Towards a complete description of the hydrologic cycle: Large-scale simulations with parallel, integrated models

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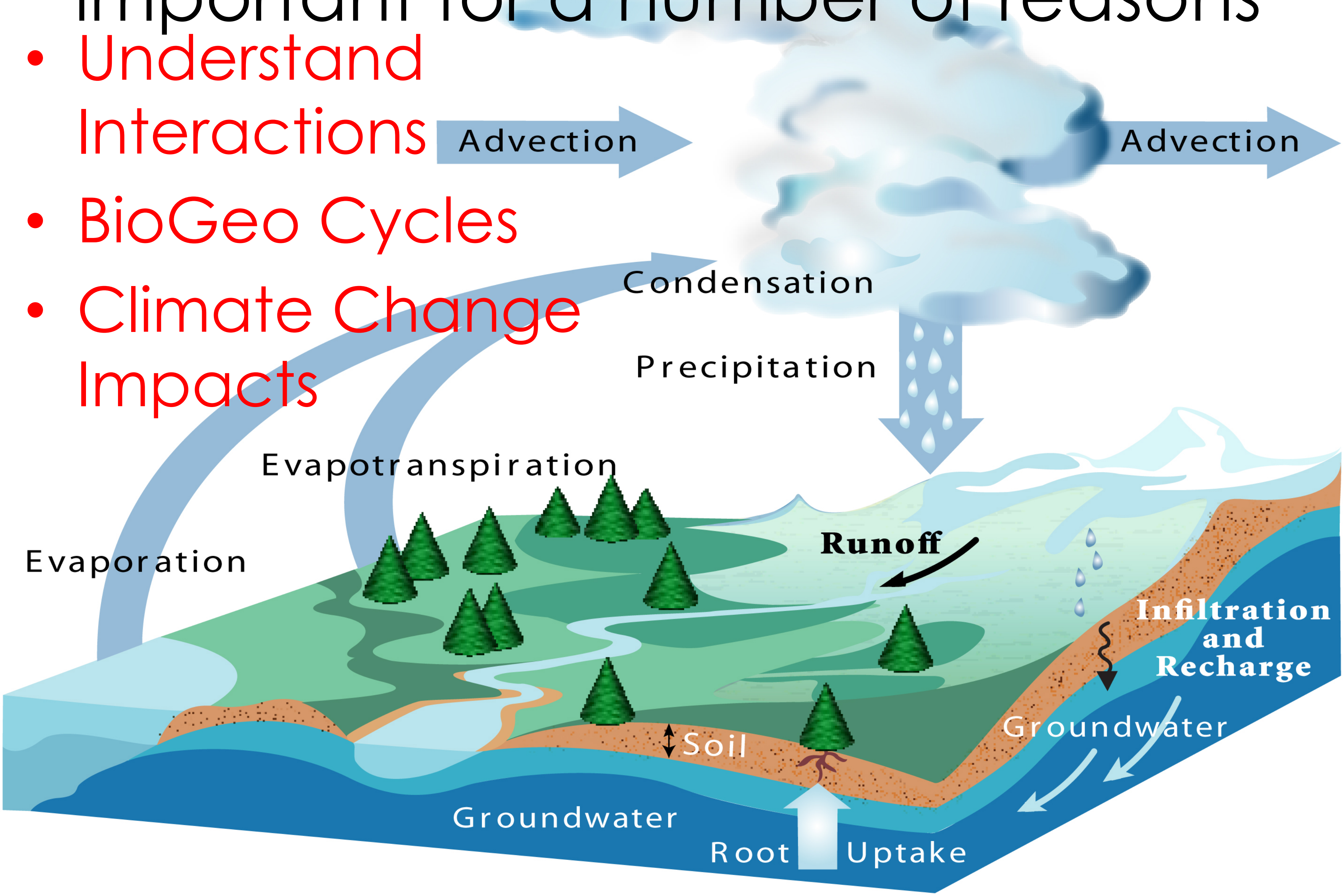
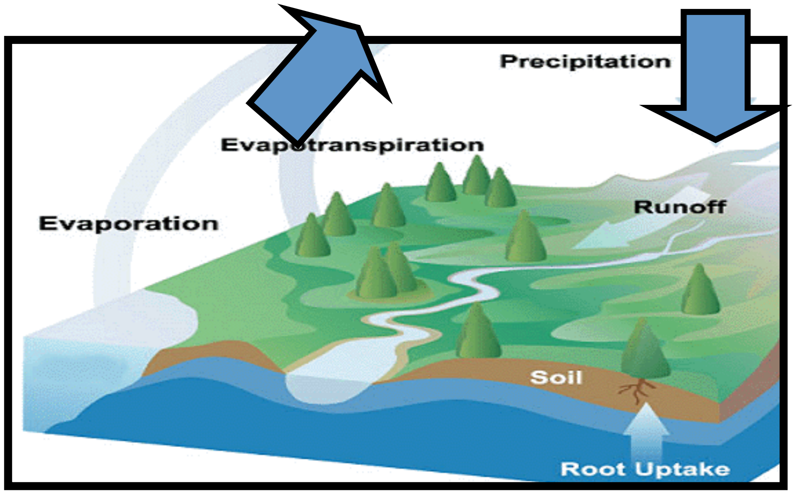
Modeling the hydrologic cycle is important for a number of reasons

