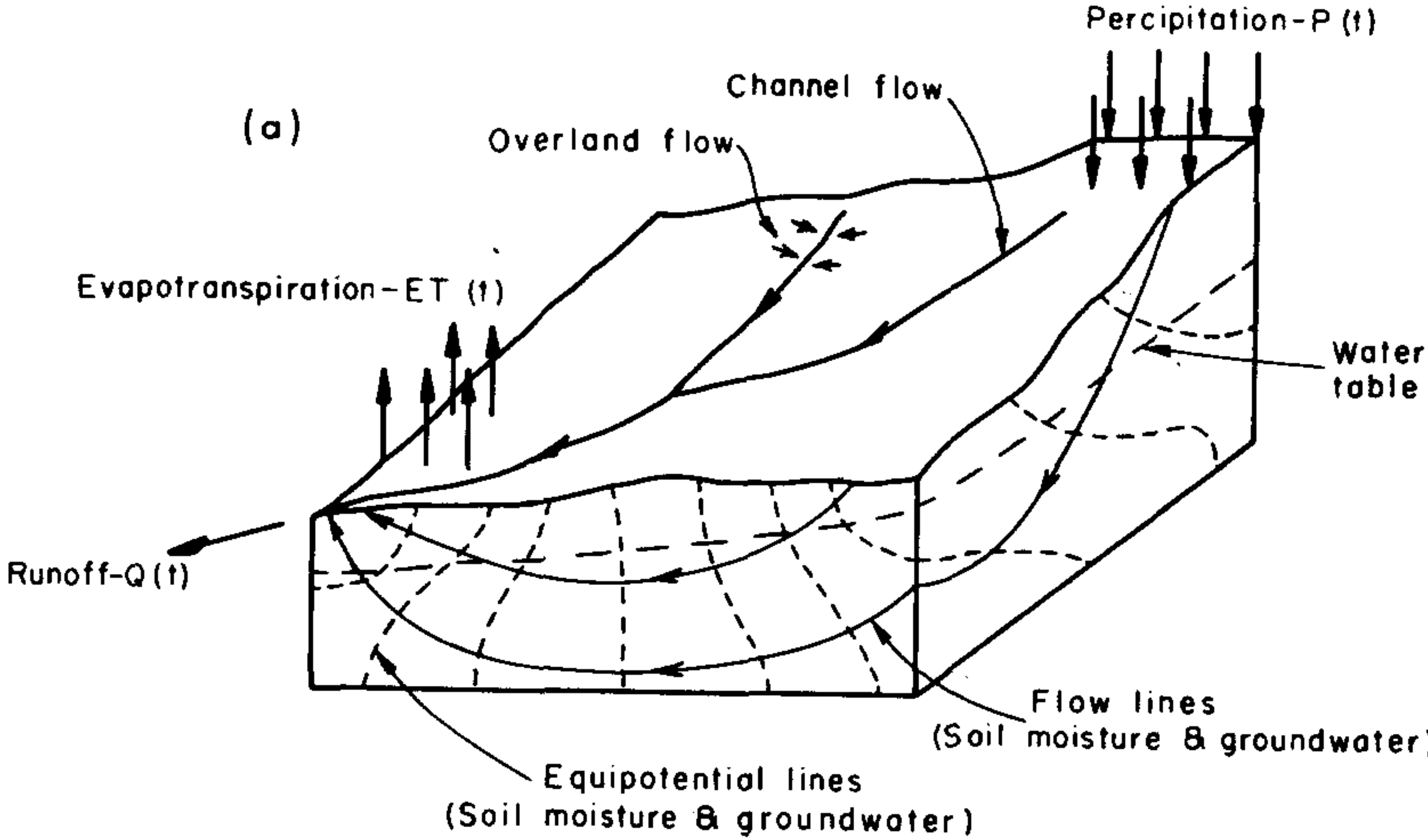


Fig. 2. A conceptual hydrologic model of the type used in the stepwise routing approach of systems hydrology.

Freeze and Harlan (1969)

They introduced a conceptual model that better represented the way we still envision hydrologic systems



Freeze and Harlan (1969)

