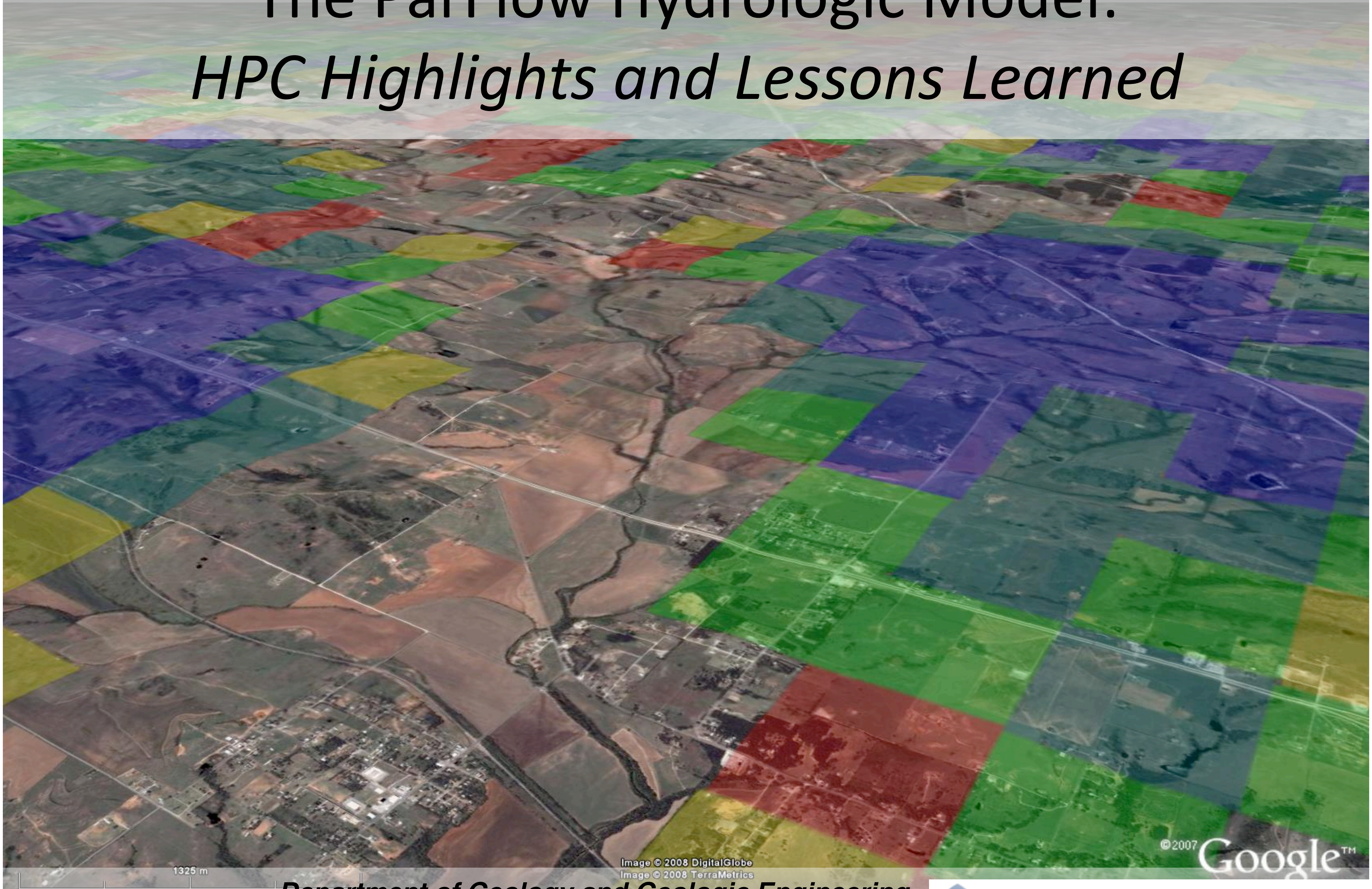
The ParFlow Hydrologic Model:
HPC Highlights and Lessons Learned



Reed Maxwell
Department of Geology and Geologic Engineering
Colorado School of Mines

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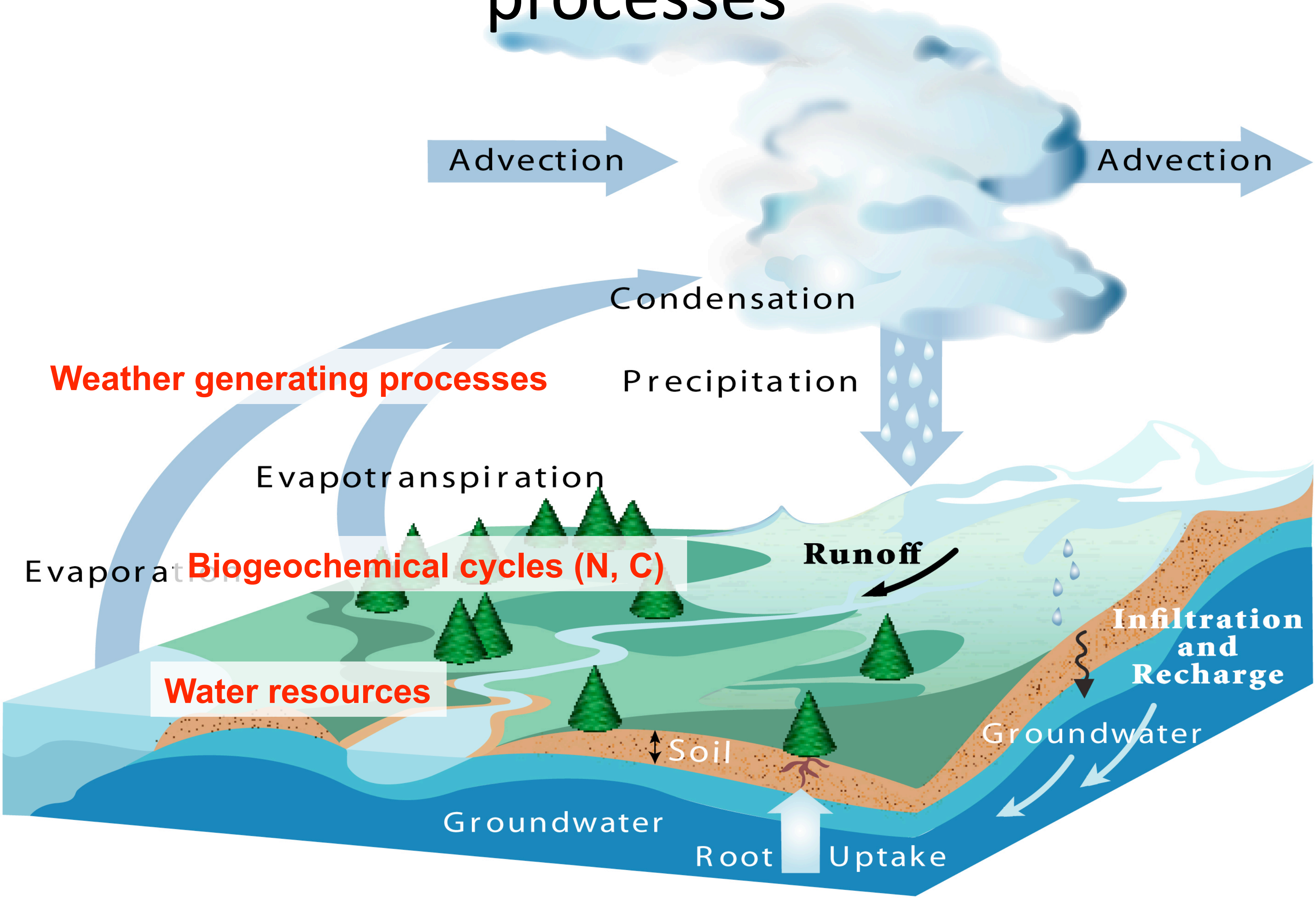
Terrestrial hydrologic cycle: many coupled processes

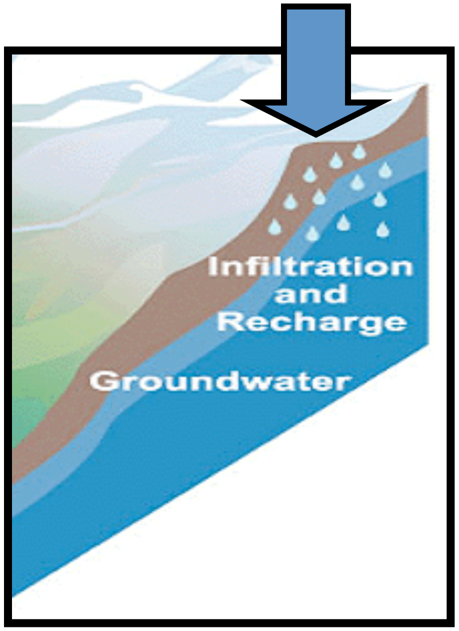


Weather generating processes

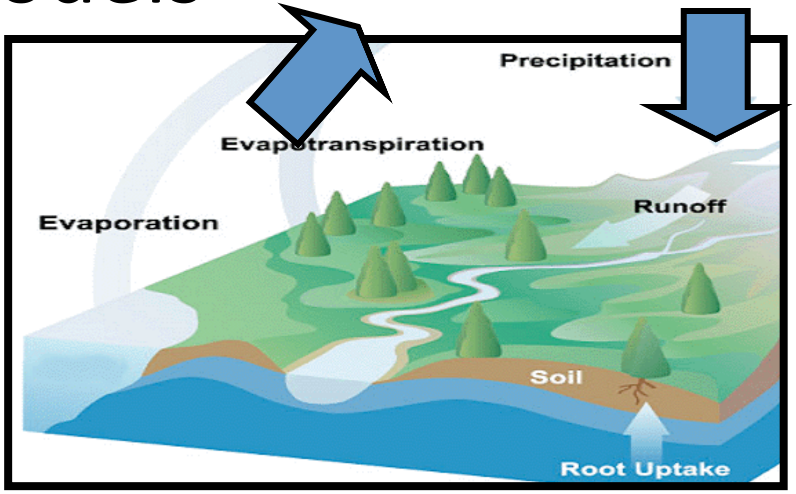
Biogeochemical cycles (N, C)

Water resources

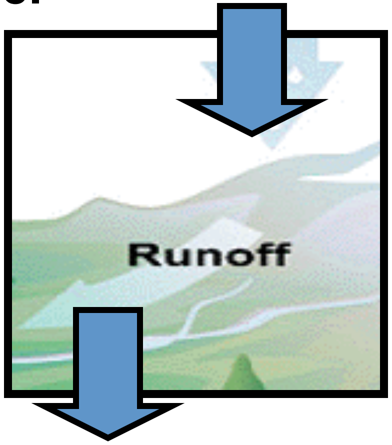
Yet it is usually simulated with disconnected models