- Understand Interactions
- BioGeo Cycles
- Climate Change Impacts

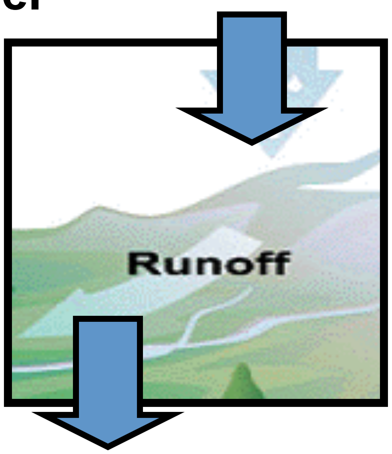


Yet it is usually simulated with disconnected models

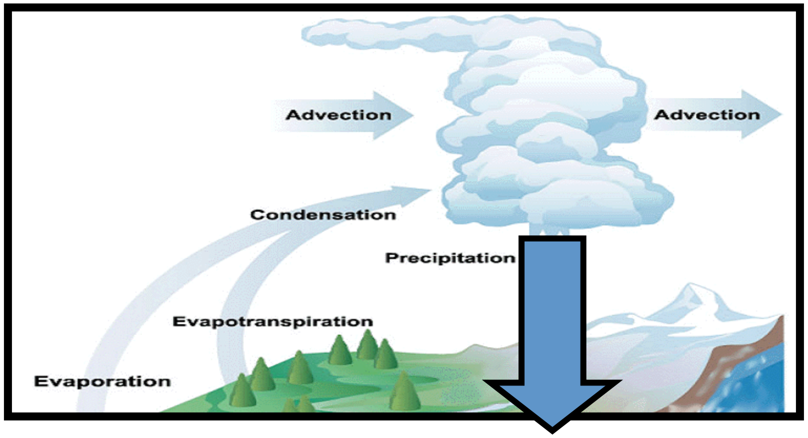
Groundwater/Vadose Model



Land Surface Model



Surface Water Model



Atmospheric Model

The water and energy balances are closely linked through ET/LE

Water Balance:

Change in Storage — Precipitation — Runoff

$$\Delta S = P - E - R$$

Evapotranspiration

Energy Balance:

$$R_n = L_e E + H + G$$

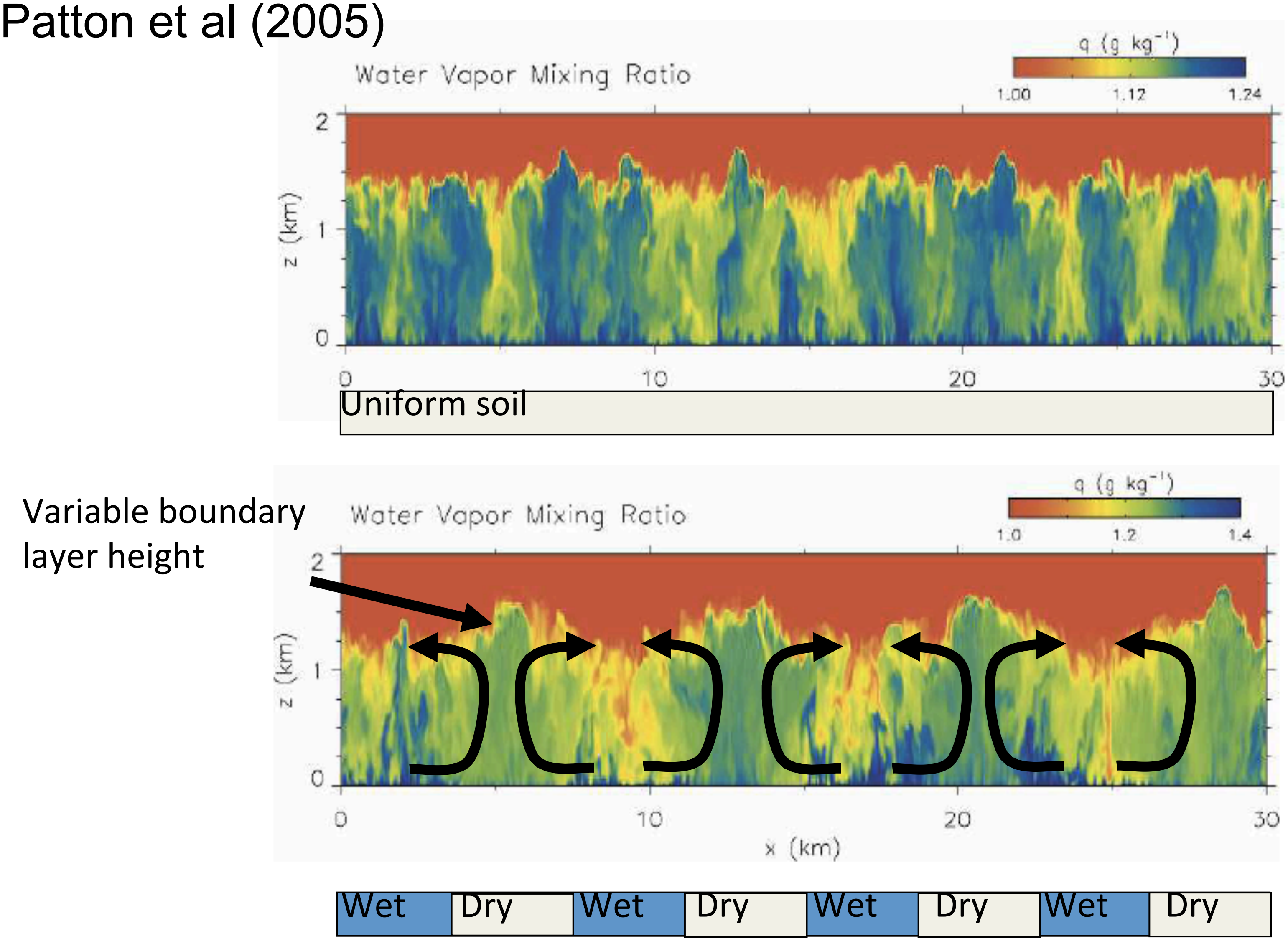
Net Radiation — Latent Heat Flux — Sensible Heat Flux — Ground Heat Flux

Land-Atmosphere interactions, particularly in modeling, have a long history in the literature

Ookouchi et al. (1984); Avissar and Pielke (1989); *Chen and Avissar (1994)*; Banta and Gannon (1995); Taylor et al (1997); Albertson and Parlange (1999); Barros and Hwu (2002); Clark et al (2003); Clark et al (2004); Amenu et al. (2005); Desai et al. (2005); *Patton et al (2005); Holt et al (2006)*; Chow et al (2006); Daniels et al (2006); Taylor et al (2007)

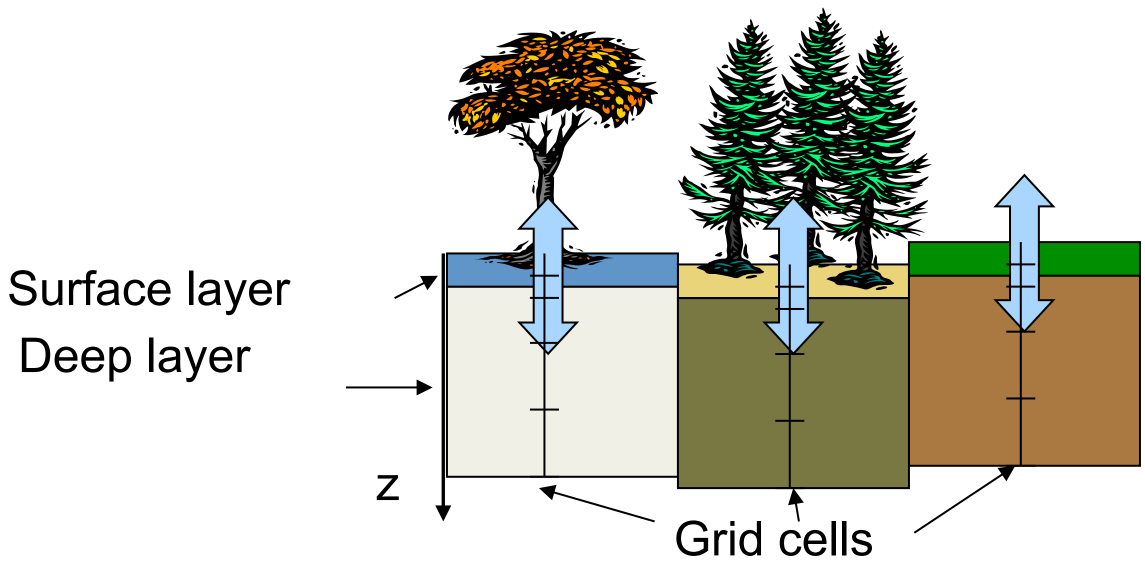
Soil moisture influences atmospheric processes (boundary layer)