ParFlow Equations: Steady Flow

$$\nabla \cdot \mathrm{q} = q_s$$

$$\mathrm{q} = -k(x)\nabla\left(\psi_p - z\right)$$

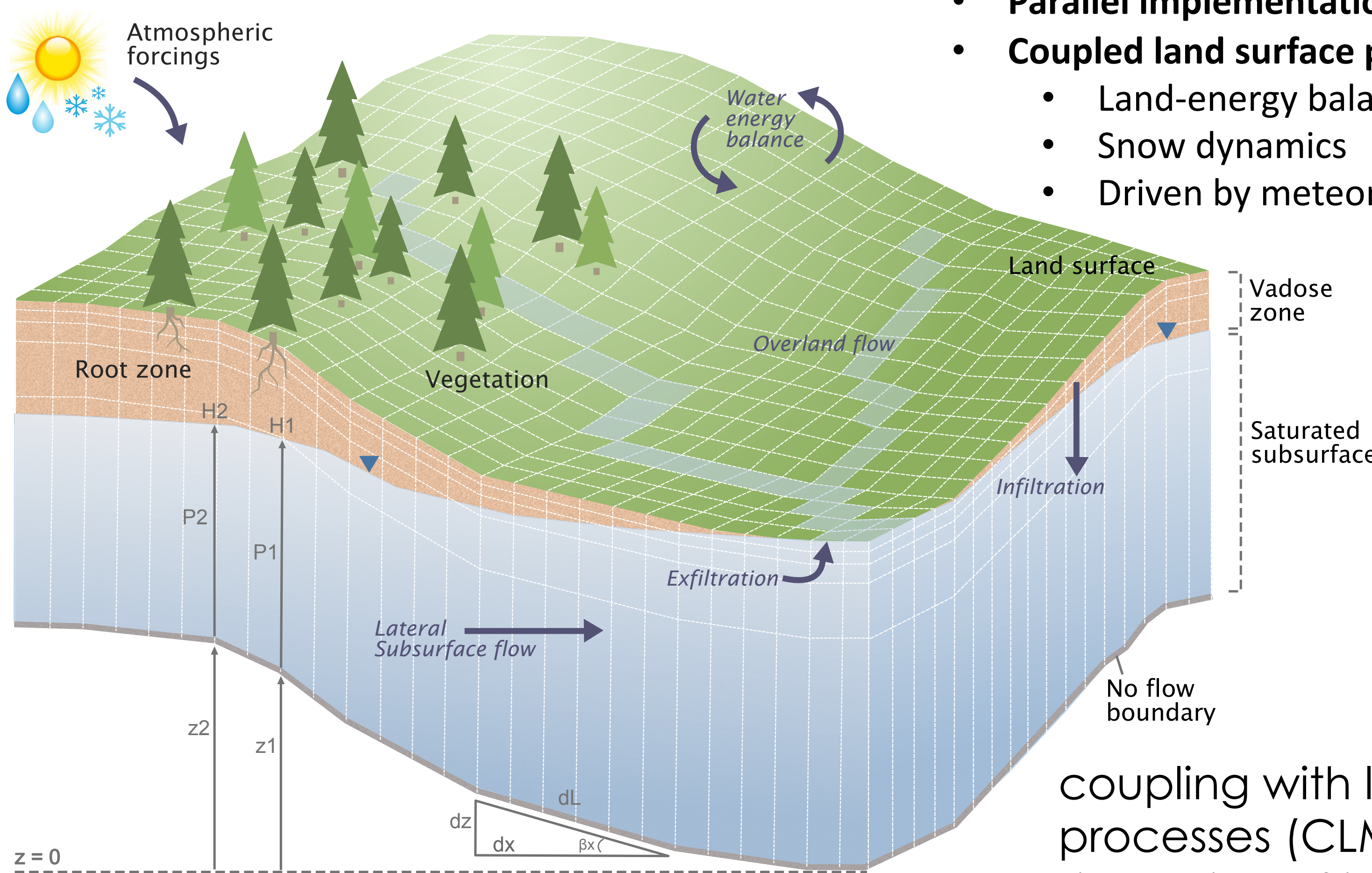
Groundwater flow and Darcy's Law

Pressure Head (L)

Saturated Hydraulic Conductivity (L/T)

The integrated hydrologic model ParFlow is a tool for computational hydrology

- Variably saturated groundwater flow
- Fully integrated surface water
- **Parallel implementation**
- **Coupled land surface processes**
    - Land-energy balance
    - Snow dynamics
    - Driven by meteorology



coupling with land surface processes (CLM) allows for simulation of interactions and connections

Maxwell (2013); Kollet and Maxwell (2008); Kollet and Maxwell (2006);Maxwell and Miller (2005); Dai et al. (2003); Jones and Woodward (2001); Ashby and Falgout (1996)

ParFlow Equations: Richards' and Overland Flow

$$S_s S_w \frac{\partial \psi_p}{\partial t} + \phi \frac{\partial S_w(\psi_p)}{\partial t} = \nabla \cdot \mathrm{q} + q_s$$

$$\boldsymbol{q} = -k(x) k_r(\psi_p) \nabla(\psi_p - z)$$

Richards' Equation

$$\frac{\partial \psi_s}{\partial t} = \nabla \vec{\mathrm{v}} \psi_s + q_r$$

$$\boldsymbol{v}_x = -\frac{\sqrt{S_{f,x}}}{n} \psi_s^{2/3}$$

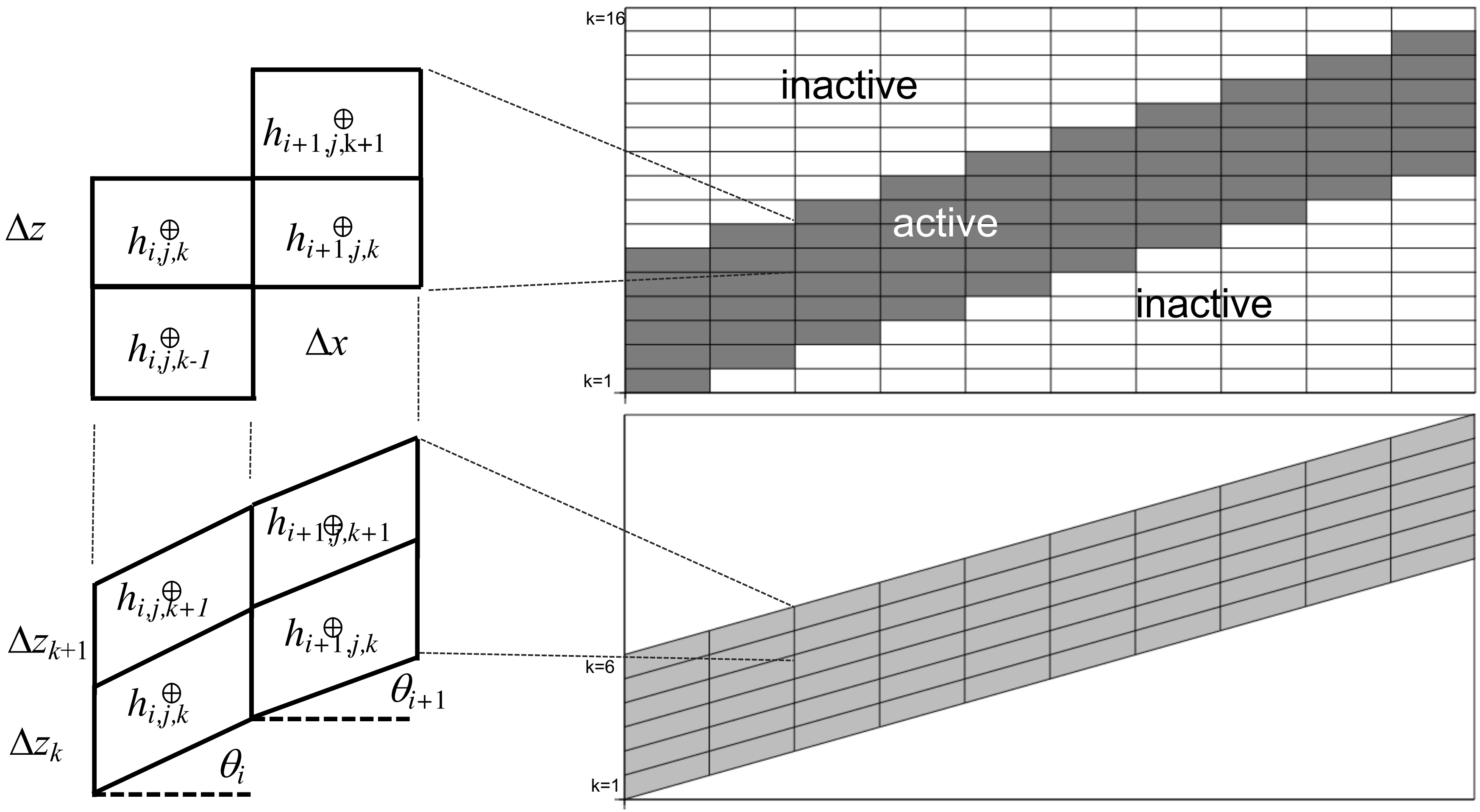
Kinematic Wave Equation

Pressure Head (L)

Saturation (-)

Saturated Hydraulic Conductivity (L/T)