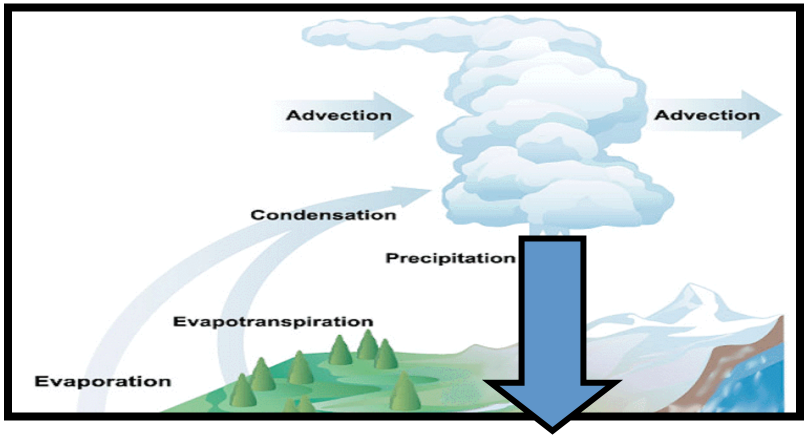
Groundwater/Vadose Model



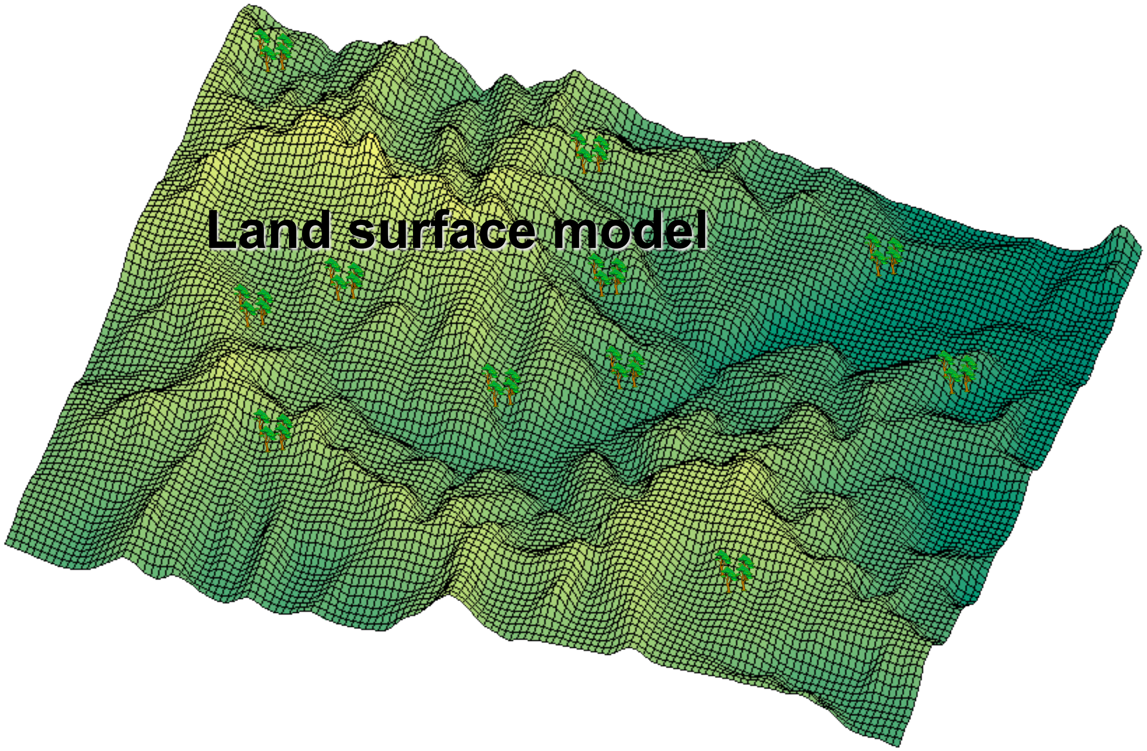
Land Surface Model

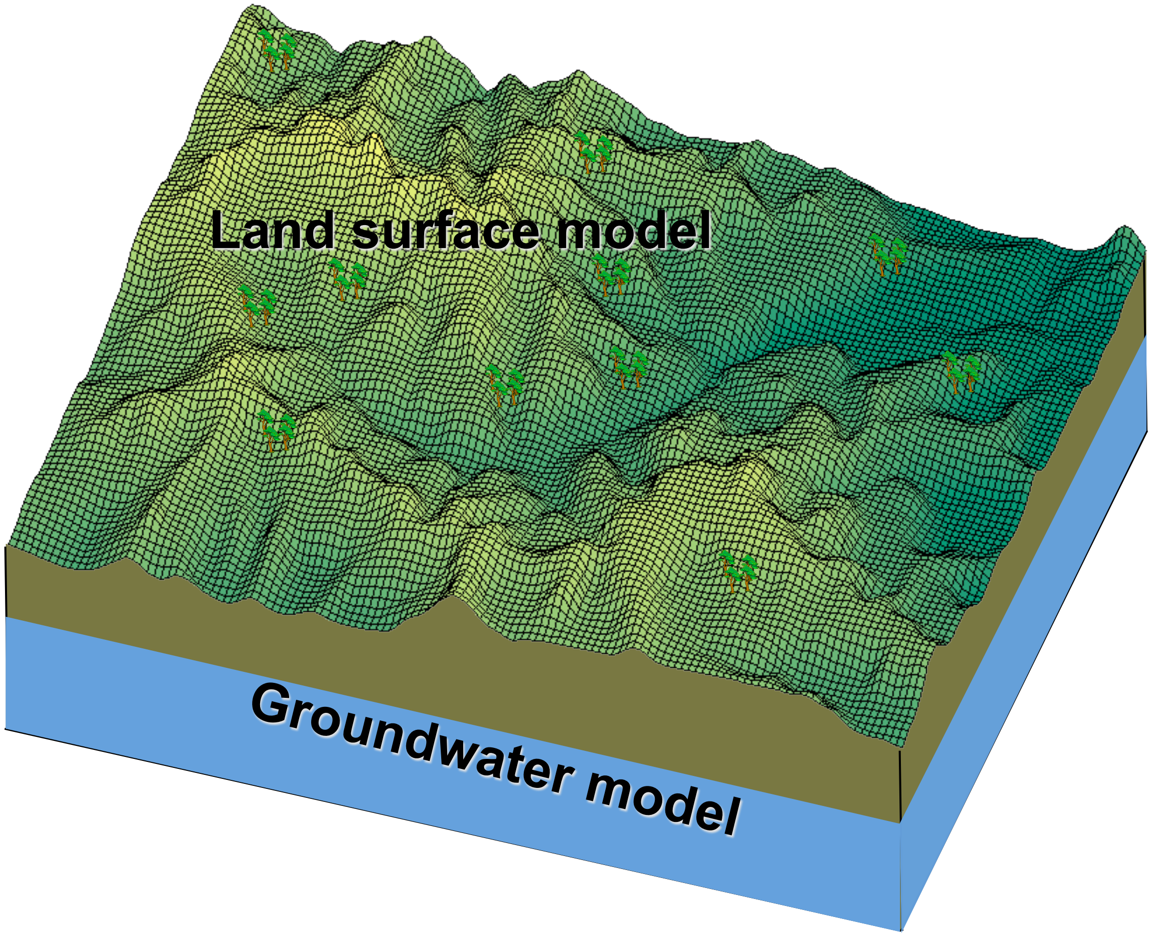


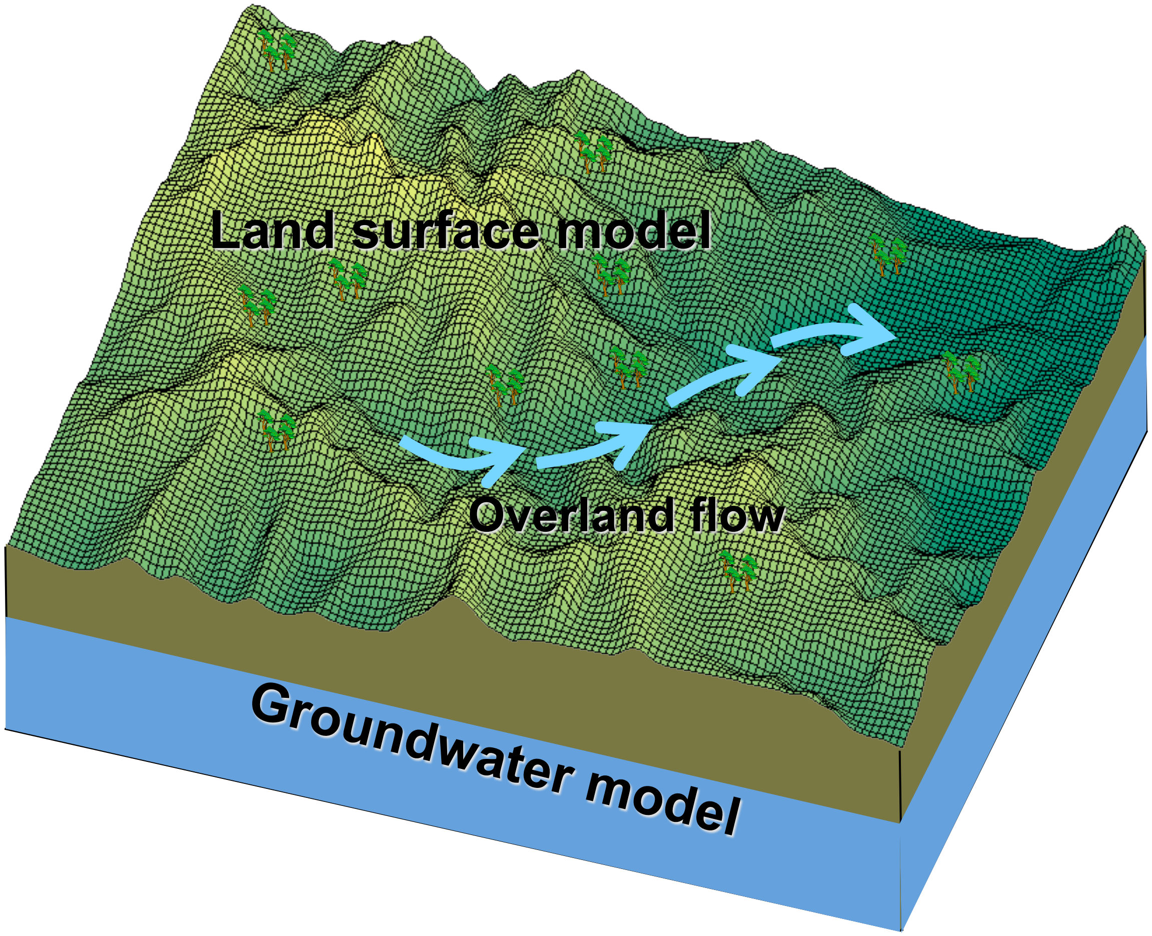
Surface Water Model

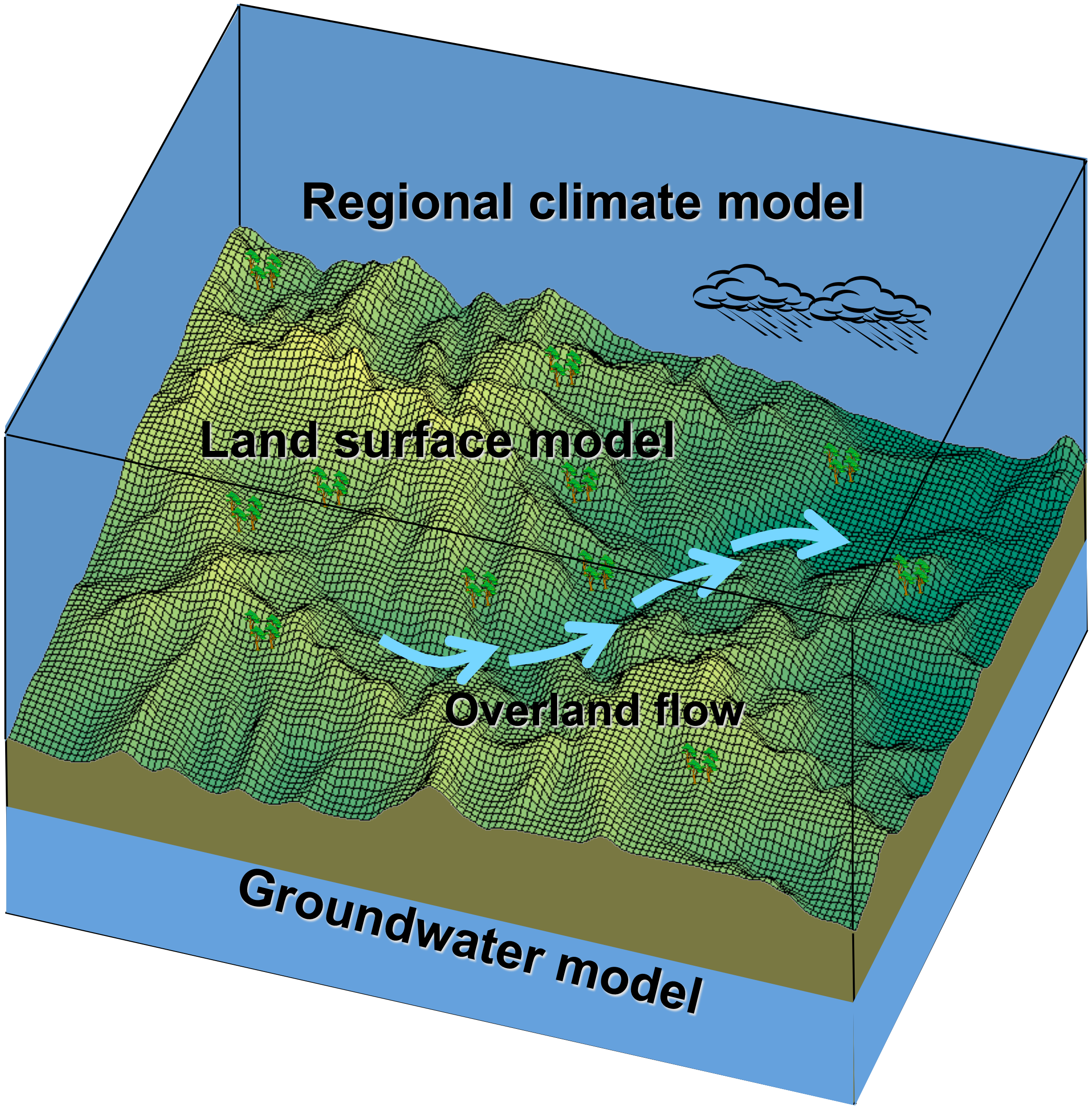


Atmospheric Model

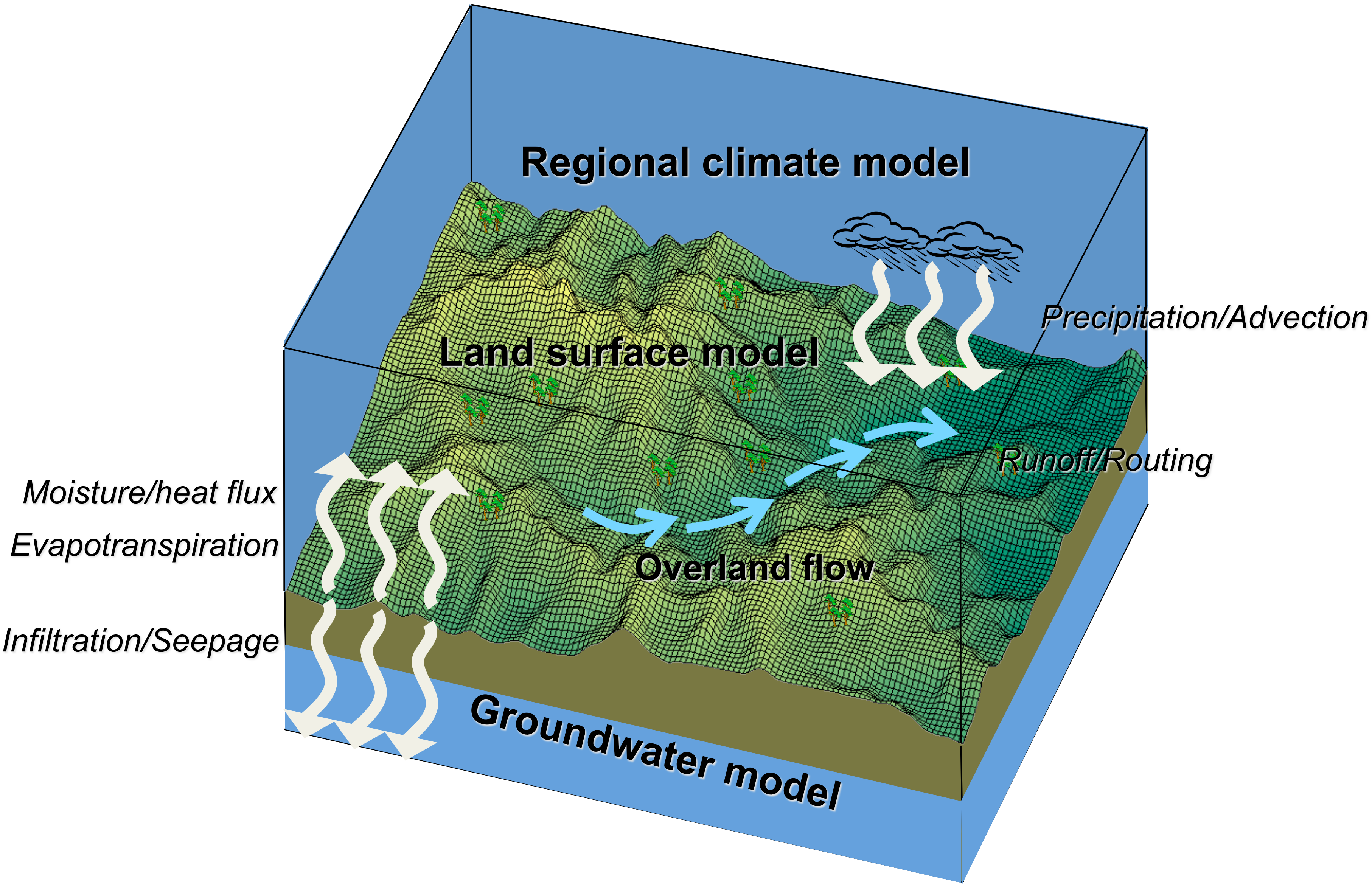

Land surface model


Land surface model
Groundwater model


Land surface model
Overland flow
Groundwater model

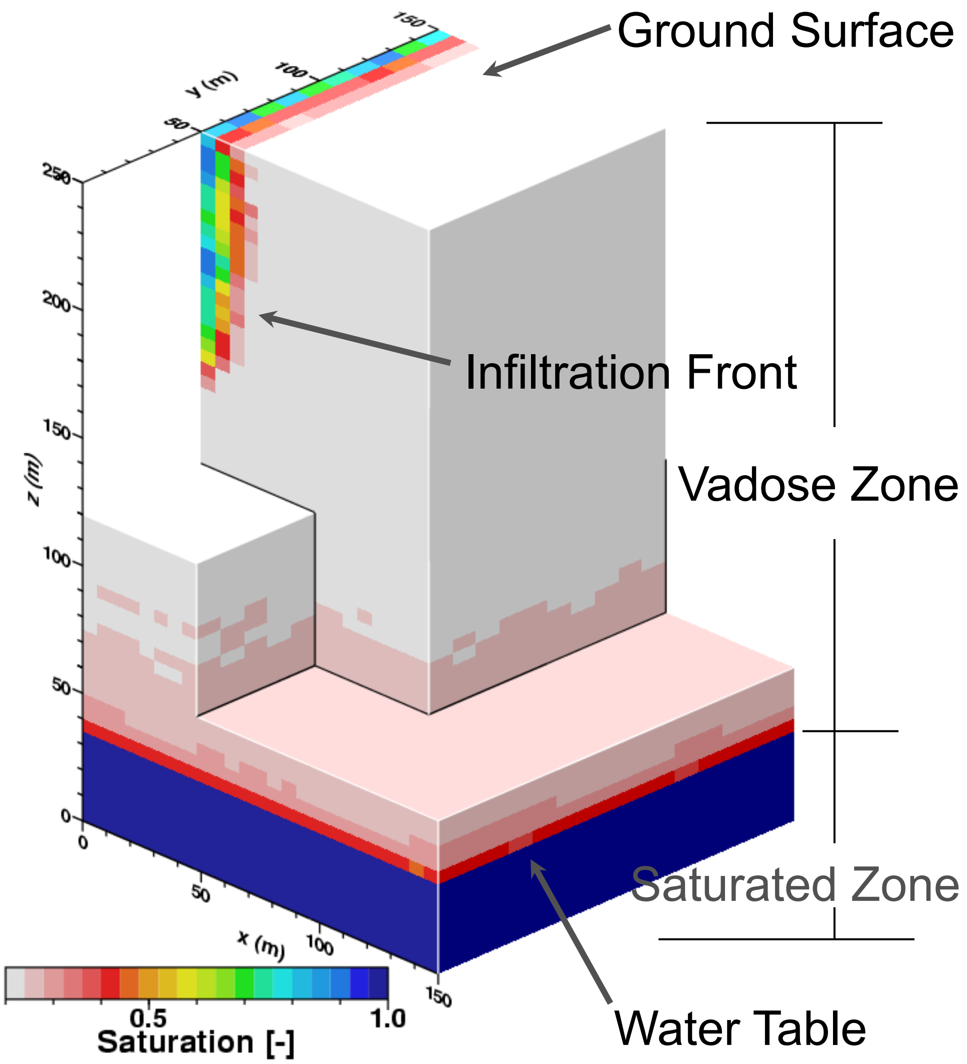

Regional climate model
Land surface model
Overland flow
Groundwater model

These models explicitly incorporate fluxes at air/land-surface/subsurface interfaces