Patton et al (2005)



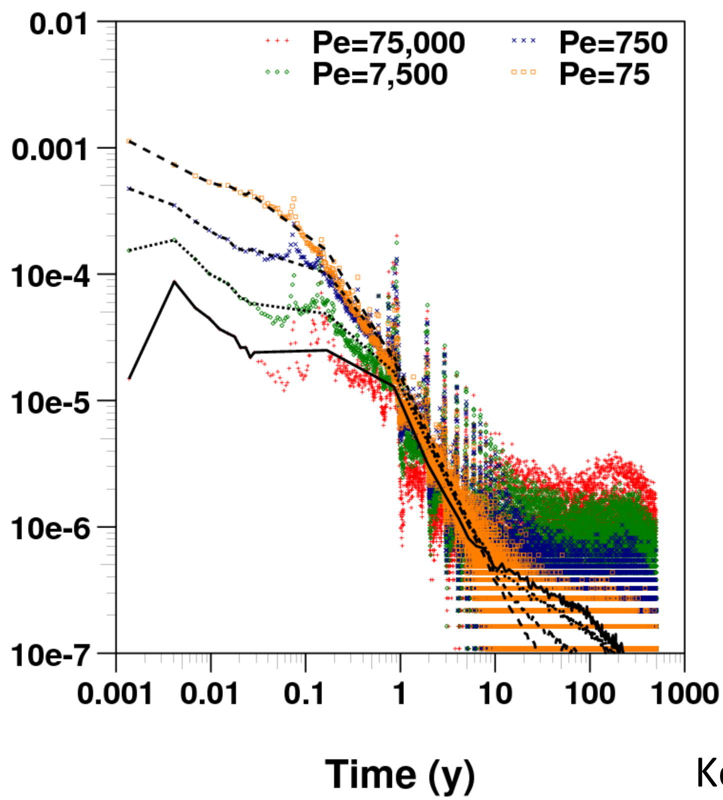
Current land-surface, groundwater models

- Land Surface Models simplify subsurface hydrology
  - Provide surface fluxes to atmosphere
  - Vertical transport only
  - Resistor-type models
  - Very shallow (~2m) subsurface, no real groundwater
  - No or simplified subsurface lateral communication or topographic effects
  - Contaminant transport not possible
- Groundwater Flow Models simplify land surface
  - Evaporation calculated operationally; no feedbacks
  - Applied only to local/regional scales; not HPC/Parallel

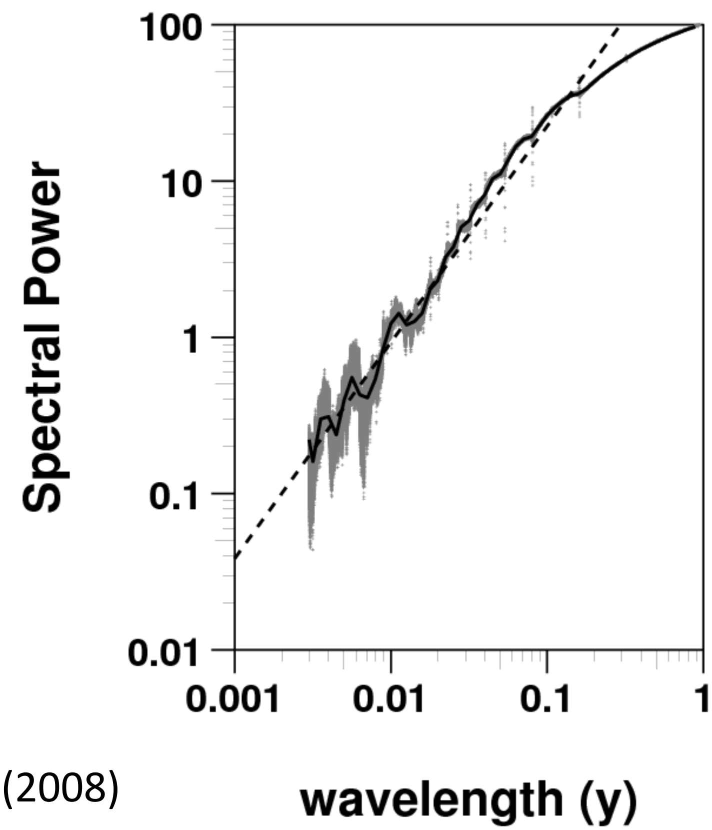


Groundwater's complications often underappreciated

- Range of paths and scales in groundwater
- Water moves as $K/\theta \sim 10^{-4}$-10^{-5} m/s
- Pressure propagates as $Kb/S_s \sim 10^{0}$-10^{1} m/s
- System responds over a wide range of scales (e.g. Kirchner et al 2000, 2001; Alley et al 2002; Haggerty et al 2002; Wörman et al 2007; Cardenas 2007; Kollet and Maxwell 2008)
- Topography and land surface processes have strong influence