ParFlow Gridding



Terrain Following Grid EQ

Modified Darcy's Law:

$$\mathbf{q} = -\mathbf{K}_s(\mathbf{x})k_r(h)[\nabla(h+z)\cos\theta_x + \sin\theta_x]$$

Slopes and fluxes:

$$\theta_x = \tan^{-1}(S_{0,x}) \text{ and } \theta_y = \tan^{-1}(S_{0,y})$$

$$q_x = -K_{s,x}(\mathbf{x})k_r(h)\left[\frac{\partial(h)}{\partial x}\cos\theta_x + \sin\theta_x\right]$$

$$= -K_{s,x}(x)k_r(h)\frac{\partial(h)}{\partial x}\cos\theta_x - K_{s,x}(x)k_r(h)\sin\theta_x$$

Diffusive Pressure Term Topographic Term

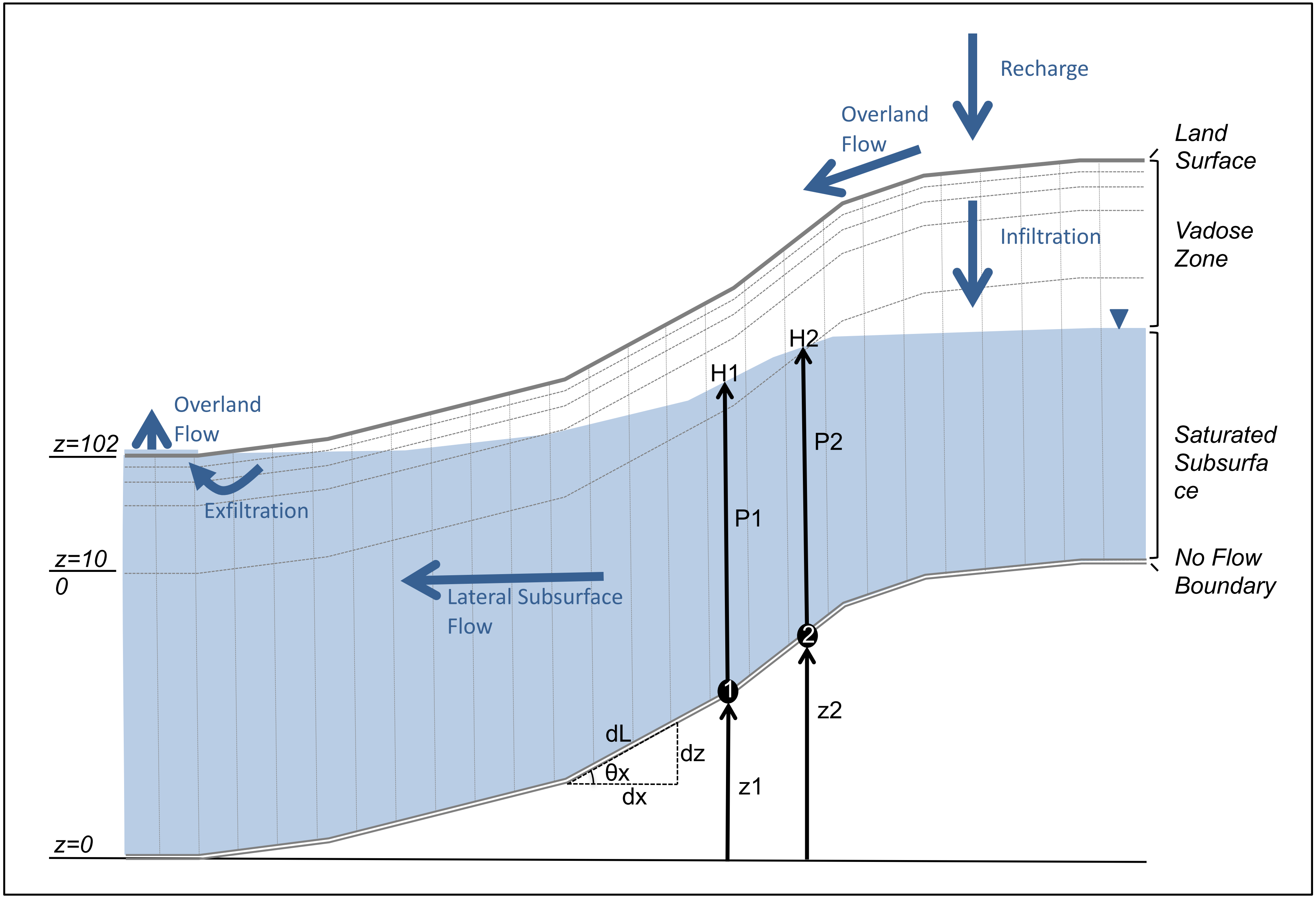
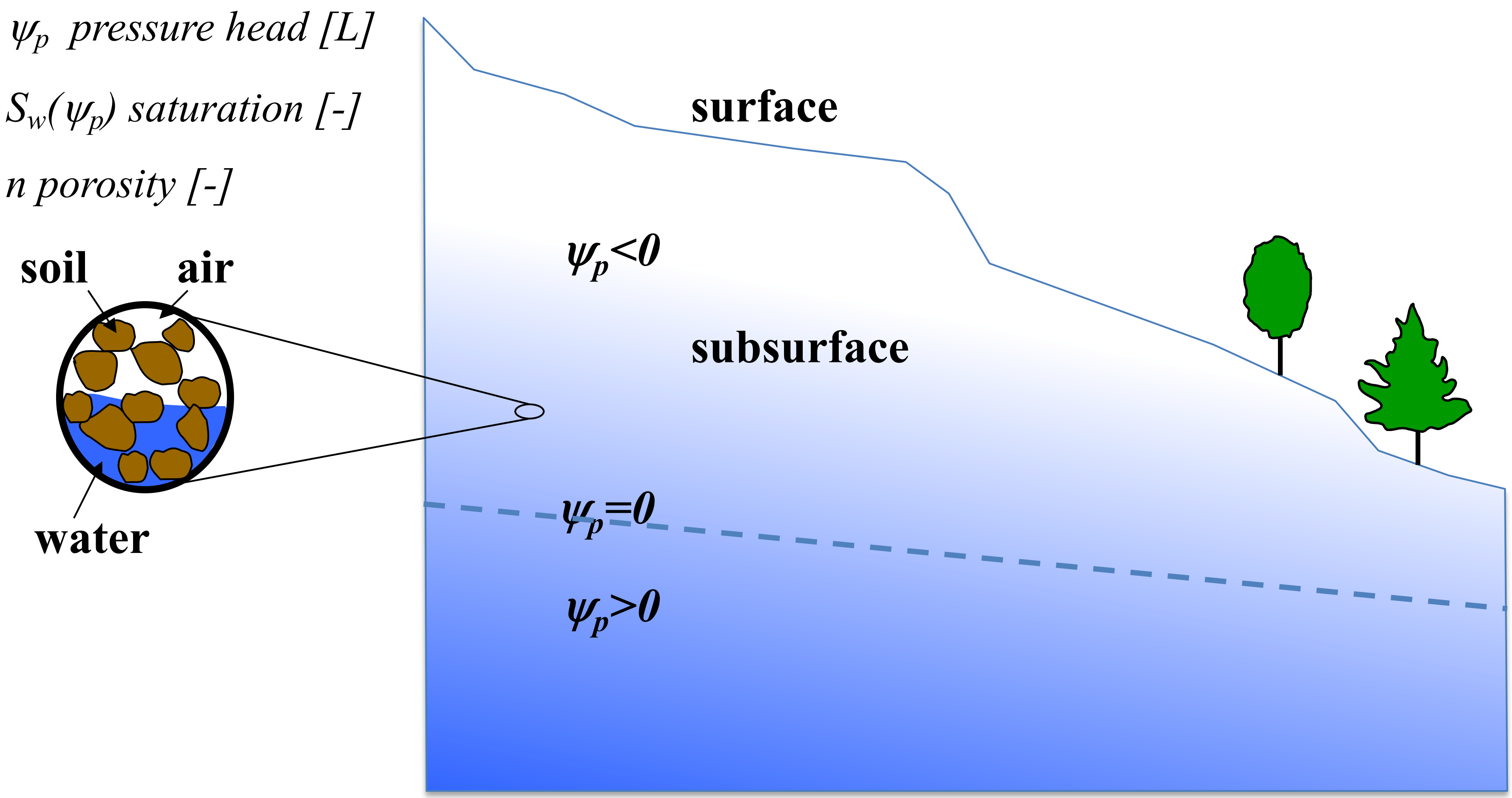