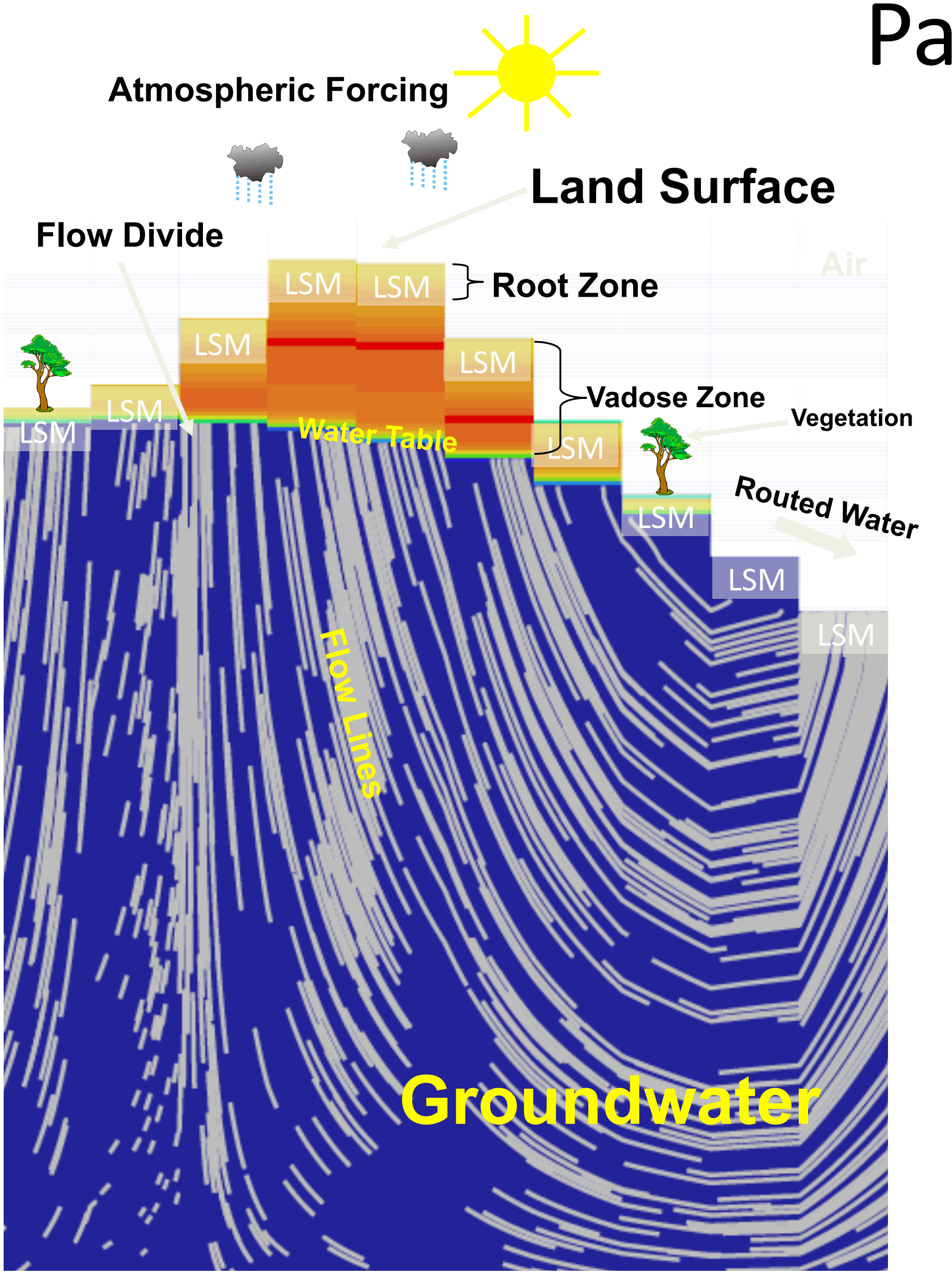


ParFlow is a combination of:

- Physics
- Solvers
- Parallelism



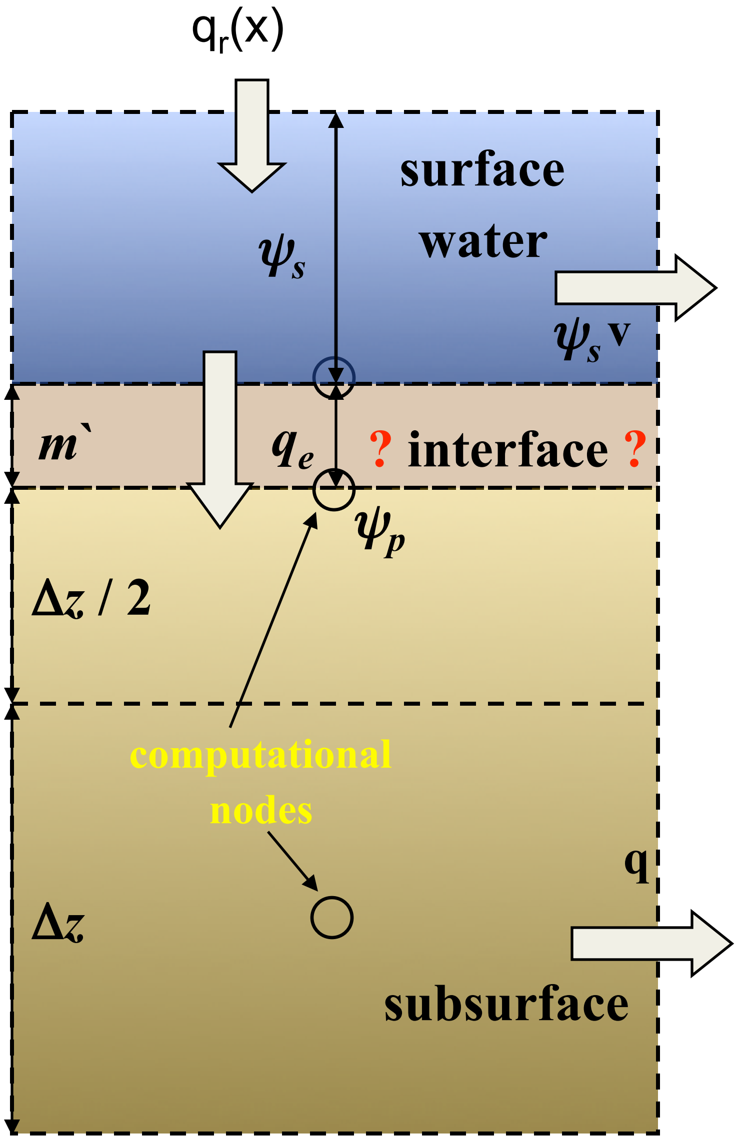
ParFlow Watershed Model



- **PF.CLM= Parflow (PF) + Common Land Model (CLM)** **Kollet and Maxwell (2008), Kollet and Maxwell (2006), Maxwell and Miller (2005), Dai et al. (2003), Jones and Woodward (2001); Ashby and Falgout (1996)**
- **Surface and soil column/root zone hydrology calculated by PF *(removed from CLM)***
- **Overland flow/runoff handled by fully-coupled overland flow BC in PF (Kollet and Maxwell, AWR, 2006)**
- **CLM is incorporated into PF as a module- fully coupled, fully mass conservative, fully parallel**

Dynamically coupled, 2D/3D OF/LS/GW Model

Overland Flow: The Conductance Concept



Kinematic wave eq

$$\frac{\partial \psi_s}{\partial t} = \nabla \cdot \psi_s \mathbf{v} - q_r(x) - q_e(x)$$

$$q_e(x) = \lambda(x)(\psi_s - \psi_p)$$

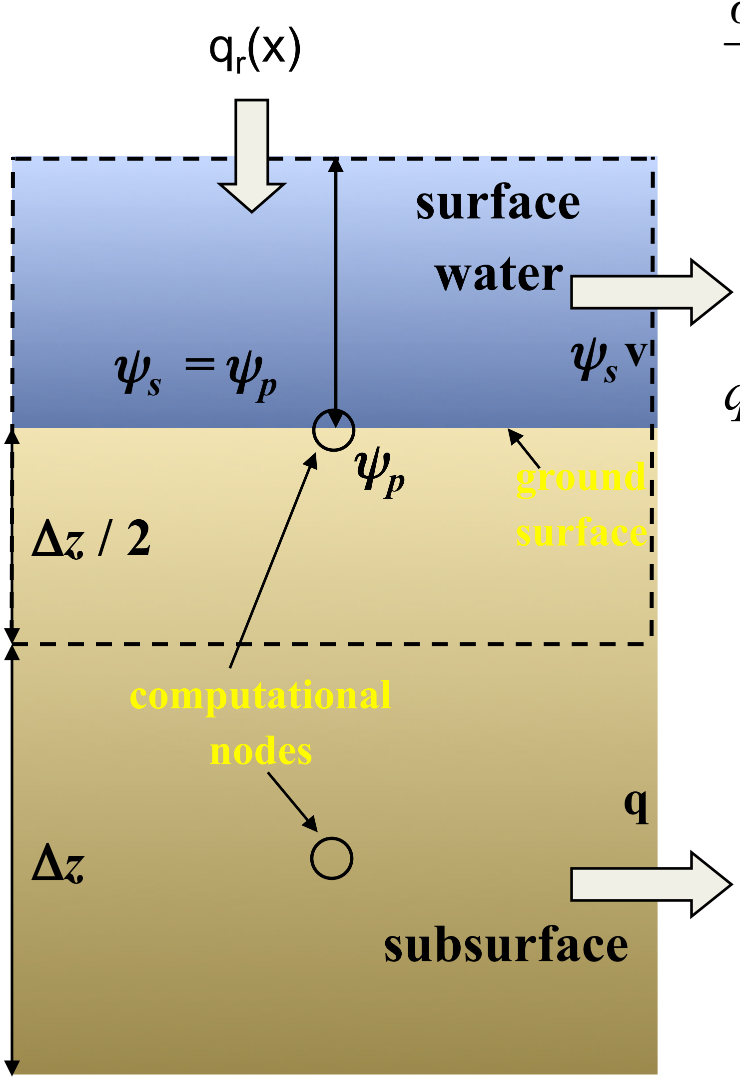
Exchange Flux

$$S_s S_w \frac{\partial \psi_p}{\partial t} + \phi \frac{\partial S_w(\psi_p)}{\partial t} = \nabla \cdot \mathbf{q} + q_s + m' q_e$$

Richards' eq

e.g. VanderKwaak and Loague (2001); Panday and Huyakorn (2004)

Overland Flow: General Pressure Formulation



$$\frac{\partial \psi_s}{\partial t} = \nabla\cdot\psi_s\mathbf{v} - q_r(x) - q_e(x)$$ Kinematic wave eq

$$\psi_s = \psi_p = \psi$$

The greater of ψ and 0

$$q_e(x) = \frac{\partial\|\psi,0\|}{\partial t} - \nabla\cdot\|\psi,0\|\mathbf{v} - q_r(x)$$

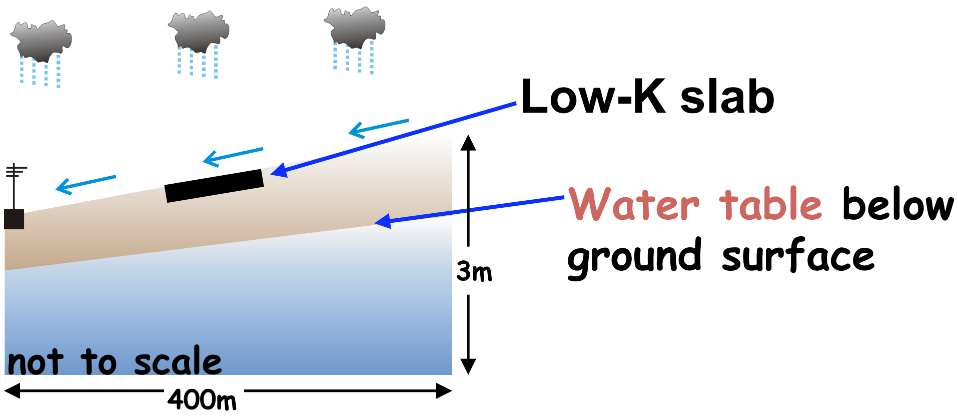
$$q_{bc} = -\mathbf{K}_s k_r(\psi)\nabla(\psi - z)$$ Neumann type BC

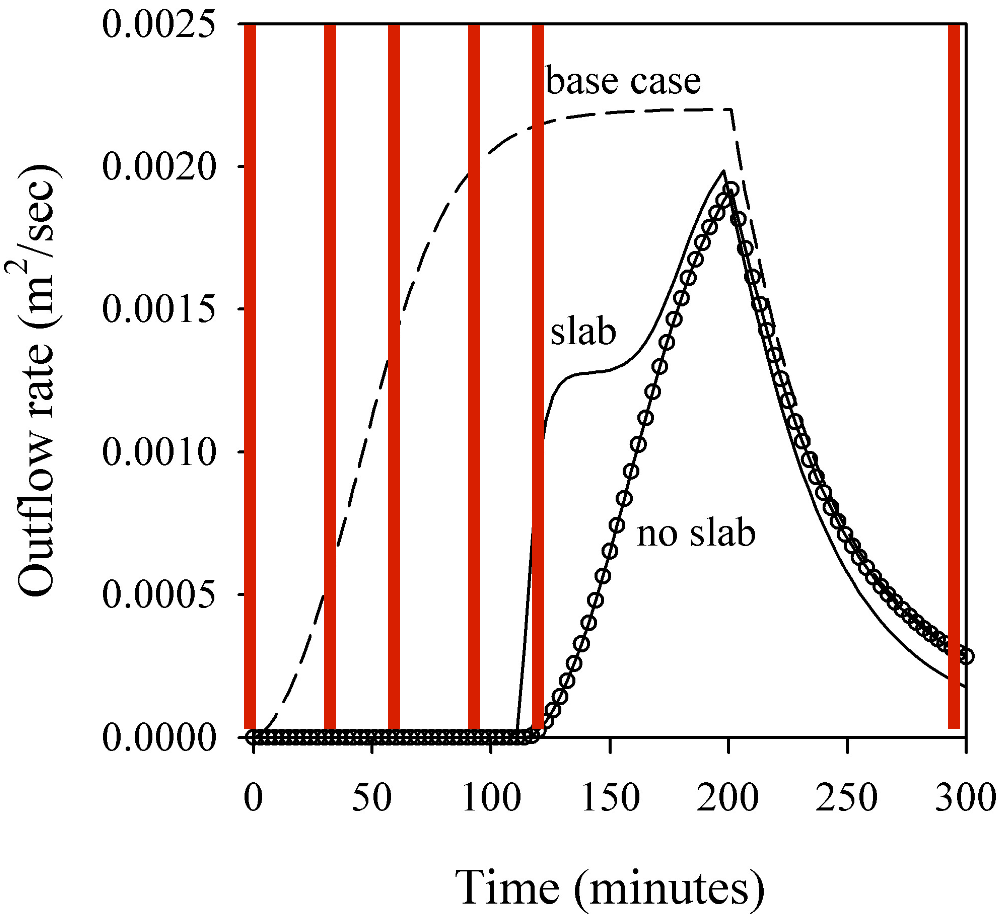
$$q_{bc}=q_e$$

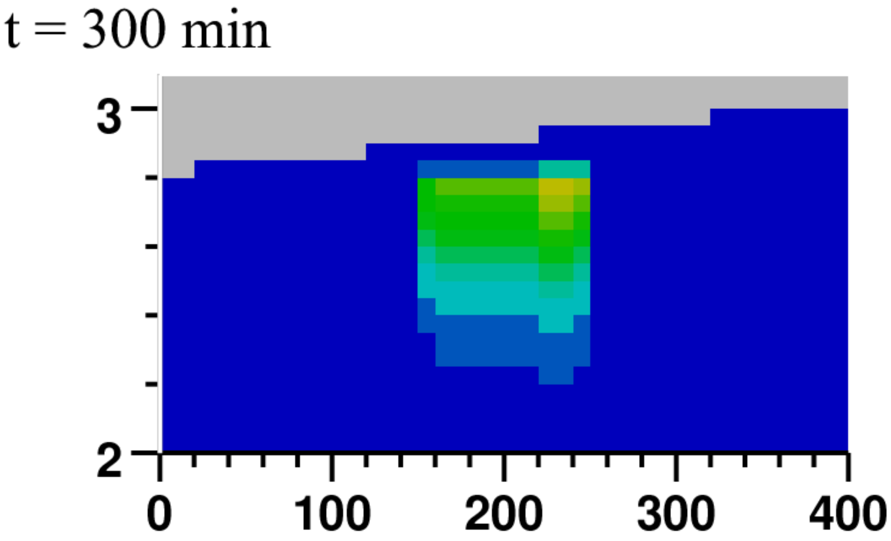
$$\boxed{-\mathbf{K}_s k_r(\psi)\nabla(\psi - z) = \frac{\partial\|\psi,0\|}{\partial t} - \nabla\cdot\|\psi,0\|\,\mathbf{v} - q_r(x)}$$