Models



Kollet and Maxwell (2008)

There have been several recent efforts to integrate terrestrial hydrology, land surface and atmospheric models

Hydrology-Atmosphere

Molders and Ruhaak (2002); Seuffert et al (2002); York et al (2002); Maxwell et al (2007); Anyah et al (2008*); Jiang et al (2009)*; Gochis and Yu (2009); Maxwell et al (2011)

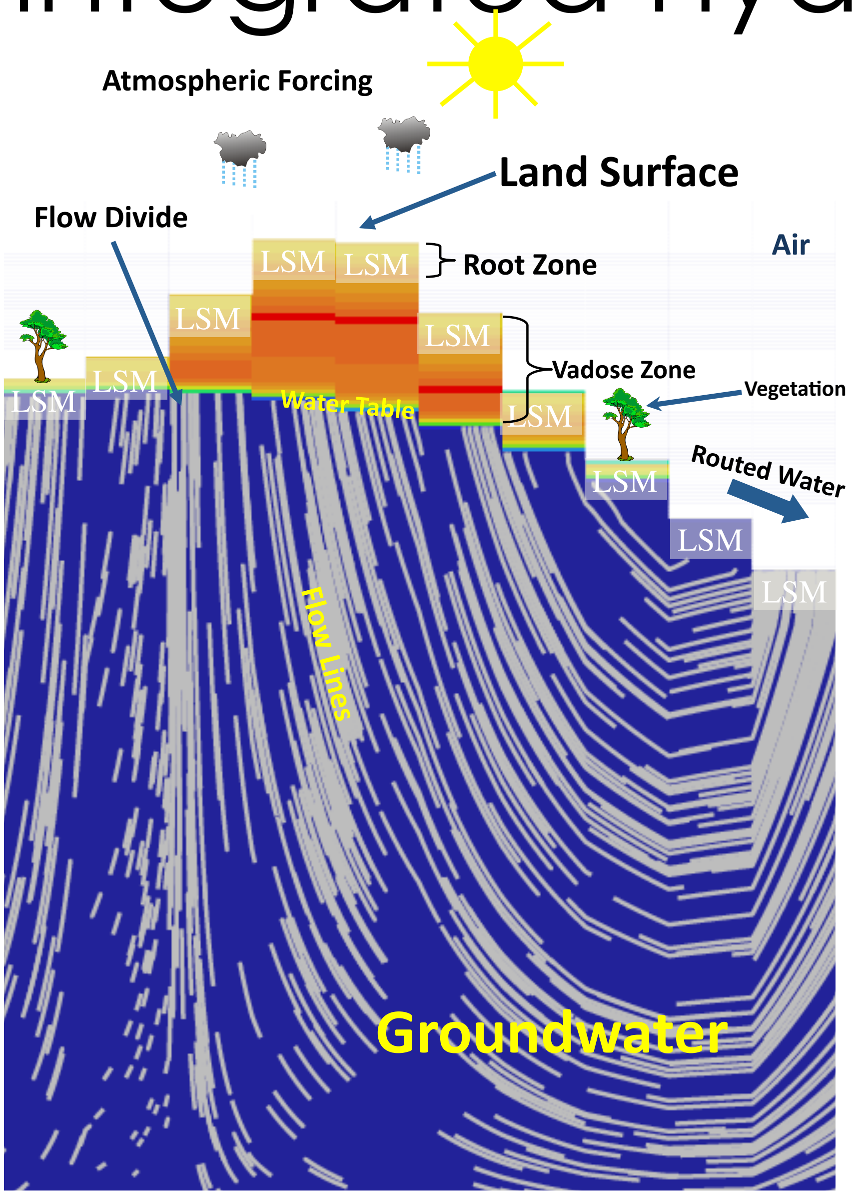
Hydrology-Land Surface

Silvapalan et al (1987); Famiglietti and Wood (1994a,b, 1995); Quinn et al. (1995); Peters-Lidard et al (1997); Endry et al (2000); Crow and Wood (2003); Liang et al (2003); Niu et al (2005); Maxwell and Miller (2005); Yeh and Eltahir (2005); Niu et al (2007); Gulden et al (2007); Fan et al (2007); Kollet and Maxwell (2008); Maxwell and Kollet (2008); Kollet (2009); Kollet et al (2009); Kollet et al (2010); Ferguson and Maxwell (2010), Maxwell (2010)

Integrated Hydrology

Freeze and Harlan (1969); VanderKwaak and Loague (2001); Panday and Huyakorn (2004); Jones et al. (2006); Kollet and Maxwell (2006); Therrien et al (2006); Qu and Duffy (2007); Kollet and Maxwell (2008); Jones et al (2008); Li et al (2008); Camporese et al (2009a,b); Dawson (2009); Ebel et al (2009); Park et al (2009); Sulis et al (2010)