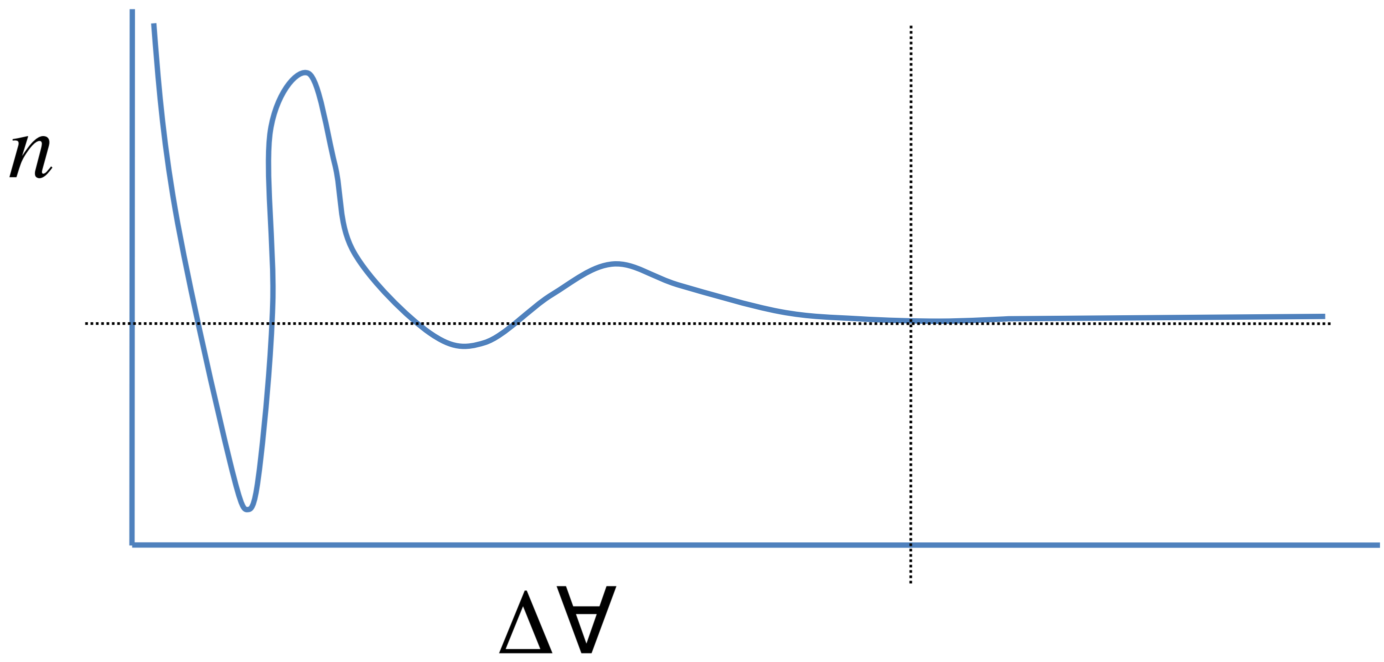
Figure 1: Illustration of a ParFlow model for an idealized hillslope using the terrain following grid formulation



ψ_p pressure head [L]
$S_w(\psi_p)$ saturation [-]
n porosity [-]
soil
air
water
surface
$\psi_p<0$
subsurface
$\psi_p=0$
$\psi_p>0$

Porosity *n* is defined by an representative elementary volume (*REV*)

$$n_0 = \lim_{\Delta\forall \to 0}\left(\frac{\text{volume of voids in } \Delta\forall}{\Delta\forall}\right)$$



ParFlow – Getting the Code, more information, help

ParFlow web page:
www.parflow.org

Github
https://github.com/parflow/parflow

ParFlow Blog
http://parflow.blogspot.com/

ParFlow User's list
parflow-users@mailman.mines.edu

ParFlow has a long development history

- *Ashby and Falgout 1996*, parallel multigrid saturated flow
- *Jones and Woodward 2001*, parallel Richards' equation flow
- *Maxwell and Miller 2005*, CLM coupling
- *Kollet and Maxwell 2006*, parallel overland flow
- *Maxwell 2013*, Terrain following grid

ParFlow is a community code, developed by several groups

- Started at Lawrence Livermore National Laboratory (LLNL)
- Center of development moved to Colorado School of Mines (CSM) in 2009
- Now active development from groups in F-Z Jülich, UniBonn, CSM, LLNL, LBL, LTHE and WSU