Kollet and Maxwell, AWR (2006)

Simulation Example



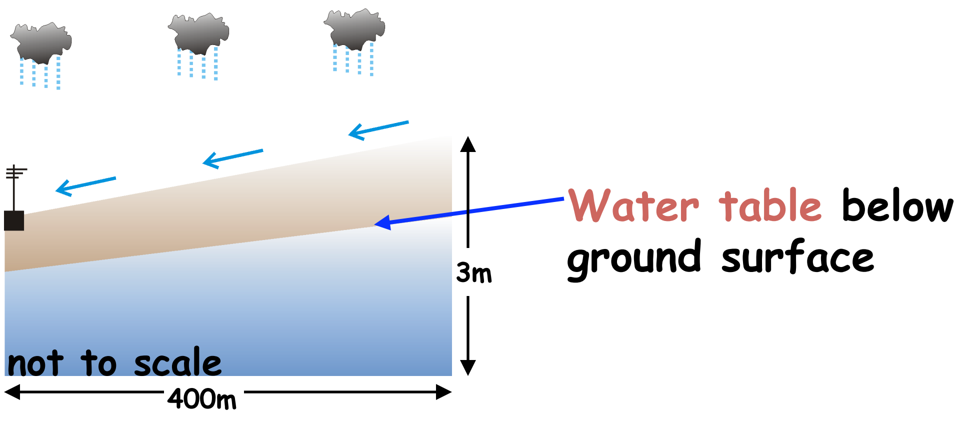




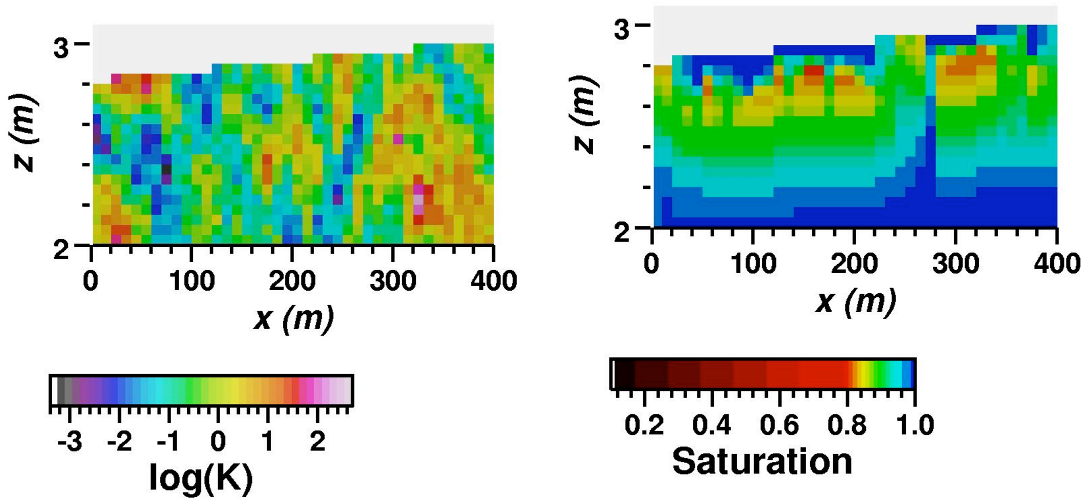
Kollet & Maxwell, AWR, 2006

Coupled Model Example: Subsurface Heterogeneity can influence the Hydrograph

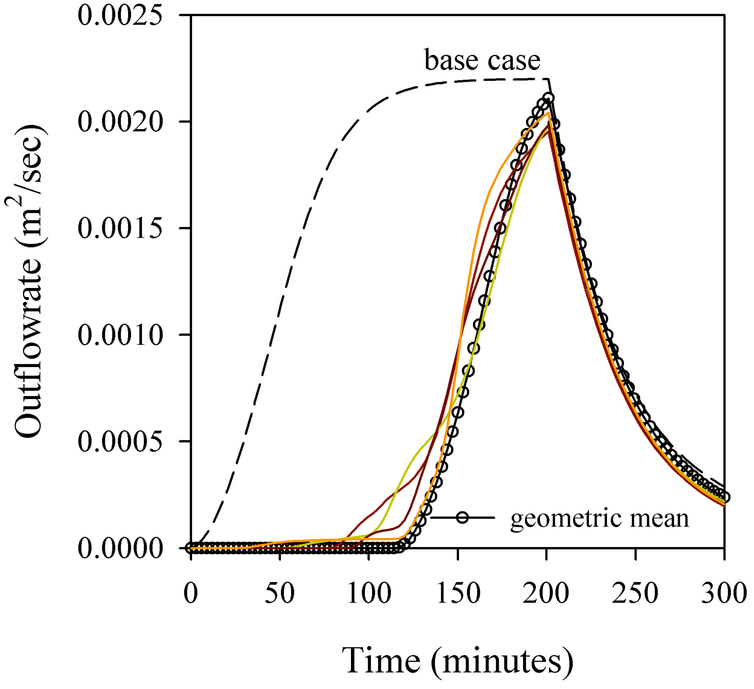
Random (Gaussian) Heterogeneity



Water table below ground surface



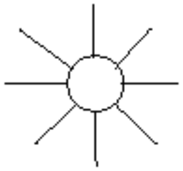
Small Monte Carlo Simulation



$$K_{geo} = q_{rain}$$

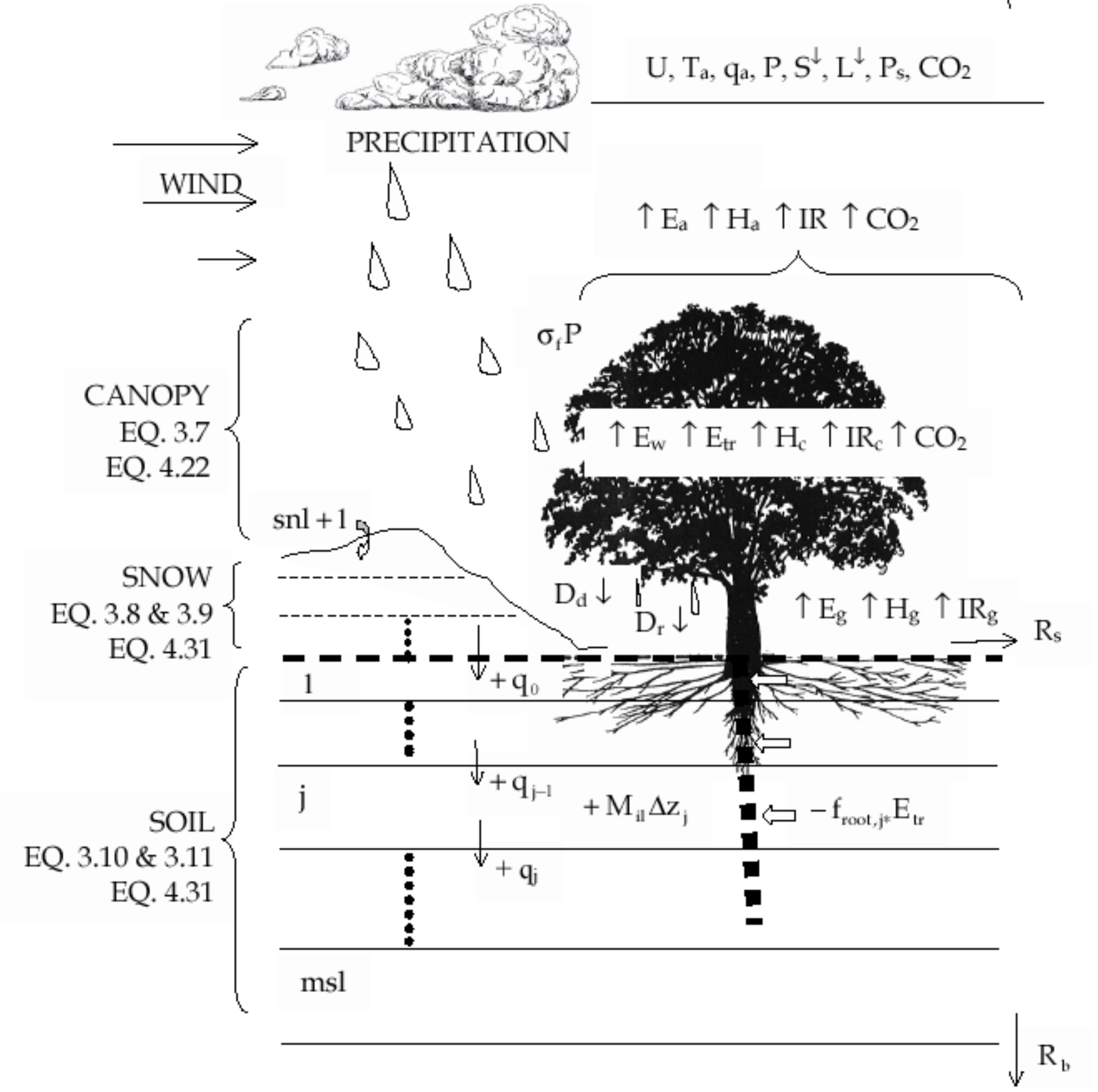
Kollet and Maxwell, AWR (2006)

Land Surface Models

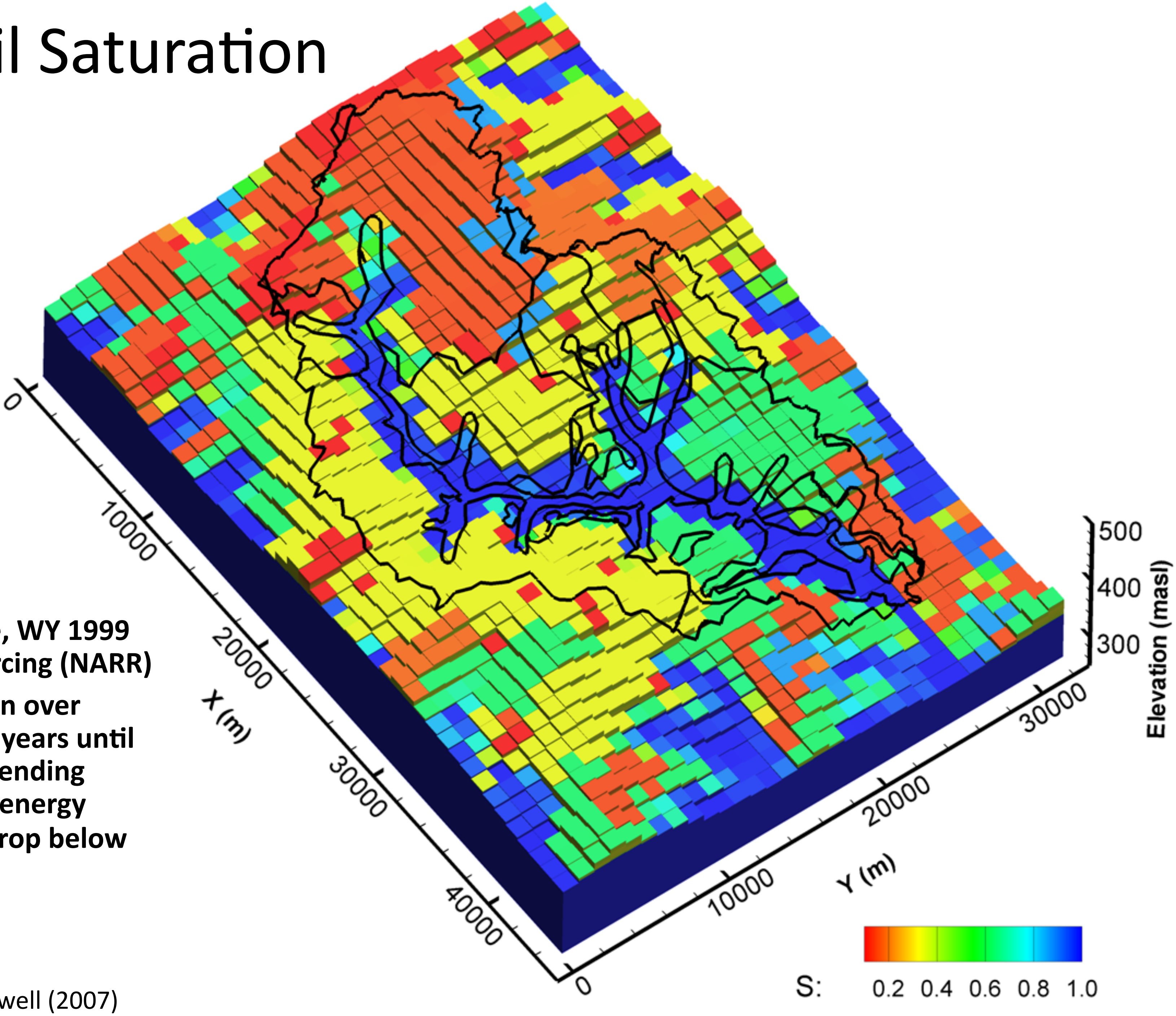


- Simulates water and energy balance near the land surface
- Single column soil-snow-vegetation biogeochemical model
- Atmospheric forcing
- Can be coupled to atmospheric models
- Simplistic, shallow, subsurface component

Baker, et al, 2003; Dia, Zeng and Dickinson, 2001



Soil Saturation



- **Run offline, WY 1999 used as forcing (NARR)**
- **Spinup: Run over successive years until beginning-ending water and energy balances drop below threshold**

Kollet and Maxwell (2007)

ParFlow Synopsis - Physics

- Fully parallel, multigrid-preconditioned, finite difference/finite volume 3D flow
- Groundwater equation (steady-state, e.g. Ashby and Falgout 1996)
- Richards' equation (transient, 3D; e.g. Jones and Woodward 2001)
- Fully-coupled overland flow (via Kollet and Maxwell 2006, overland flow boundary condition approach)
- NCAR-Land Surface Model CLM integrated into ParFlow as module, all biogeophyiscal, energy budget at land surface, snow/snowmelt/compaction, some dynamic plant interactions