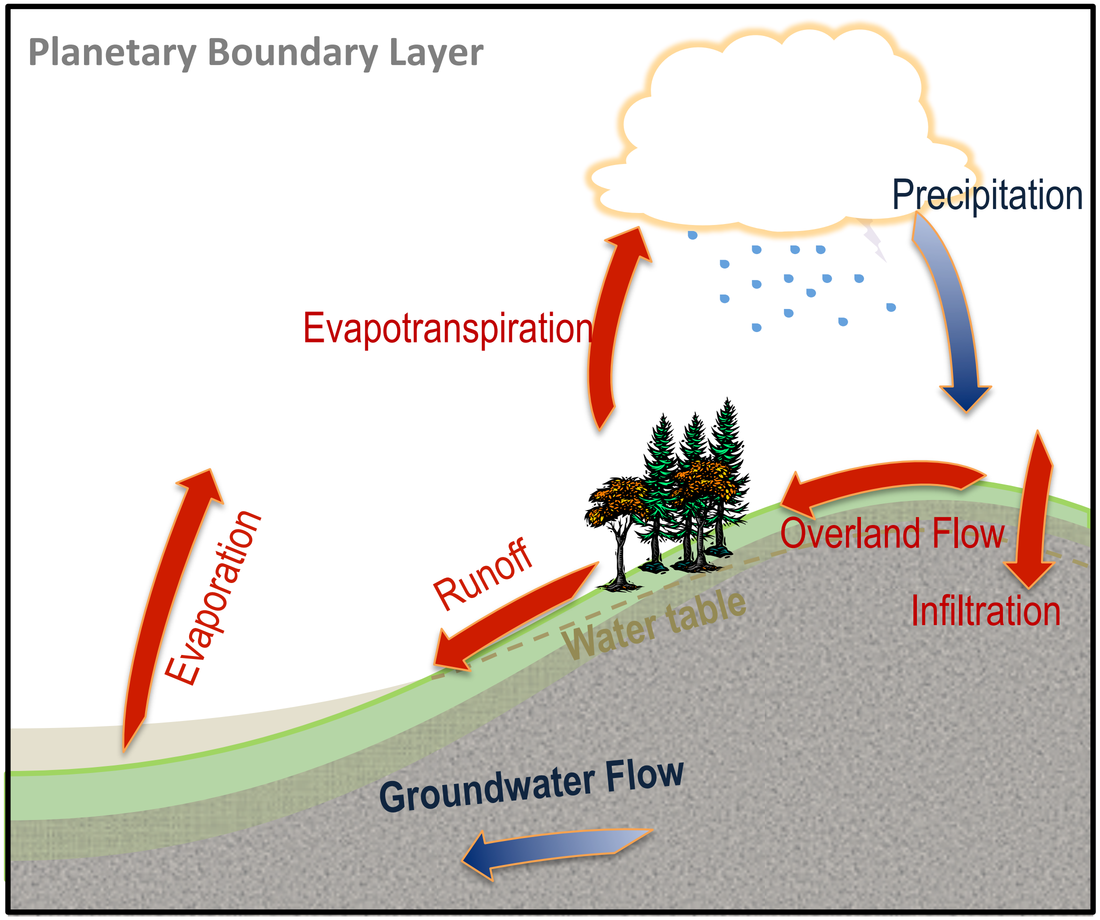
We use ParFlow: a fully-integrated hydrology model



- Growing number of *integrated* SW-GW models: HGS, CATHY, OGS, PIHM, InHM, we use/develop ParFlow
- Groundwater flow: variably-saturated three-dimensional Richards equation
- Overland flow/surface runoff: free-surface overland flow boundary condition (continuity + Mannings + kinematic/diffusive wave)
- Land surface water and energy fluxes: Common Land Model (CLM), canopy and vegetation processes, and coupled water-energy balance
- Fully-coupled, mass conservative, parallel implementation