Rheinische Friedrich-Wilhelms-Universität Bonn

ParFlow has been used in many studies

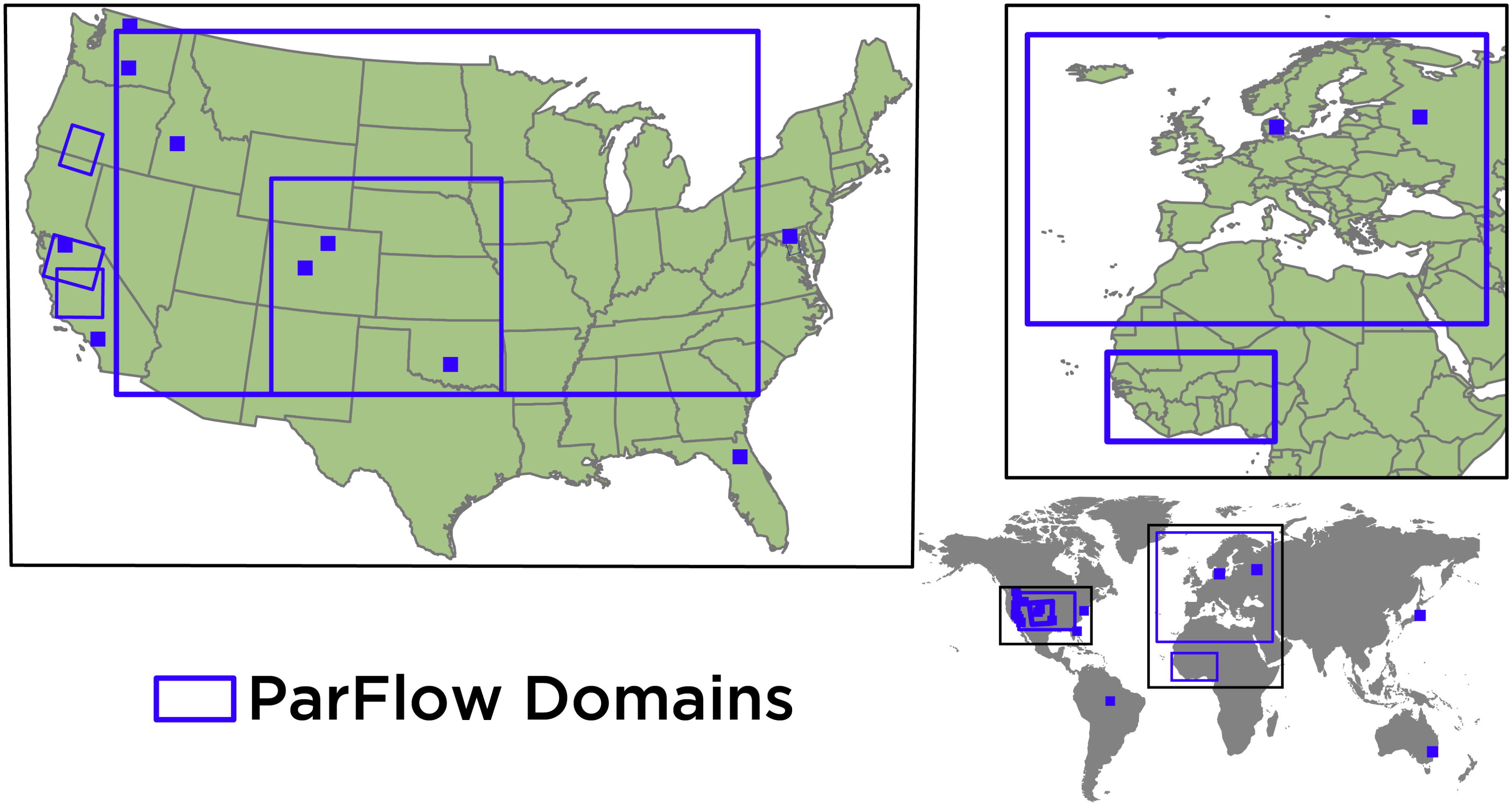
Table 1.1- 1.6 in the ParFlow manual lists most of the published studies to date and some details about them

1.2. *PUBLISHED STUDIES THAT HAVE USED* PARFLOW 3

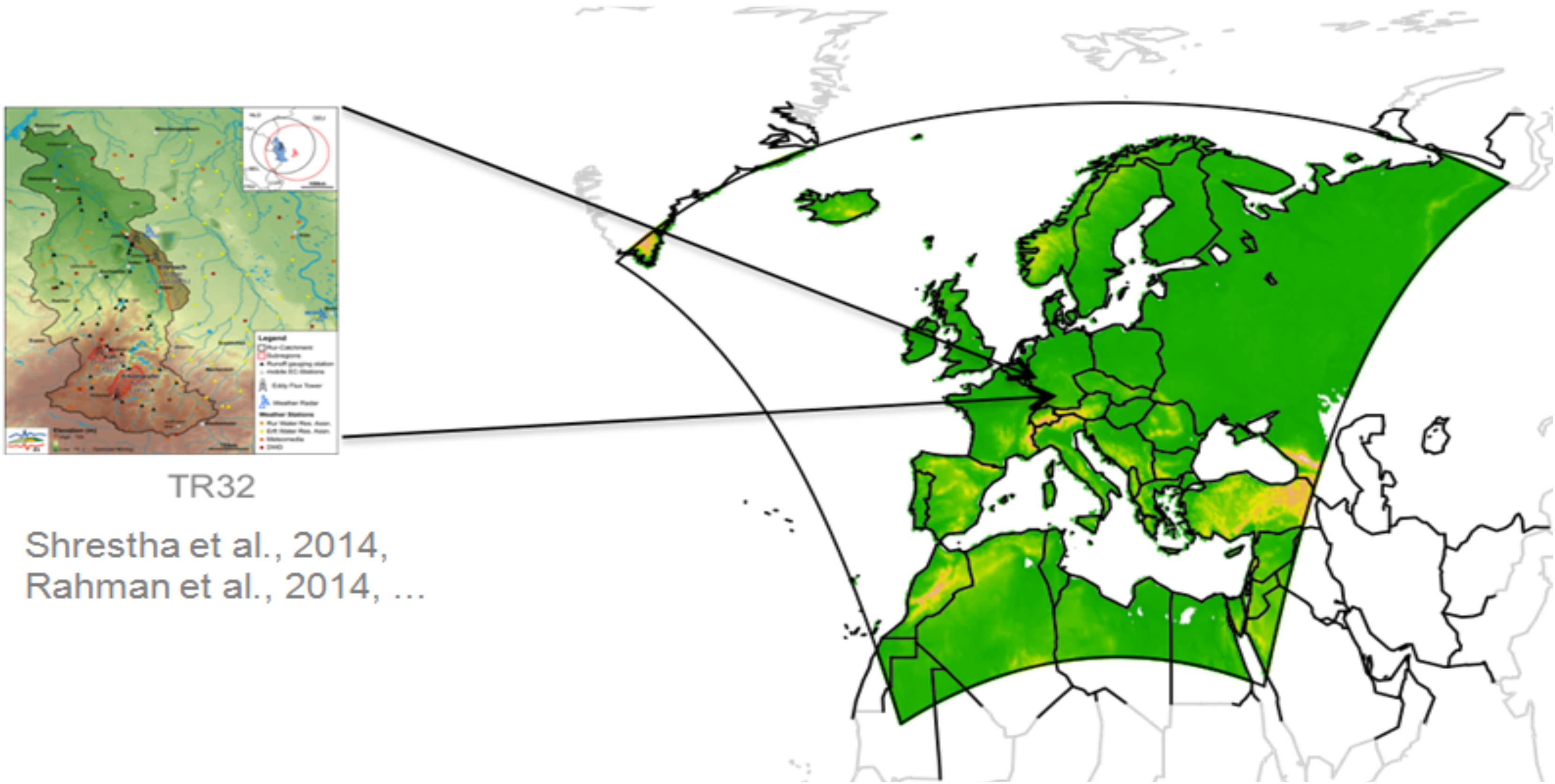
Table 1.1: List of ParFlow references with application and process details.