ParFlow Synopsis – Physics (cont)

- Coupled to U of Oklahoma mesoscale atmospheric code ARPS (e.g. Maxwell, Chow, Kollet 2007)
- Coupled to NCAR Weather Research and Forecasting (WRF) Code (Maxwell et al 2009)
- Couples to (integrates with) Lagrangian contaminant transport code (SLIM)

ParFlow- performance

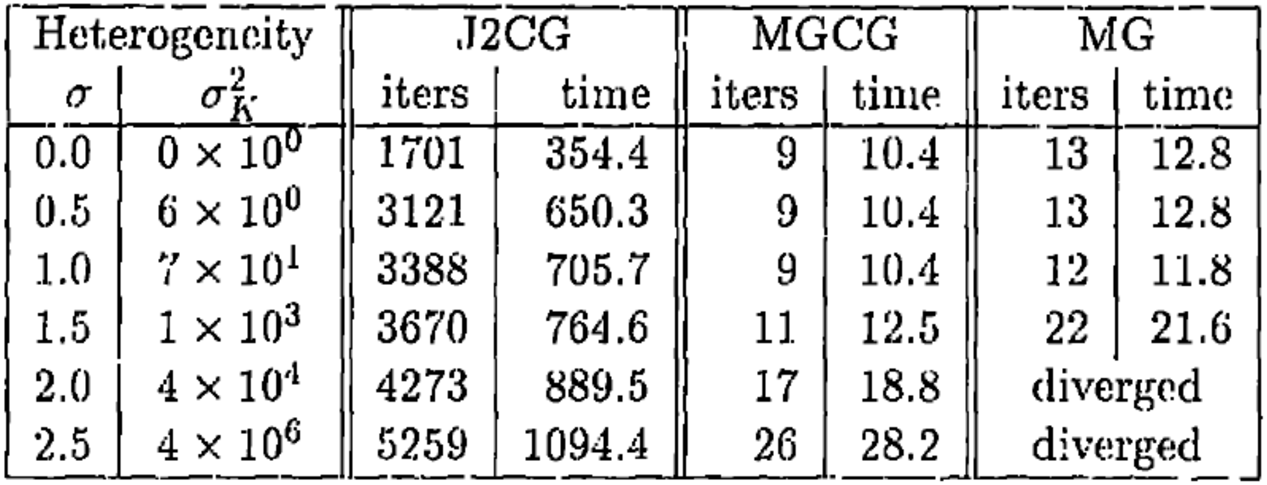
- Efficient implementation results from
  - efficient linear preconditioning (HyPre)
  - efficient nonlinear solver (Kinsol –SUNDIALS)
  - efficient coupling and code operation/architecture
- All implementations scale linearly with problem size
- All implementations demonstrate excellent parallel scaling to large (~1000) processors
- For 3D, Steady-state groundwater ~100 X faster than typical GW code
- For 2D, transient Richards' variably saturated ~10X faster than typical var-sat codes in 2D, *much greater speedup in 3D*

Performance: Making the problem "harder"

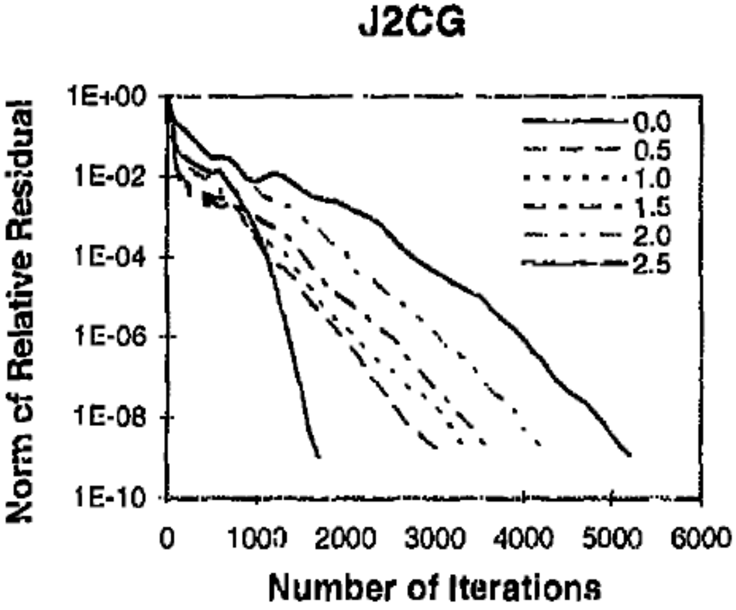
Ashby and Falgout (1996)

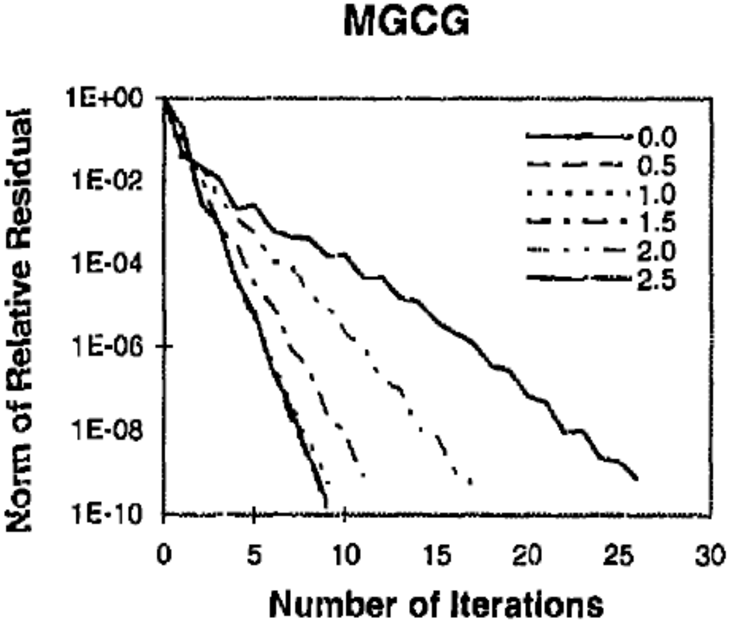
TABLE 5.5

Varying the degree of heterogeneity.



Heterogeneity		J2CG		MGCG		MG	
σ	σ_K^2	iters	time	iters	time	iters	time
0.0	0×10^0	1701	354.4	9	10.4	13	12.8
0.5	6×10^0	3121	650.3	9	10.4	13	12.8
1.0	7×10^1	3388	705.7	9	10.4	12	11.8
1.5	1×10^3	3670	764.6	11	12.5	22	21.6
2.0	4×10^4	4273	889.5	17	18.8	diverged	
2.5	4×10^6	5259	1094.4	26	28.2	diverged	





Performance: Making the problem bigger

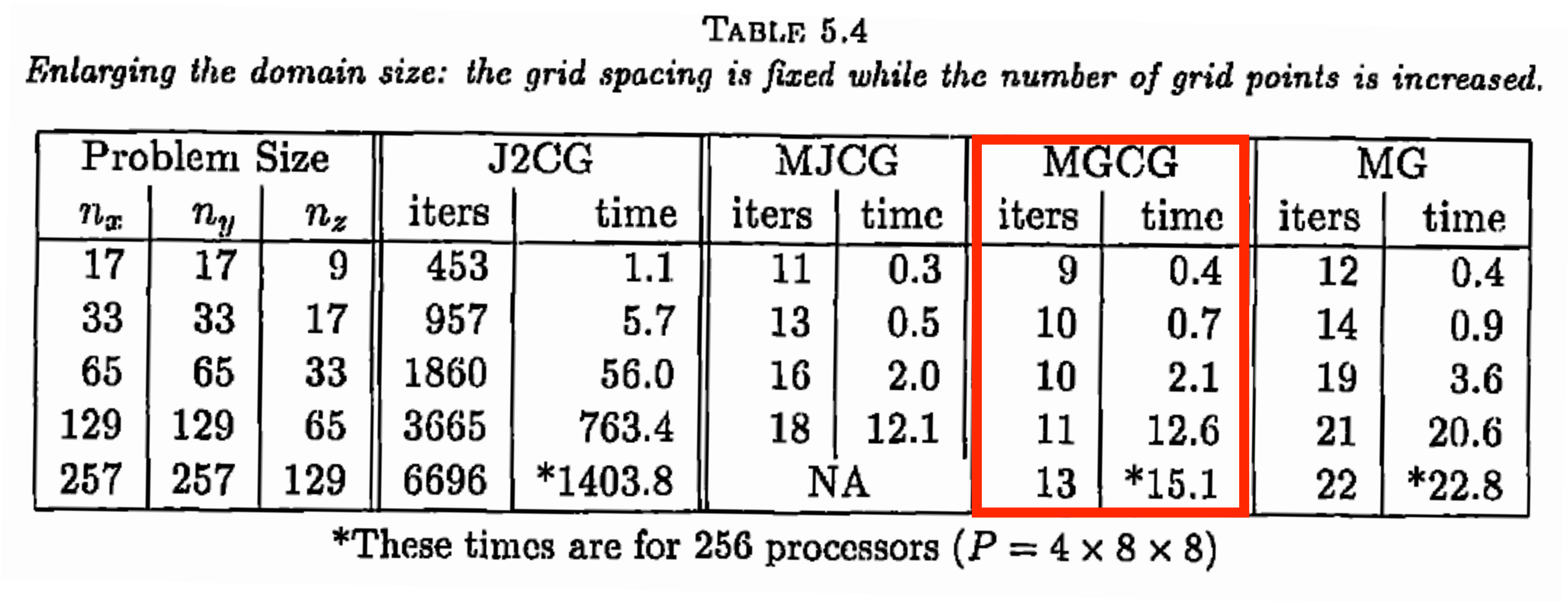


TABLE 5.4

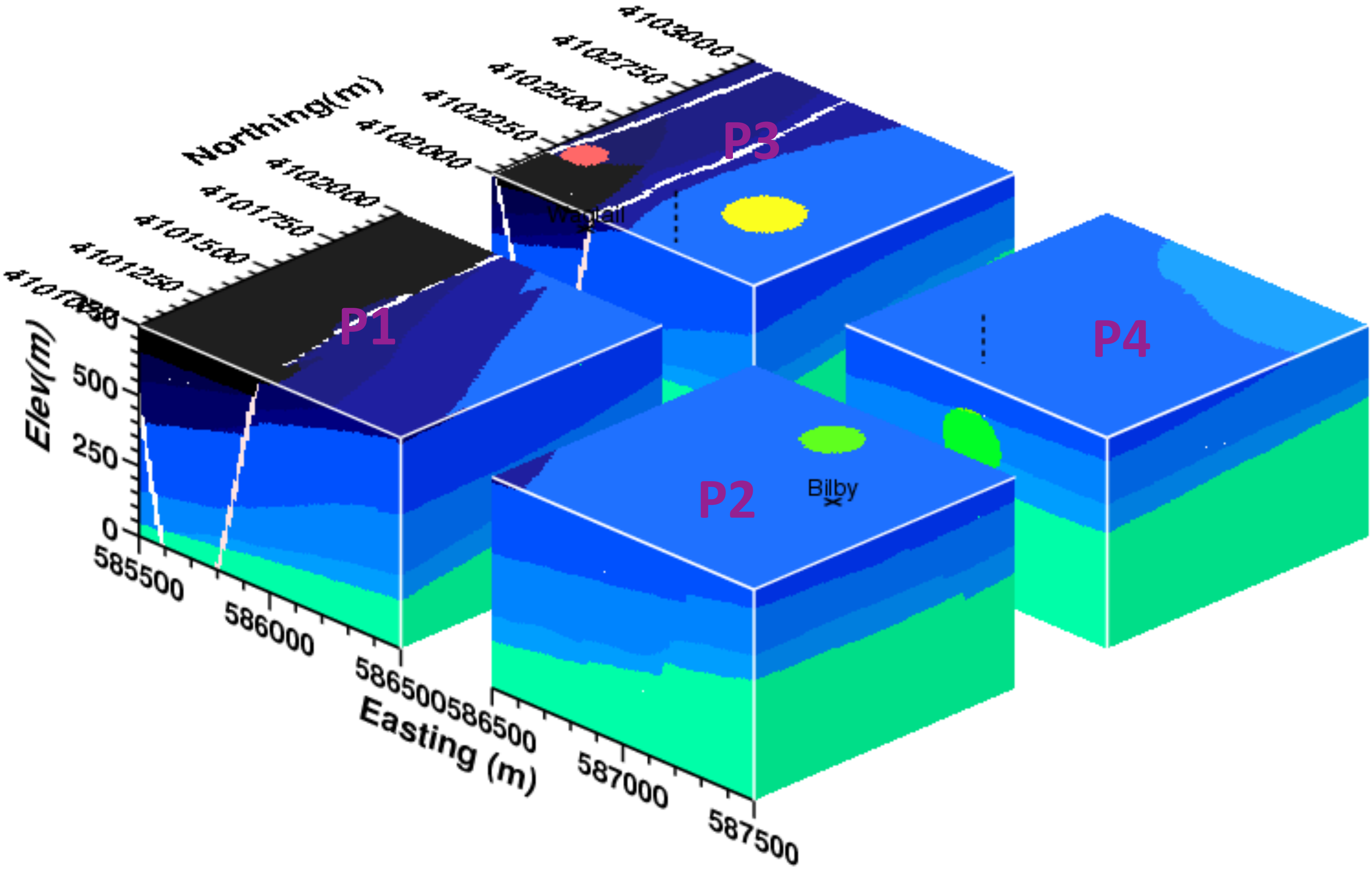
Enlarging the domain size: the grid spacing is fixed while the number of grid points is increased.