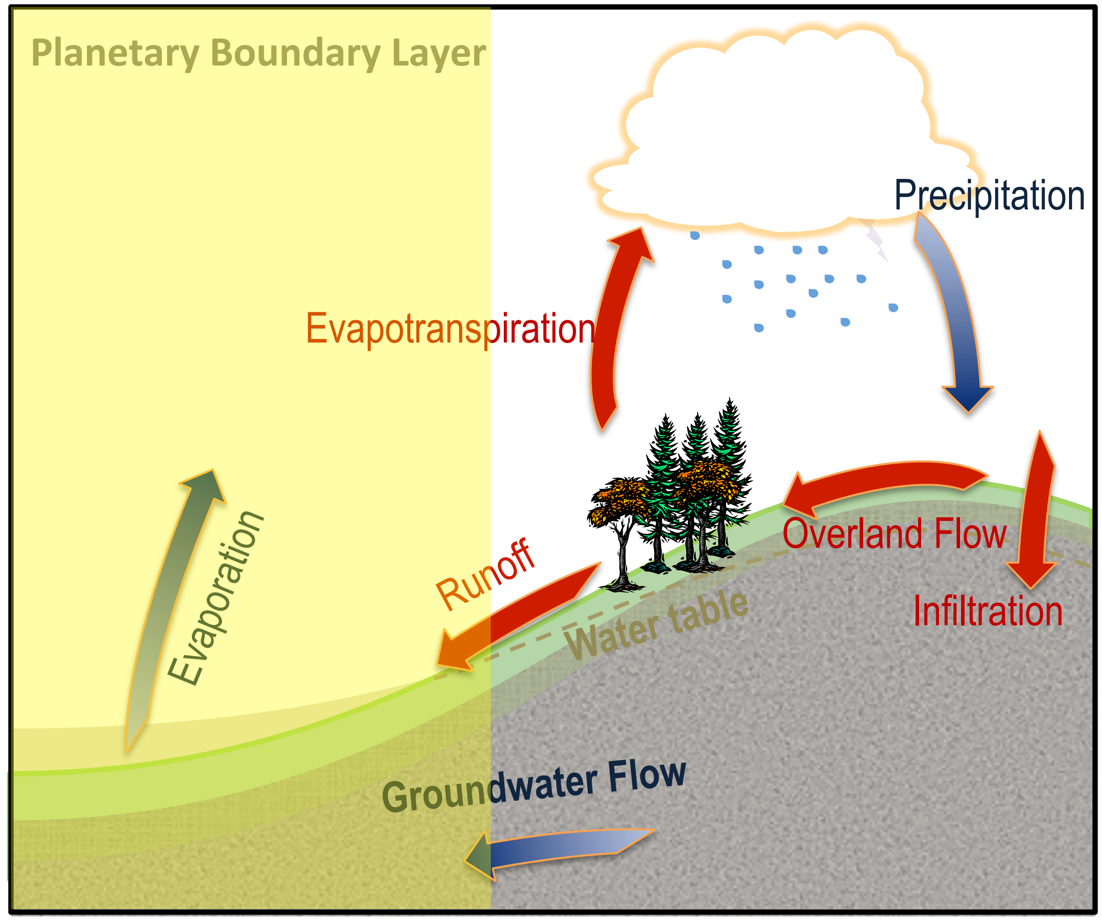
Kollet and Maxwell (2008), Kollet and Maxwell (2006), Maxwell and Miller (2005), Dai et al. (2003), Jones and Woodward (2001); Ashby and Falgout (1996)