Reference	**Coupled Model**	**Application**	**Scale**	**Domain**	**TB**	**TFG**	**VS**	**Vdz**
[9] Bearup et al. (2016)		Hillslope Hydrologic Response; MPB	Hillslope	Idealized			X	
[52] Maxwell et al. (2016)		Residence Time Distributions	Continental	CONUS			X	X
[68] Reyes at al. (2015)	CLM	Surface Heterogeneity, Surface Energy Budget (SEB)	Urban Watershed Ballona Creek Watershed, CA		X	X	X	
[17] Condon and Maxwell (2015)		Subsurface Heterogeneity (groundwater fluxes and topography)	Continental	CONUS			X	X
[33] Jefferson et al. (2015)	CLM	Active subspaces; Dimension reduction; Energy fluxes	Hillslope	Idealized				
[32] Jefferson and Maxwell (2015)	CLM	Sensitivity Analysis (evap-	Column	Idealized				

ParFlow has been applied at many sites worldwide



ParFlow has been used to model watersheds around the world at a wide range of scales



TR32

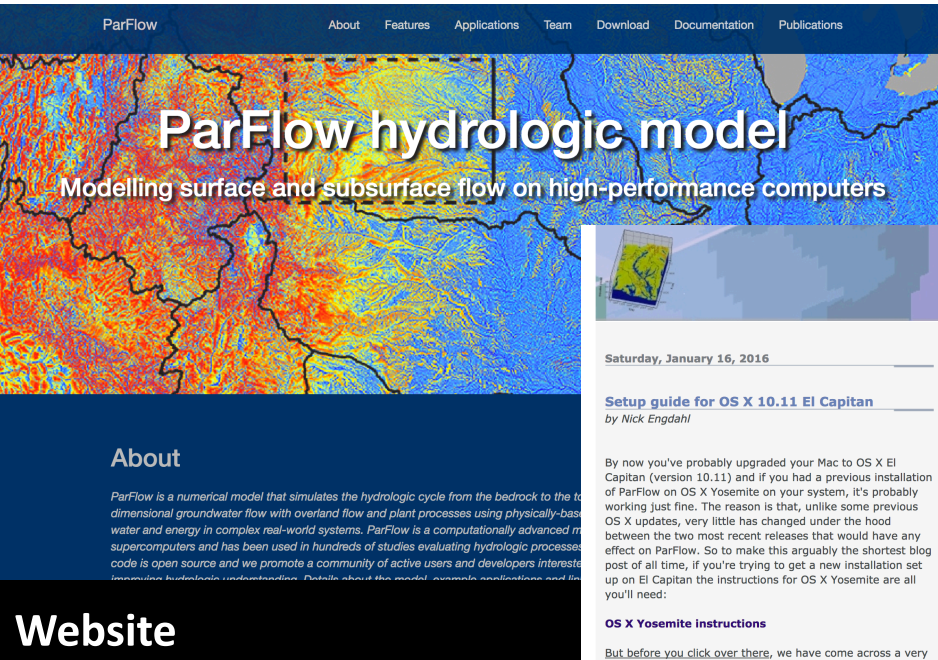
Shrestha et al., 2014,
Rahman et al., 2014, …

Including Big Thompson (CO), Chesapeake (MD), CONUS, CORDEX, East Inlet (CO), East River (CO), Klamath (OR), Little Washita (OK), Rur (Germany), San Joaquin (CA), Sante Fe (FL), Skjern (Denmark), Wüstebach (Germany)

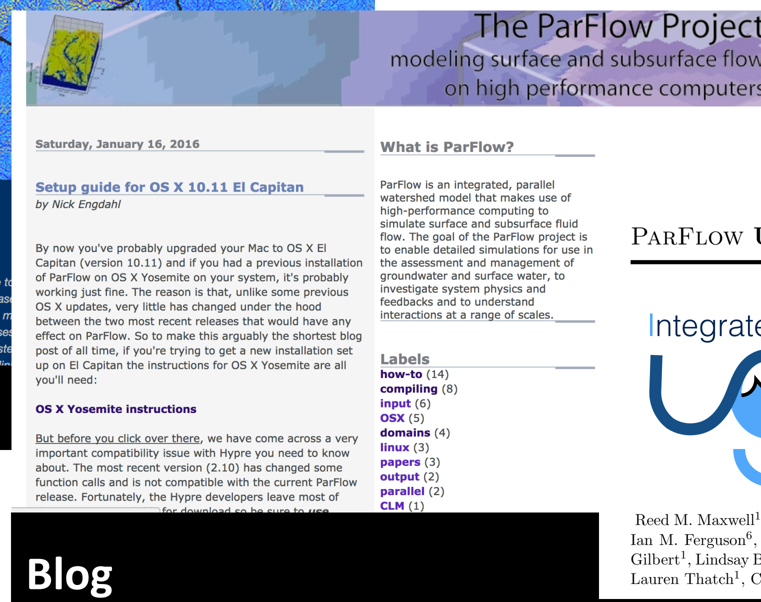
ParFlow – Getting the Code, more information, help

Online Resources

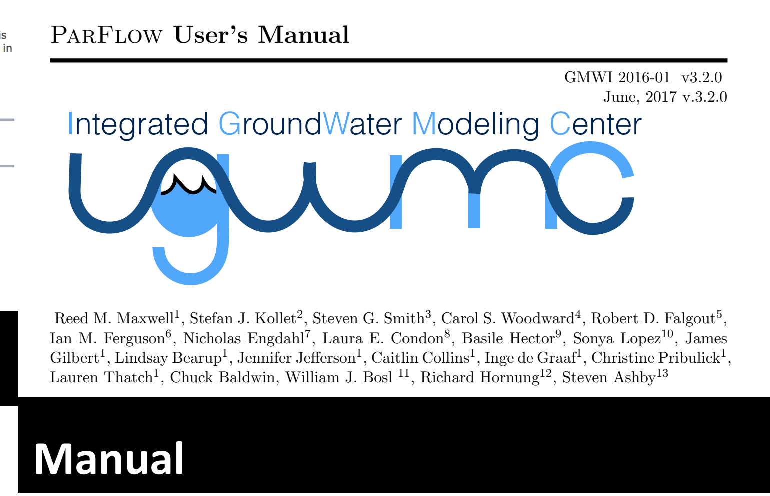
Variety of resources to accommodate users with a range of technical experience