Problem Size			J2CG		MJCG		MGCG		MG	
n_x	n_y	n_z	iters	time	iters	time	iters	time	iters	time
17	17	9	453	1.1	11	0.3	9	0.4	12	0.4
33	33	17	957	5.7	13	0.5	10	0.7	14	0.9
65	65	33	1860	56.0	16	2.0	10	2.1	19	3.6
129	129	65	3665	763.4	18	12.1	11	12.6	21	20.6
257	257	129	6696	*1403.8	NA		13	*15.1	22	*22.8

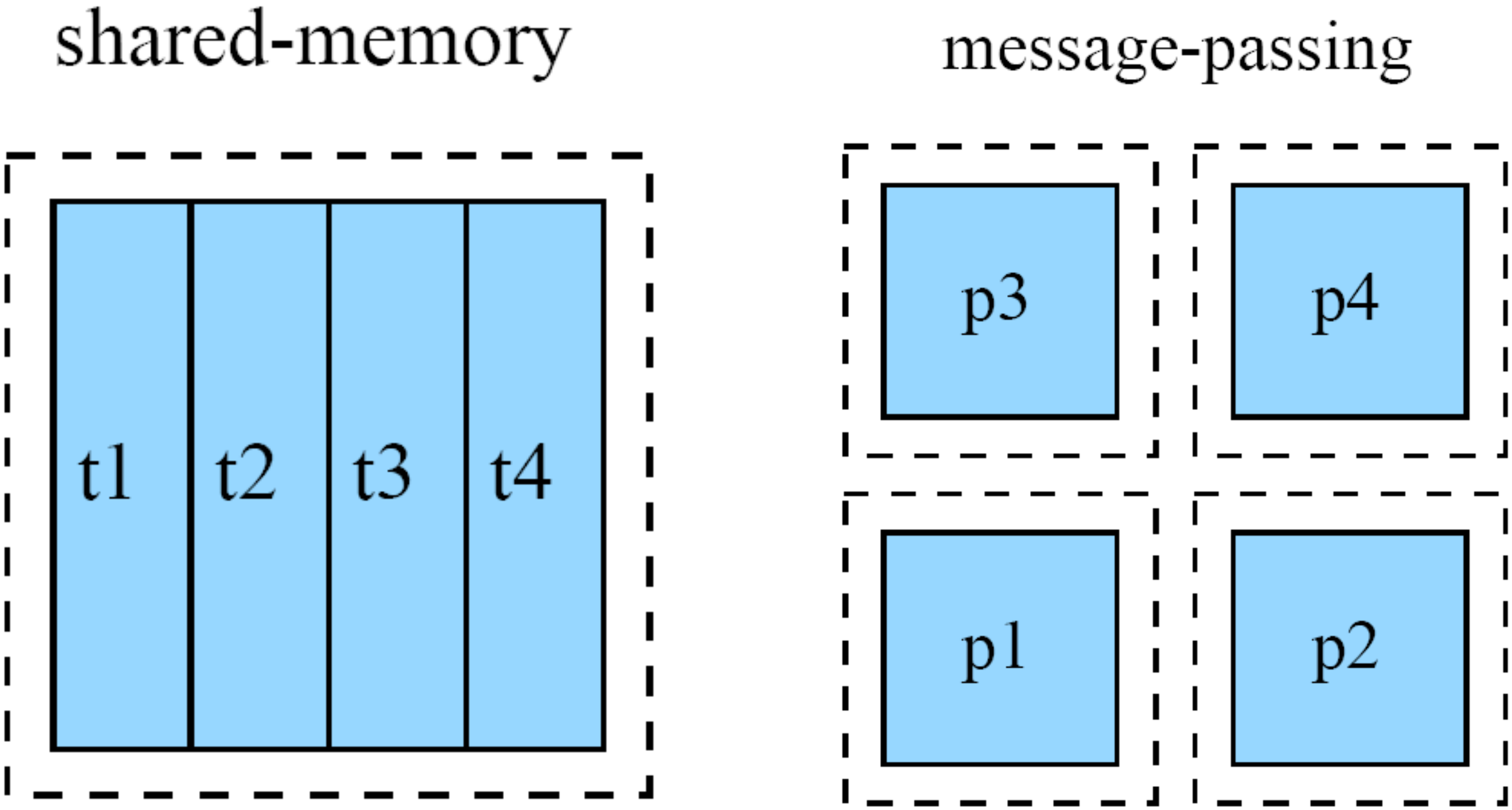
*These times are for 256 processors ($P = 4 \times 8 \times 8$)

Ashby and Falgout (1996)

Parallelization

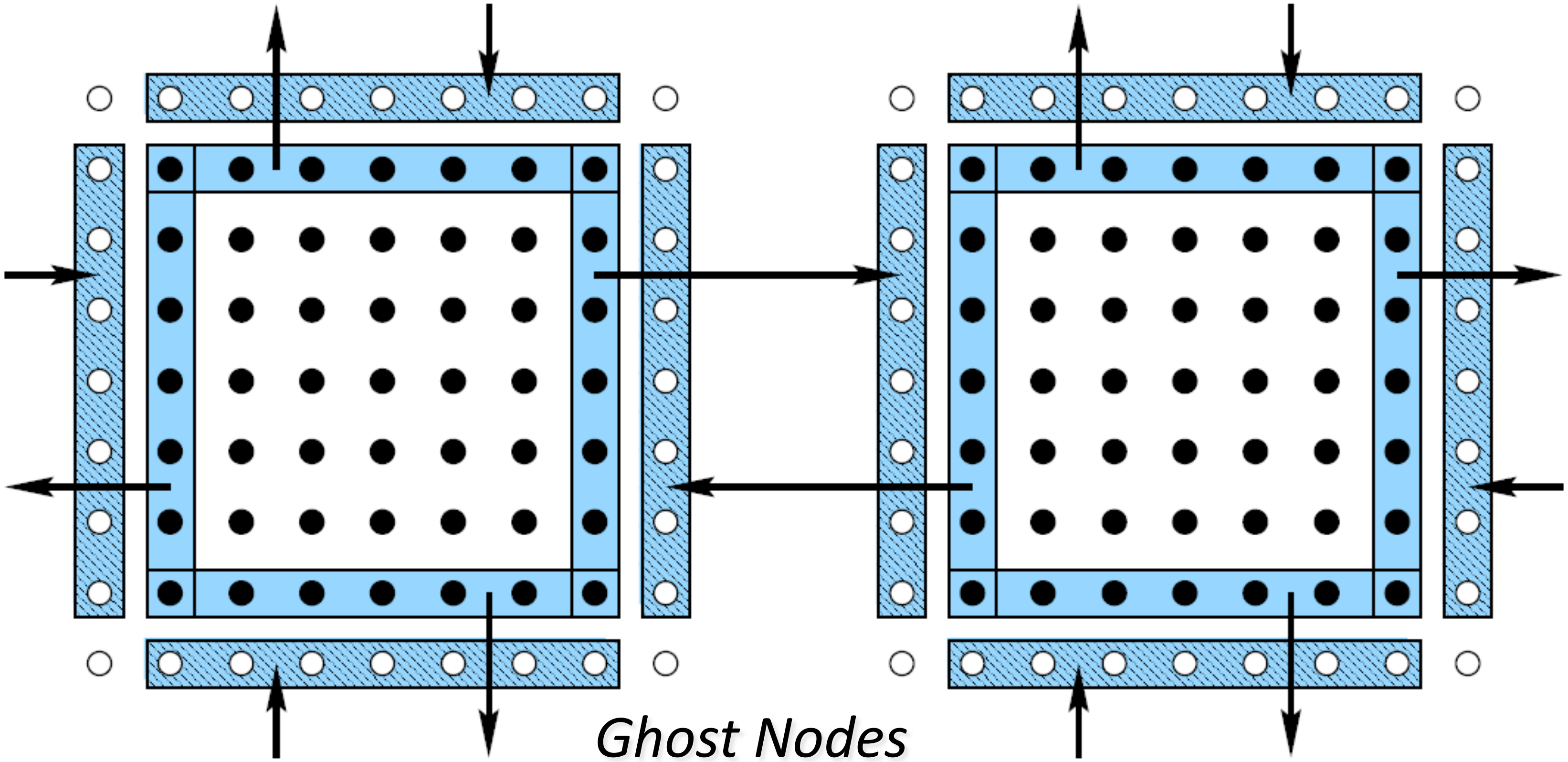


Parallelization



Falgout and Jones (1999)

Parallelization- Distributed Memory



Ghost Nodes

P1

P2

Falgout and Jones (1999)

Performance: Serial and Parallel

- Performance and parallel performance are intricately linked
- To get good parallel performance the numerical algorithm must scale linearly with problem size
- If we want to run large problems and our solver does not scale parallel performance will not be sustained

Scaled Parallel Efficiency- Scaled Speedup

Scaled parallel efficiency, *E,* is defined as the ratio of time to run a problem of varying size as we keep the per-processor work constant

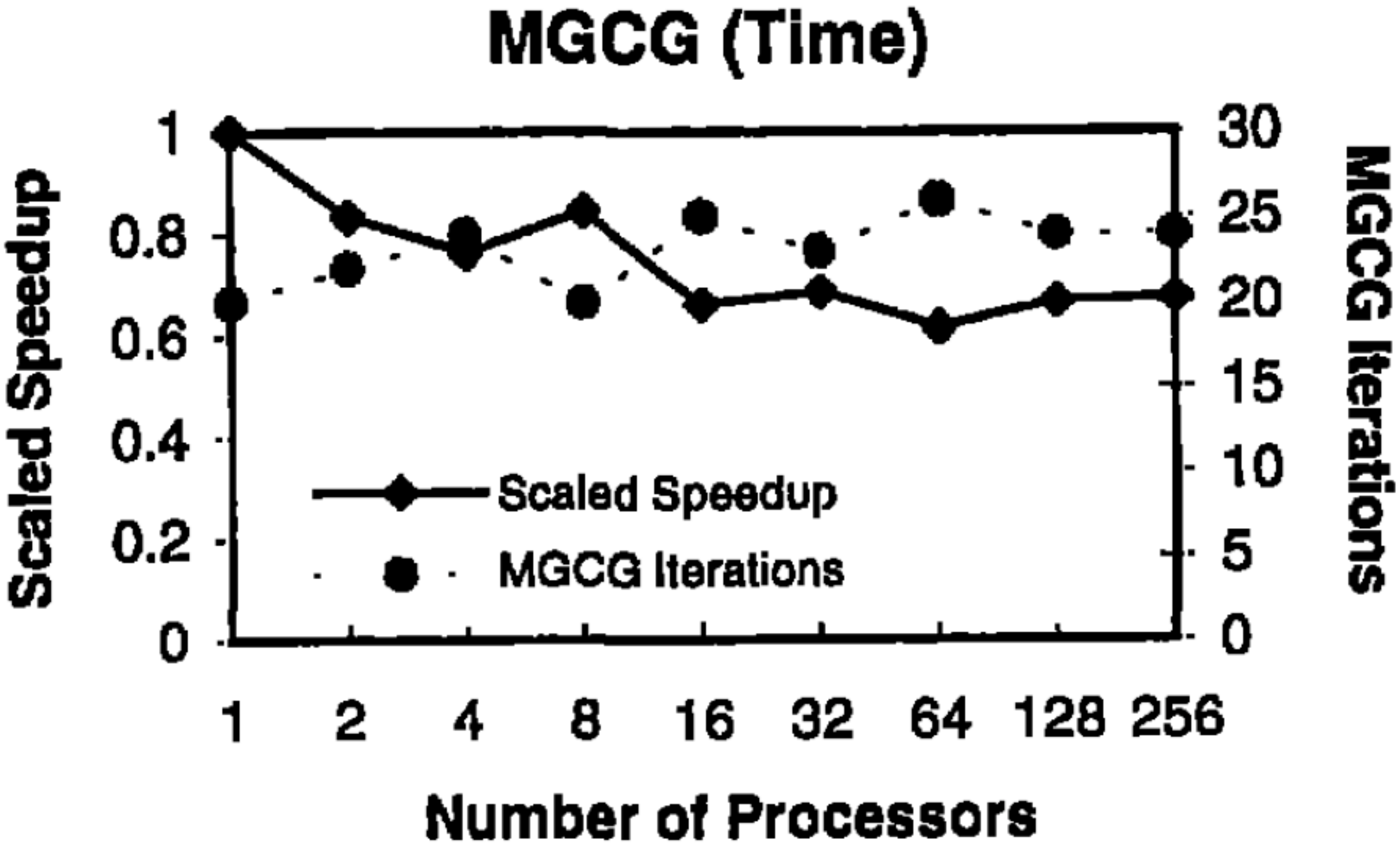
$$E(n,p) = \frac{T(n,1)}{T(pn,p)}$$

T = run time

n = problem size

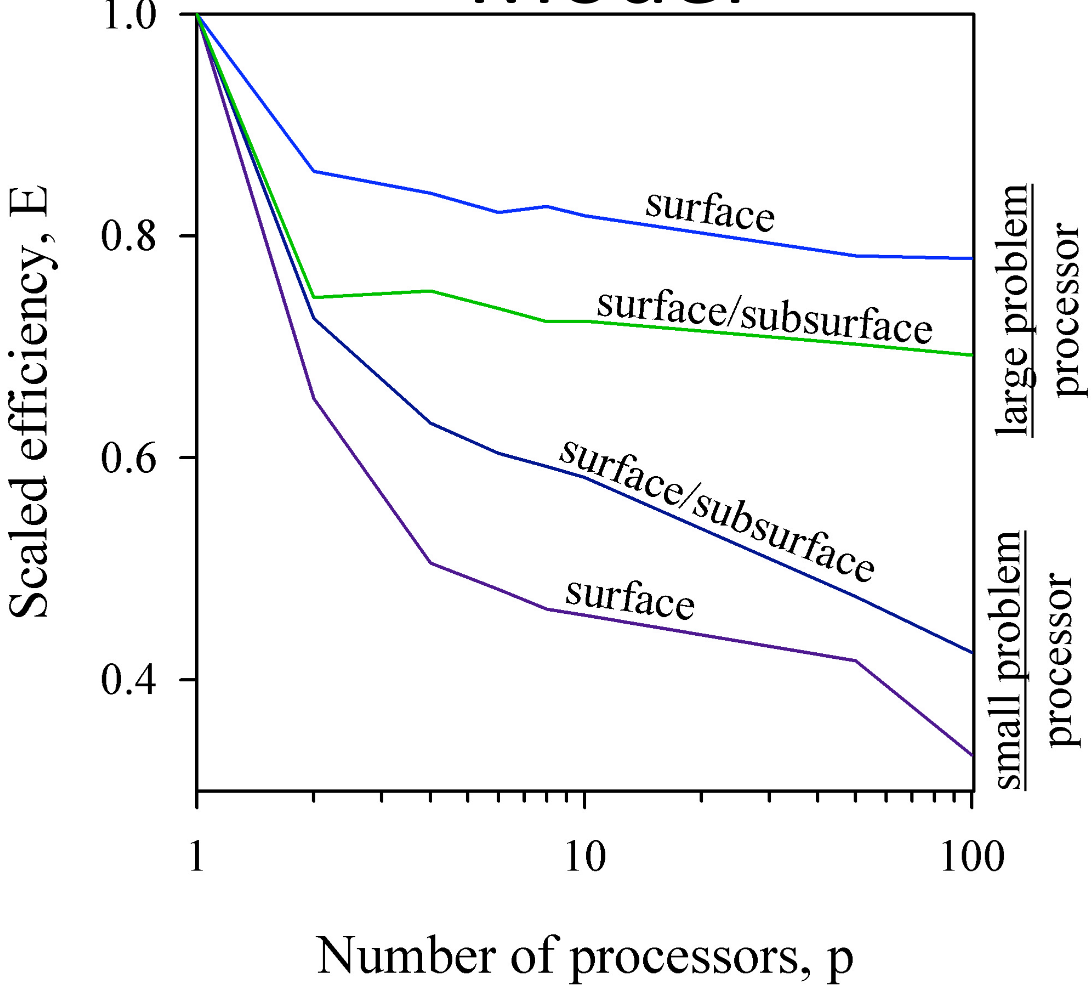
p = number of processors

Parallel Performance: Scaled Speedup of the Linear Problem



Ashby and Falgout (1996)

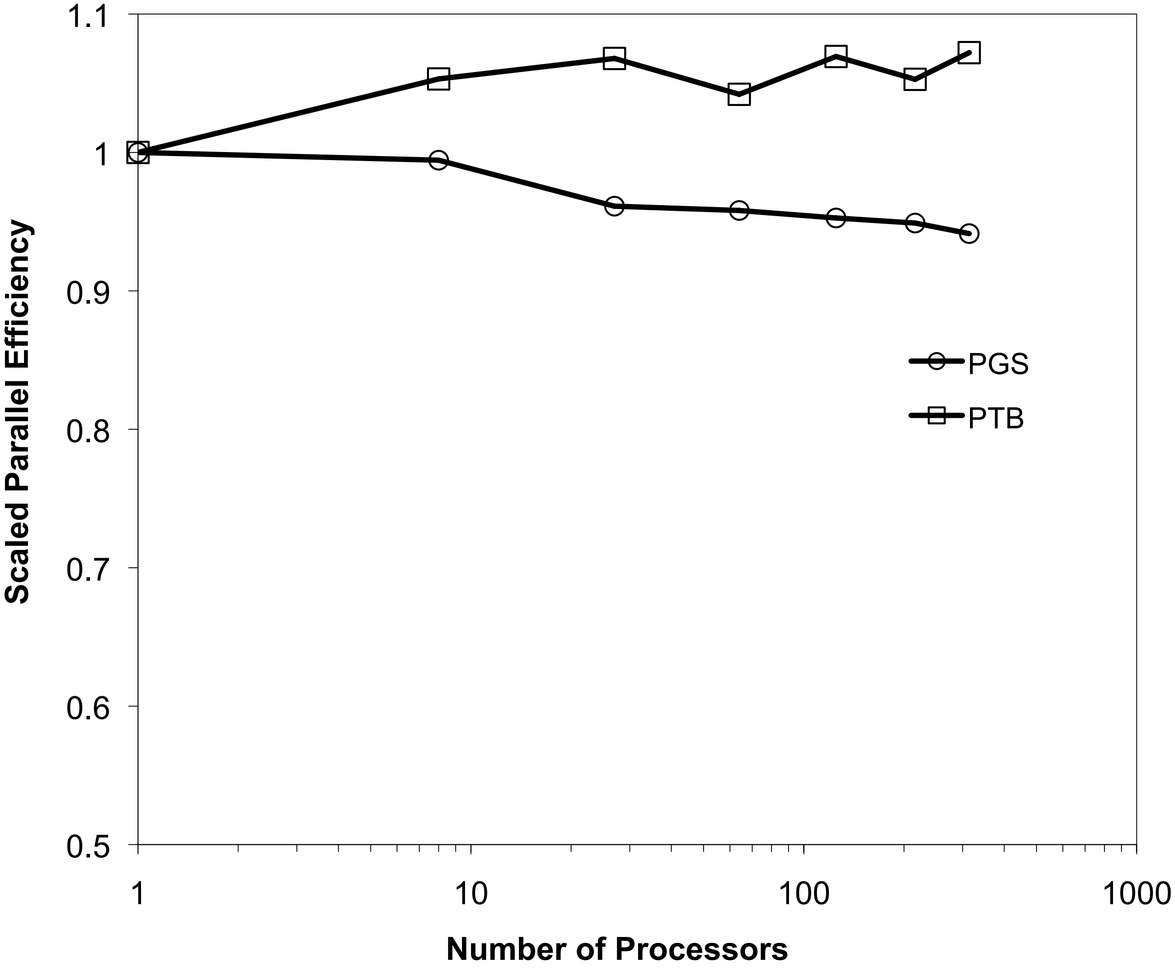
Scaled Parallel Efficiency of Coupled Model



Perfect efficiency: double problem size and processor #
same run time => E = 1

Kollet and Maxwell, AWR (2006)

Parallel Performance: Correlated GRF Simulation



ParFlow Synopsis- code operation

- ParFlow written in *ANSI* C with object-oriented structure
- Parallel from "bottom-up" with ability to handle many communication sublayers (serial, shared-memory and distributed memory implementation from one common physics core)
- OctTree technique to allow any general domain shapes and geometries (topography, large-intermediate-scale geology)
- TCL/TK scripting interface w/ object-oriented structure
- Parallel Gaussian and Parallel Turning Bands stochastic random field generators with ability to follow any geometry (e.g. Maxwell et al 2009)

ParFlow Synopsis- code operation (cont)

- Recently released under GNU LPGL license, open-source, free software
- Multiplatform, “Laptop to supercomputer” with OSX, Windows and Linux Unix porting
- Build system now handled by GNU Autoconf makes porting simple
- Robust toolset (PFTOOLS) to manipulate/post-process files
- Output now fully integrated with VISIT visualization system among others

Model Input Structure

- 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

Computational Grid (Input File)

Comment character for tcl/tk

```
#-----------------------------------------------------------
# Computational Grid
#-----------------------------------------------------------
pfset ComputationalGrid.Lower.X                 0.0
pfset ComputationalGrid.Lower.Y                 0.0
pfset ComputationalGrid.Lower.Z                 0.0

pfset ComputationalGrid.NX                      30
pfset ComputationalGrid.NY                      30
pfset ComputationalGrid.NZ                      30

pfset ComputationalGrid.DX                        10.0
pfset ComputationalGrid.DY                     10.0
pfset ComputationalGrid.DZ                           .05
```

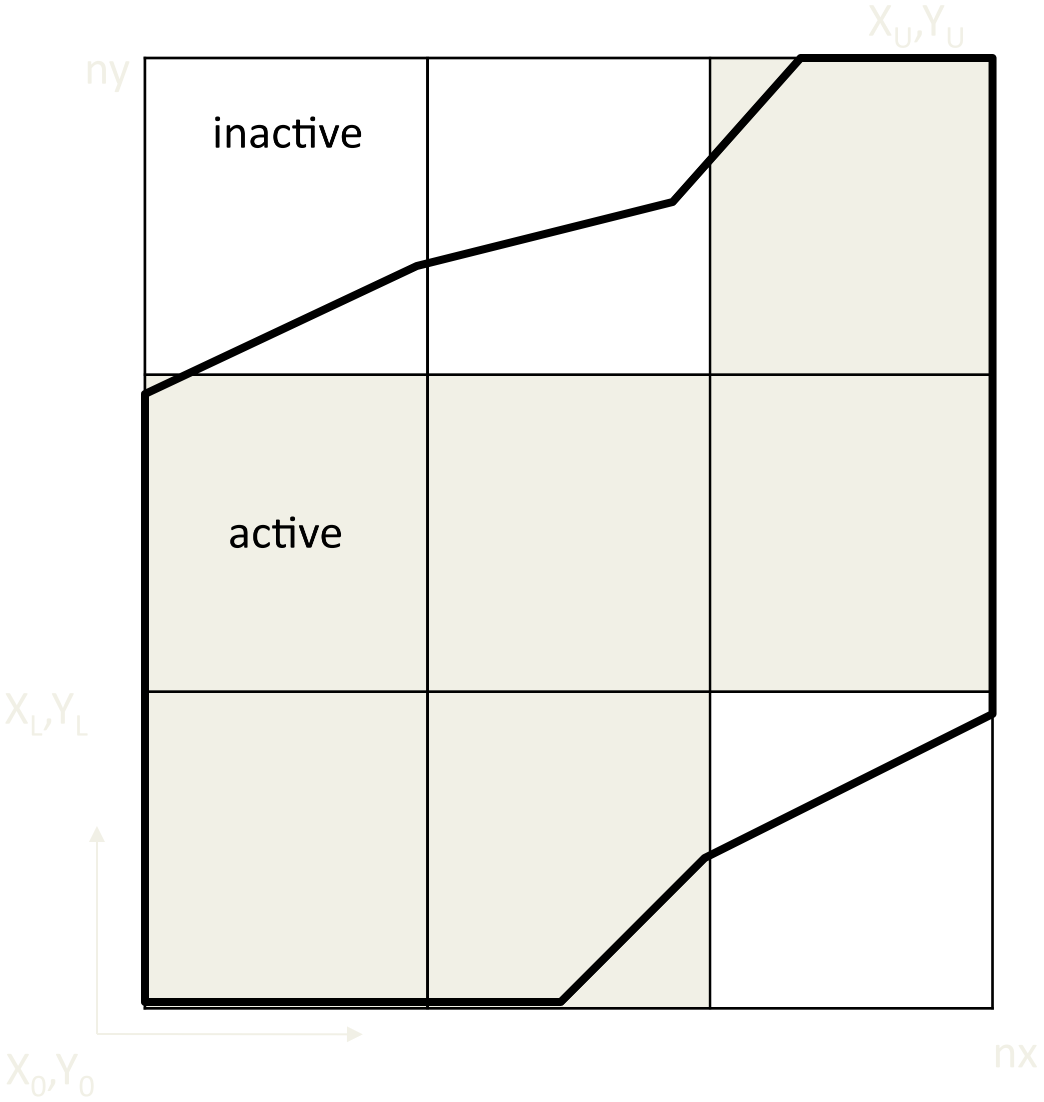
Coordinates (length units)

Grid dimensions (integer)

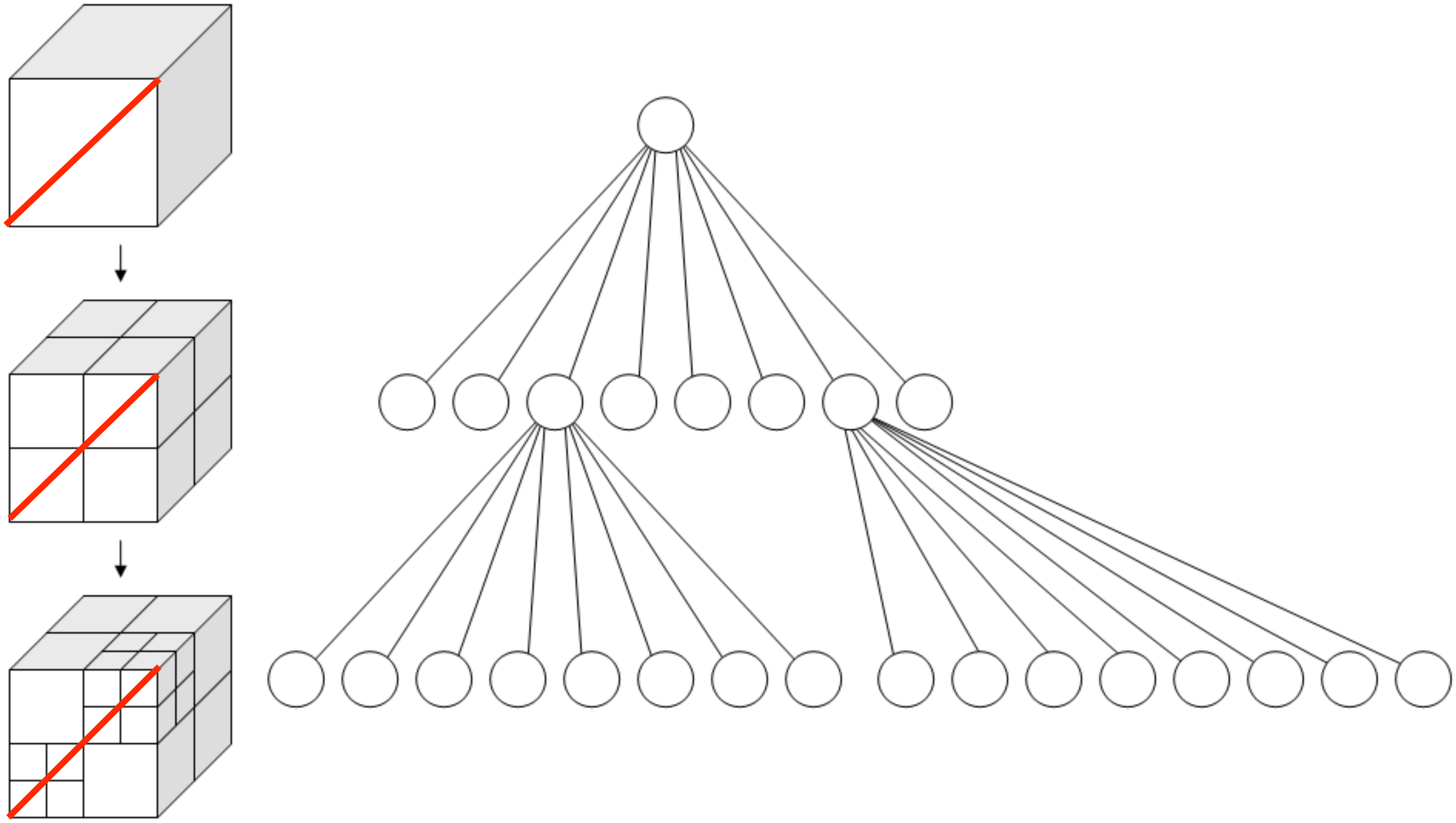
Cell size (length units)

SolidFile Geometry

- A triangulated information network file that can delineate geometries of any shape
- Read in as a .pfsol file
- Geometries and patches are defined from within the file
- May be used to delineate active and inactive cells

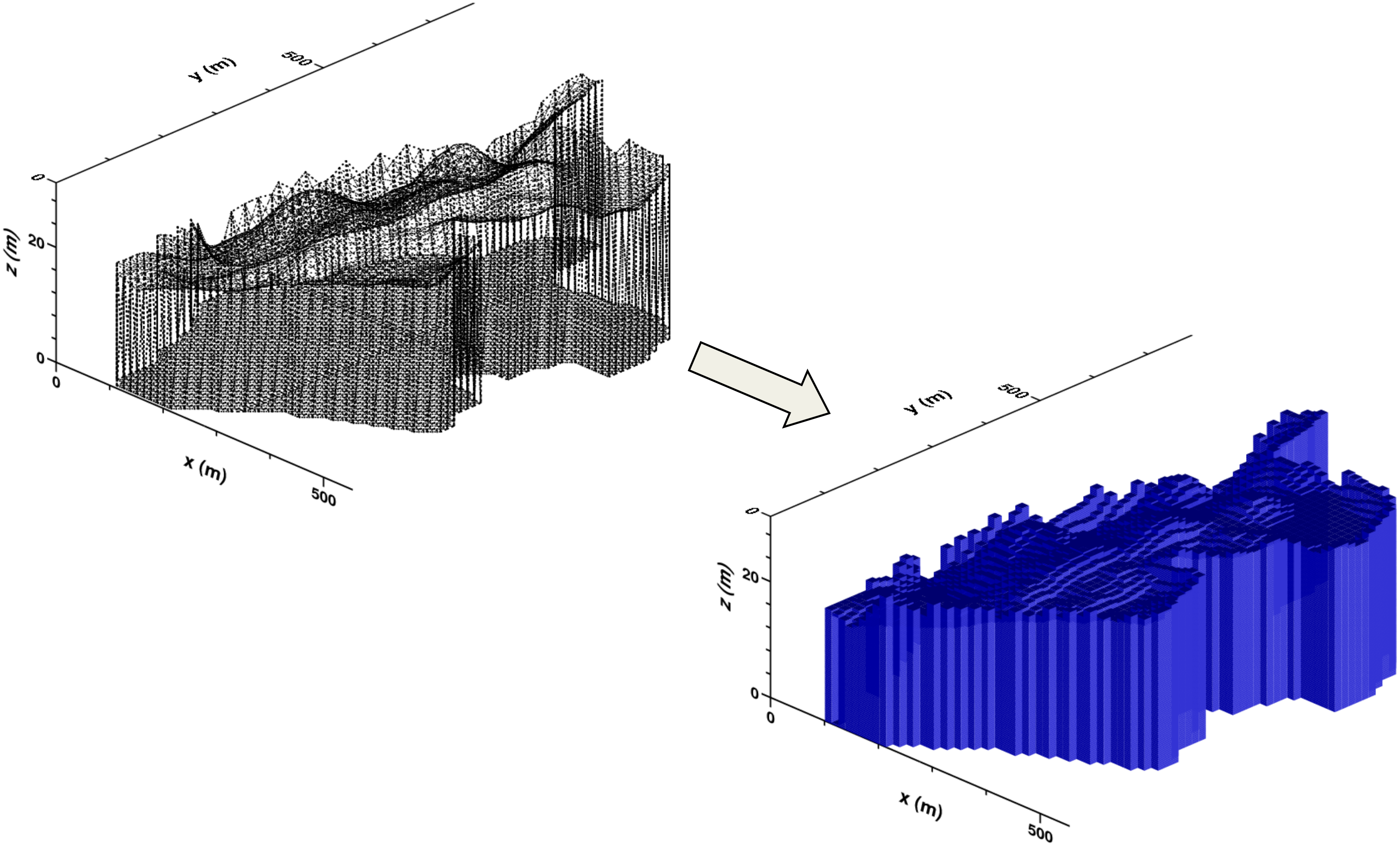


Octree used to delineate geometries



Source: Wikipedia

SolidFile Geometry



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

ParFlow – Bibliography (Model Physics Papers in bold)

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13. S. F. Ashby, W. J. Bosl, R. D. Falgout, S. G. Smith, A. F. B. Tompson, and T. J. Williams (1999), A numerical simulation of groundwater flow and contaminant transport on the CRAY T3D and C90 supercomputers, International Journal of High Performance Computer Applications, 13(1), 80-93
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15. **S. F. Ashby and R. D. Falgout, (1996), A parallel multigrid preconditioned conjugate gradient algorithm for groundwater flow simulations, Nuclear Science and Engineering, 124(1), 145-159.**