Website



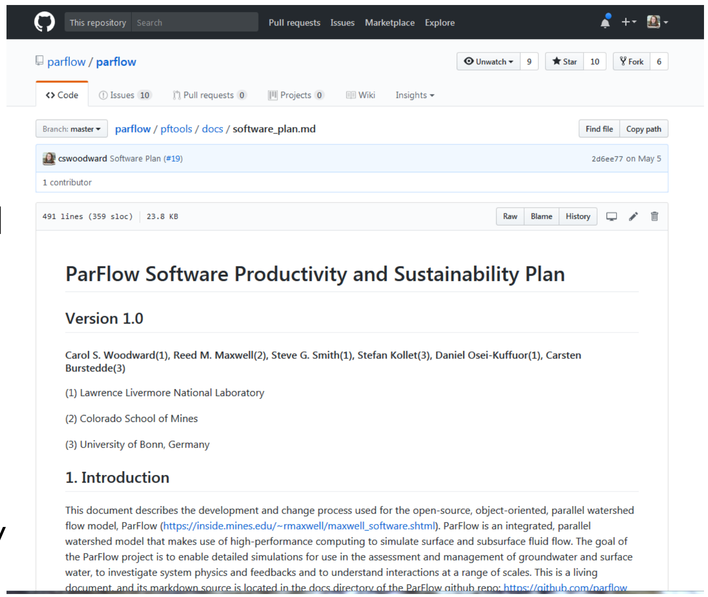
Blog



Manual

We developed a software productivity and sustainability plan for ParFlow

- This plan lays out formal processes that contributors to ParFlow are expected to follow
  - Requirements for design documents and project review of new feature and capability enhancements
  - Establishes a Git workflow for submission of new code and its review
  - Establishes documentation requirements for new code
  - Describes testing practices
  - Establishes practices for external package usage and testing
- This document helps prevent conflicting features, poorly designed, and untested code from creeping into ParFlow
- This is a living document, expected to be updated and changed as ParFlow continues to evolve



ParFlow Software Productivity and Sustainability Plan

Version 1.0

Carol S. Woodward(1), Reed M. Maxwell(2), Steve G. Smith(1), Stefan Kollet(3), Daniel Osei-Kuffuor(1), Carsten Burstedde(3)

(1) Lawrence Livermore National Laboratory

(2) Colorado School of Mines

(3) University of Bonn, Germany

1. Introduction

This document describes the development and change process used for the open-source, object-oriented, parallel watershed flow model, ParFlow (https://inside.mines.edu/~rmaxwell/maxwell_software.shtml). ParFlow is an integrated, parallel watershed model that makes use of high-performance computing to simulate surface and subsurface fluid flow. The goal of the ParFlow project is to enable detailed simulations for use in the assessment and management of groundwater and surface water, to investigate system physics and feedbacks and to understand interactions at a range of scales. This is a living document, and its markdown source is located in the docs directory of the ParFlow github repo: https://github.com/parflow

https://github.com/parflow/parflow/blob/master/pftools/docs/software_plan.md

Centralized version control and development is critical

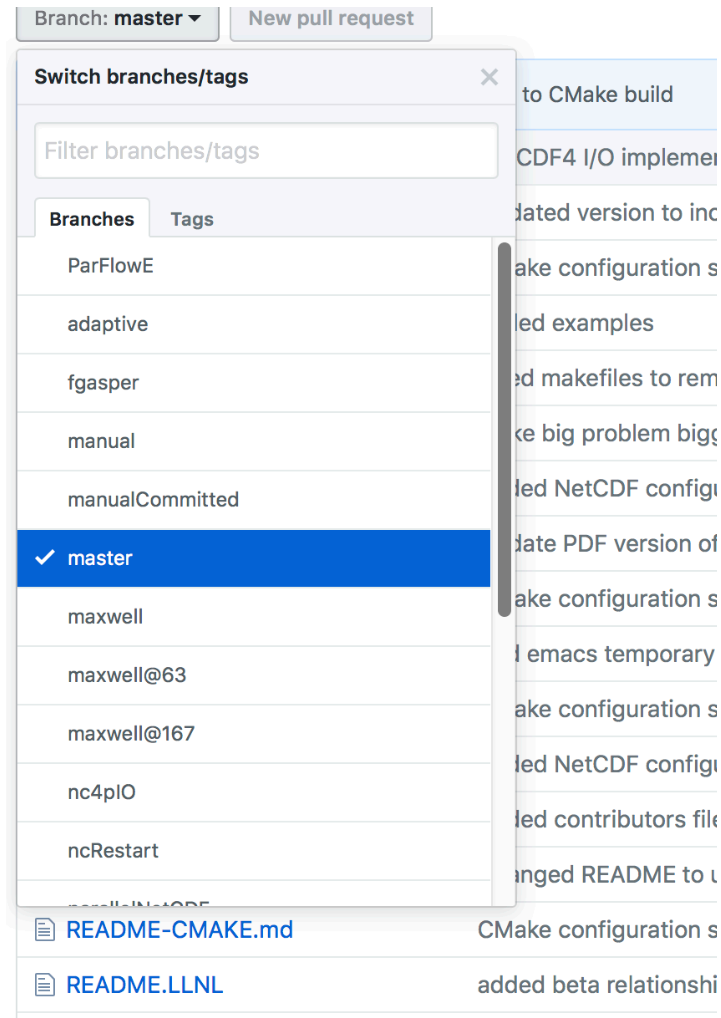
- ParFlow is hosted on GitHub
  - Git repository used for
    - Source code
    - Test cases
    - Documentation
  - Issue tracking
    - Not heavily used yet
    - Transitioning users to submitting issues rather than emails for better tracking