ParFlow Development Team

- Reed M. Maxwell: *Department of Geology and Geologic Engineering, Colorado School of Mines Golden, CO, USA*: rmaxwell@mines.edu
- Stefan J. Kollet: *Meteorological Institute, Bonn University, Bonn, Germany*: stefan.kollet@uni-bonn.de
- Steven G. Smith: *Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA. USA*: sgsmith@llnl.gov
- Carol S. Woodward: *Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA, USA*: cswoodward@llnl.gov
- Robert D. Falgout: *Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA, USA*
- William J. Bosl: *Children's Hospital Informatics Program, Harvard Medical School, Boston, MA, USA*
- Chuck Baldwin, *Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA, USA*
- Richard Hornung: *Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA, USA*
- Steven Ashby: *Pacific Northwest National Laboratory, Richland, WA, USA.*

ParFlow – Getting the Code, more information

Old (LLNL) ParFlow web page:

https://computation.llnl.gov/casc/parflow/parflow_home.html

Reed Maxwell's web page (code section updated soon w/ PF download, etc)

http://inside.mines.edu/~rmaxwell/

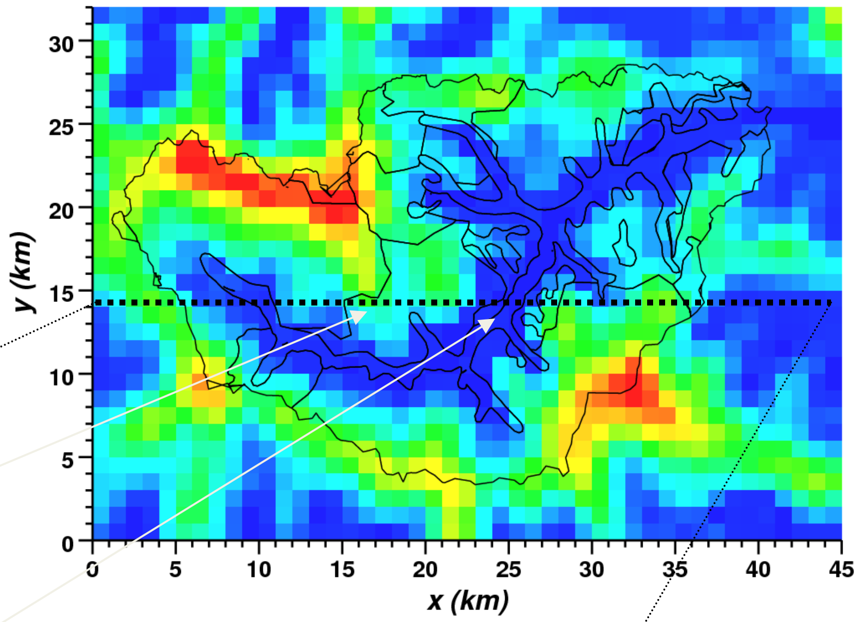
ParFlow Blog

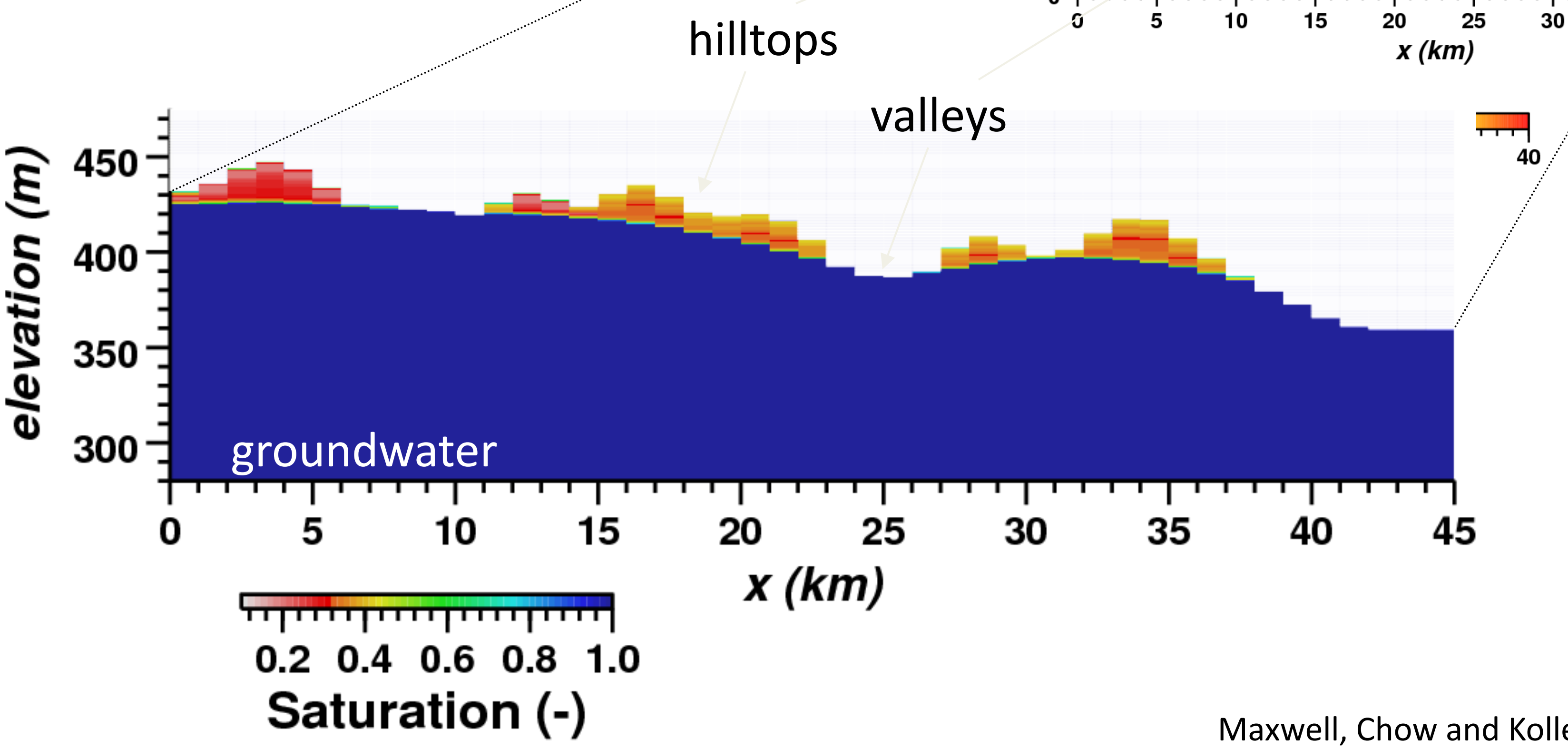
http://parflow.blogspot.com/

Email: rmaxwell@mines.edu

Water Table Depth, Cross Section

- **Water table driven by topography**
- **Very deep (~40m) at hilltops (*drier*)**
- **Very shallow in valleys (*wetter*)**
- **Cross section shows variation of WT and Saturation**

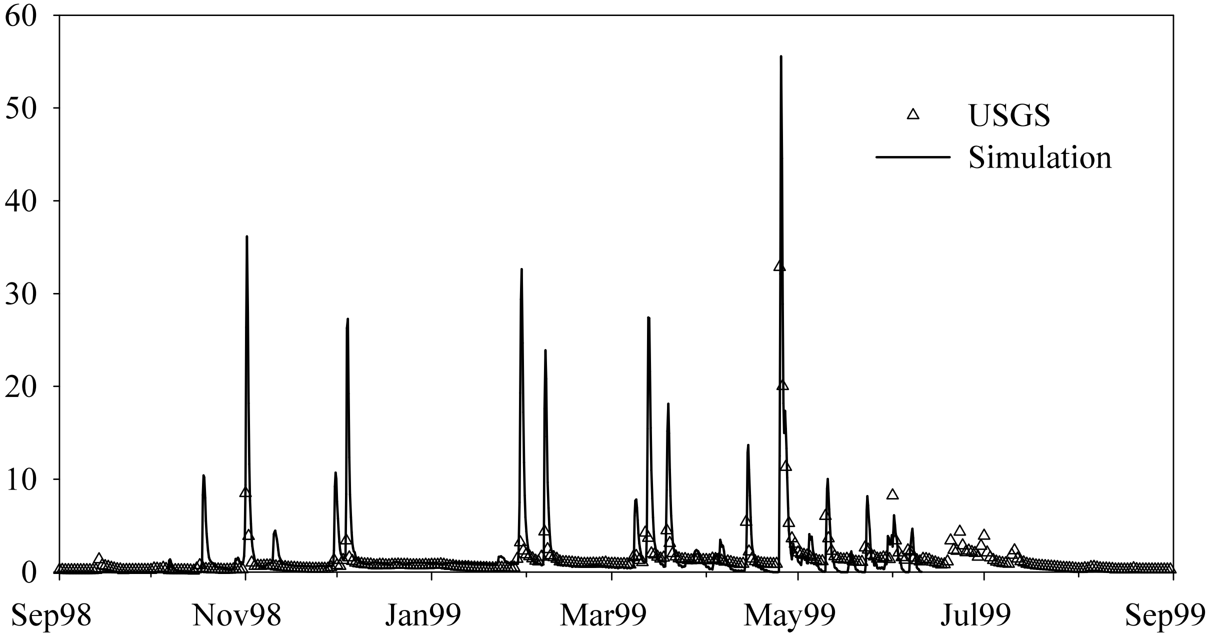


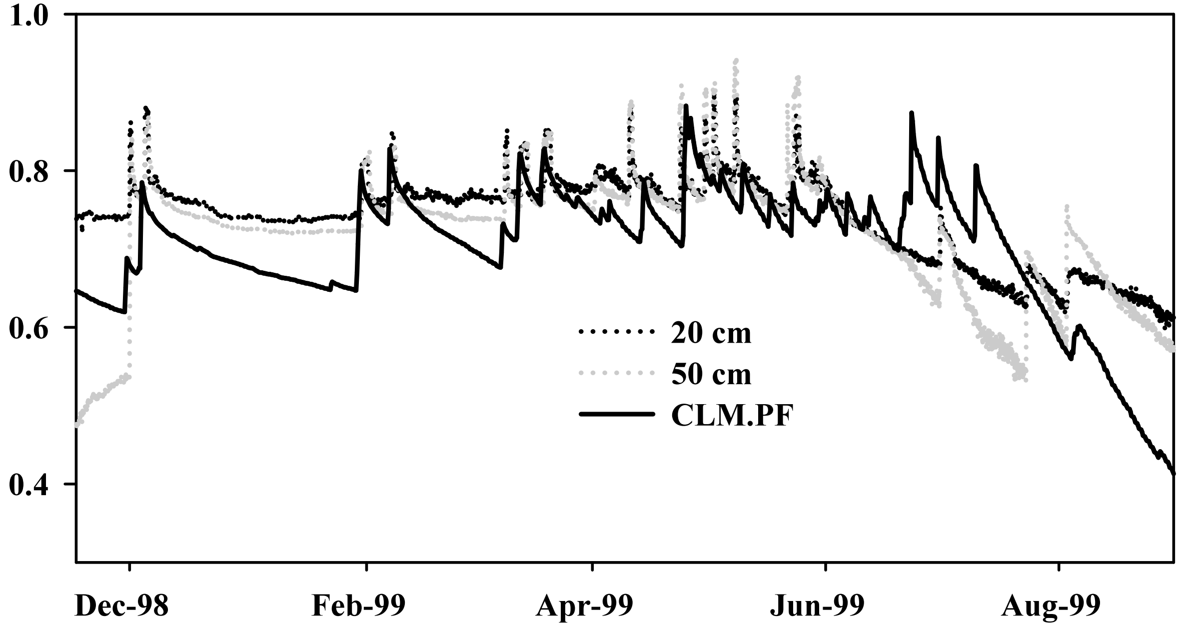


Maxwell, Chow and Kollet, AWR (2007)

Comparison to outflow and saturation observations

- **Overall favorable comparisons**
- **Trends (particularly SM) match very well**
- **Difficulty comparing due to resolution and scale of observations**
- **Intent *not* to calibrate/predict but to understand process**

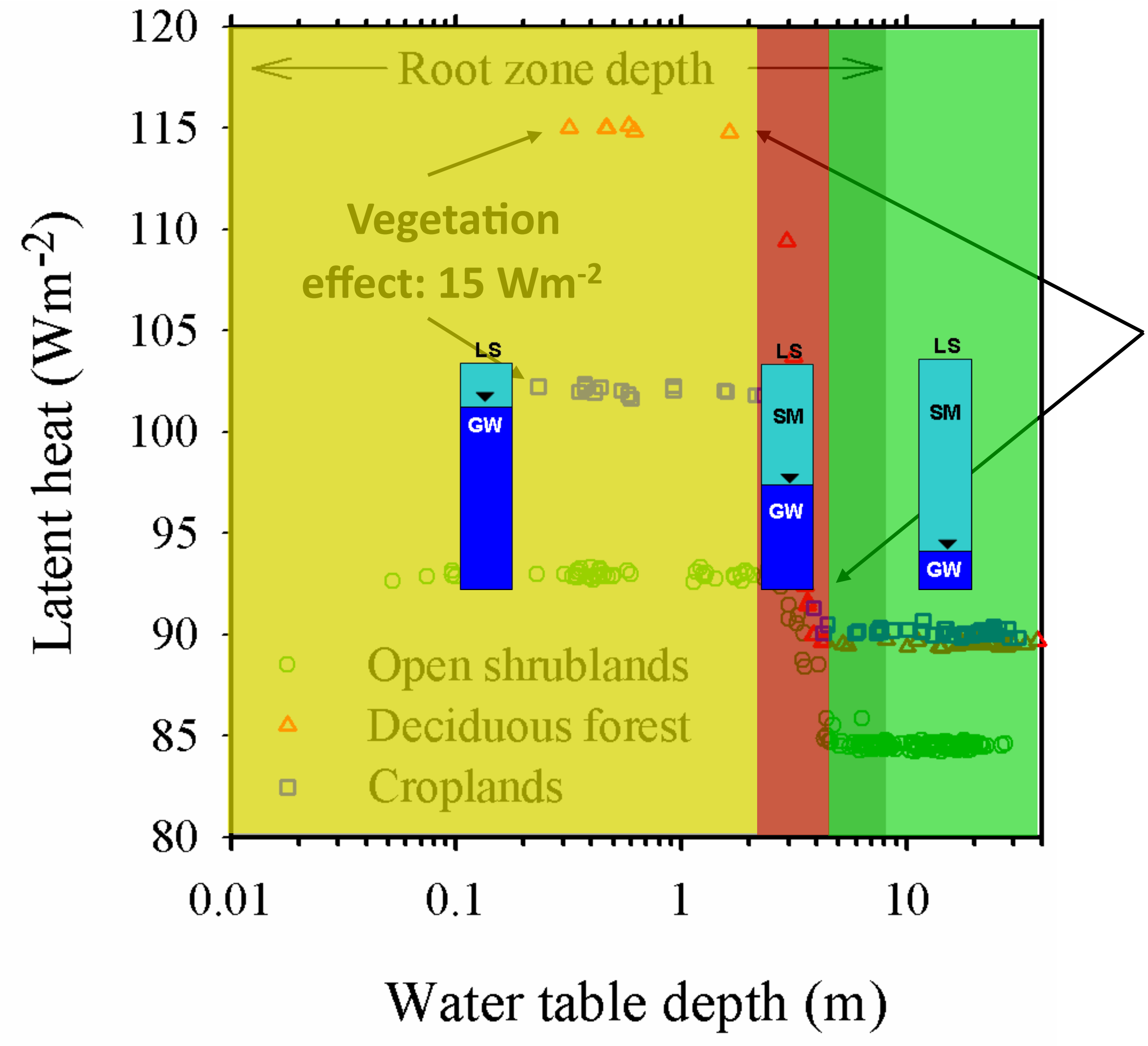




Kollet and Maxwell (2007)

Influence of Groundwater Dynamics on Energy Fluxes

(yearly averaged)



Groundwater effect: 25 Wm^{-2}

Kollet and Maxwell (2008)