GitHub

https://github.com/parflow

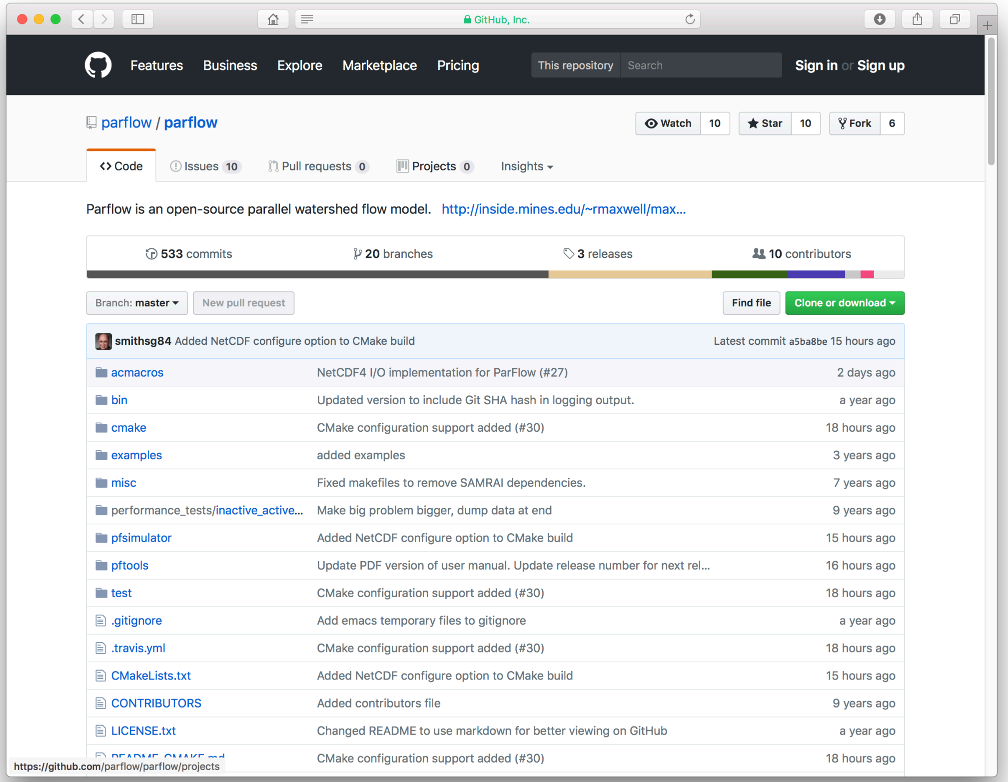
With 20 active development branches the development plan is important

- **Branches** span range and scope
- New **features** must play well with each other
- **Versioning** and backward compatibility



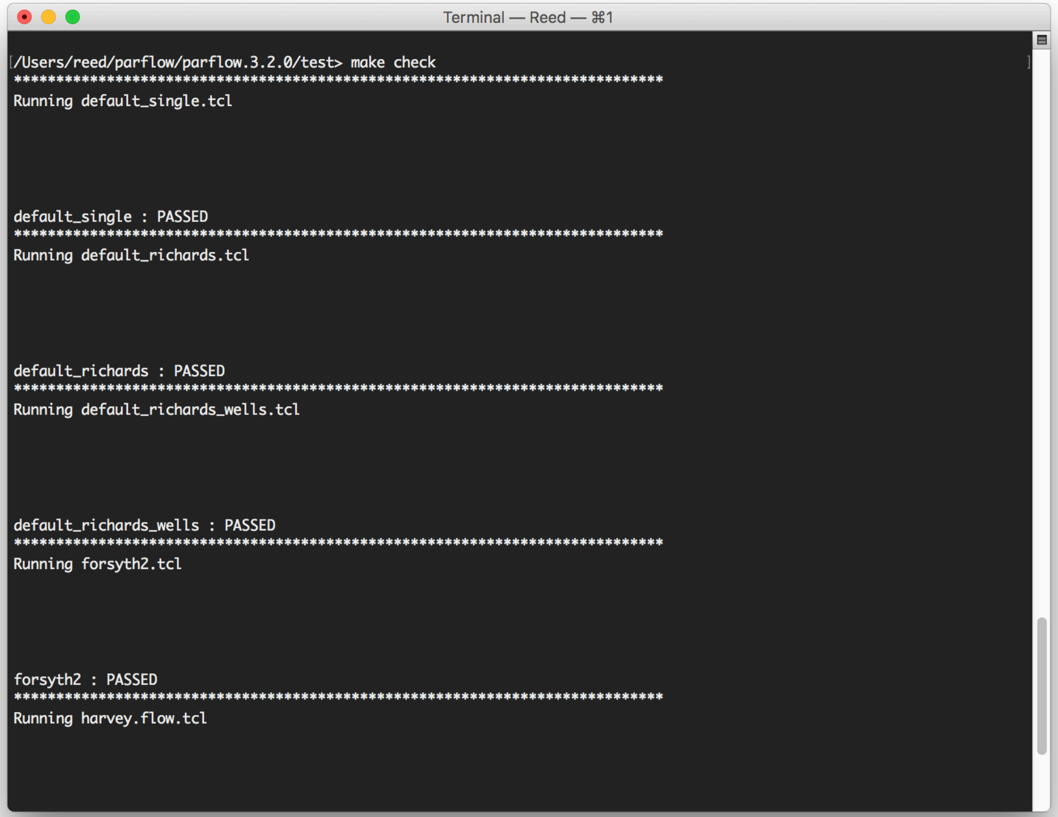
GitHub provides a mechanism to enforce the development plan

- Standard GitHub Pull request model is used for code submissions
  - Development is done on branches or GitHub repository forks
    - Only lead maintainers have write access to master branch
  - Pull requests are reviewed by lead maintainers
    - Correctness
    - Consistency with coding style
    - Verify test for new feature was added
    - Regression tests pass



Automated test cases provide code verification mechanism

- Suite of test cases testing solvers and code features
- Contributed with each new major update
- Testing allows check for backward compatibility of new code
- Tests provide examples for new users



Automated testing allows us to predict hardware software incompatibilities

- Automated set of integration/regression tests
  - Tests major features/code paths
  - Easy to execute “make test”
- TravisCI integration with GitHub used for continuous integration
  - Currently testing Linux
  - Enables small scale parallel tests (MPI is available in images).
  - Investigating adding MacOS
- Manually launching test suite on larger parallel machines (LLNL/LBNL)
  - Would like to fully automate integrate with GitHub but don’t have a mechanism for this yet

Travis CI

The model input structure is a novel aspect

- TCL/TK scripting language
- All parameters input as keys using pfset command
- Keys used to build a database that ParFlow uses
- ParFlow executed by pfrun command
- Since input file is a script may be run like a program

Take Home Messages…

- We can strive towards an integrated picture, model and understanding of the hydrologic cycle
- This requires new equations, process descriptions, solvers and parallel architecture
- This enables new understanding about connections between components

IBM BG/Q released in 2012
JüQueen 5 PFLOPS

Seymore-Cray 7600 released in 1969
10 MFLOPS

Apple iPad 1: 40 MFLOPS
Apple iPad Air: 1 GFLOP
iPhone 4s: 170 MFLOPS
iPhone 6/6+: ~3 GFLOPS