Land Surface Processes –Conceptual Model



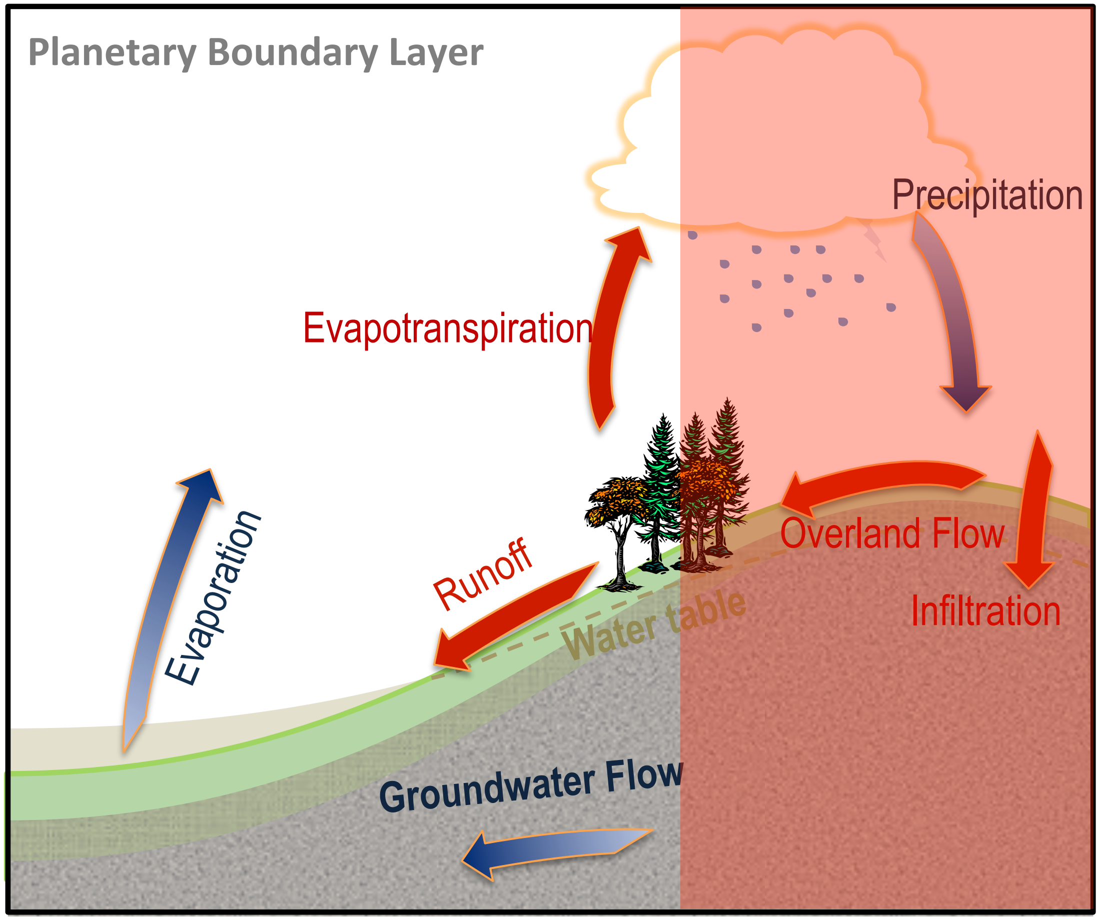
Land Surface Processes

Land surface processes non-soil moisture limited.



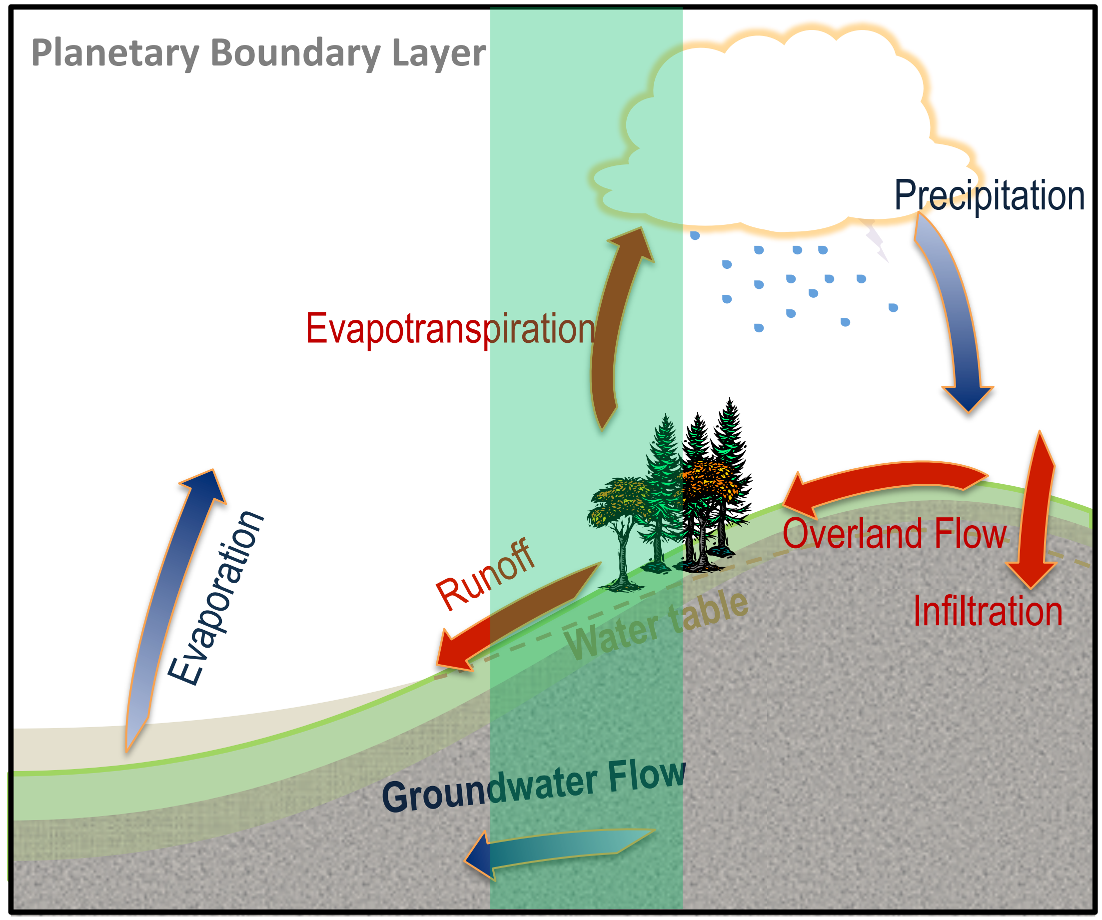
Land Surface Processes

Land surface processes decoupled from water table.



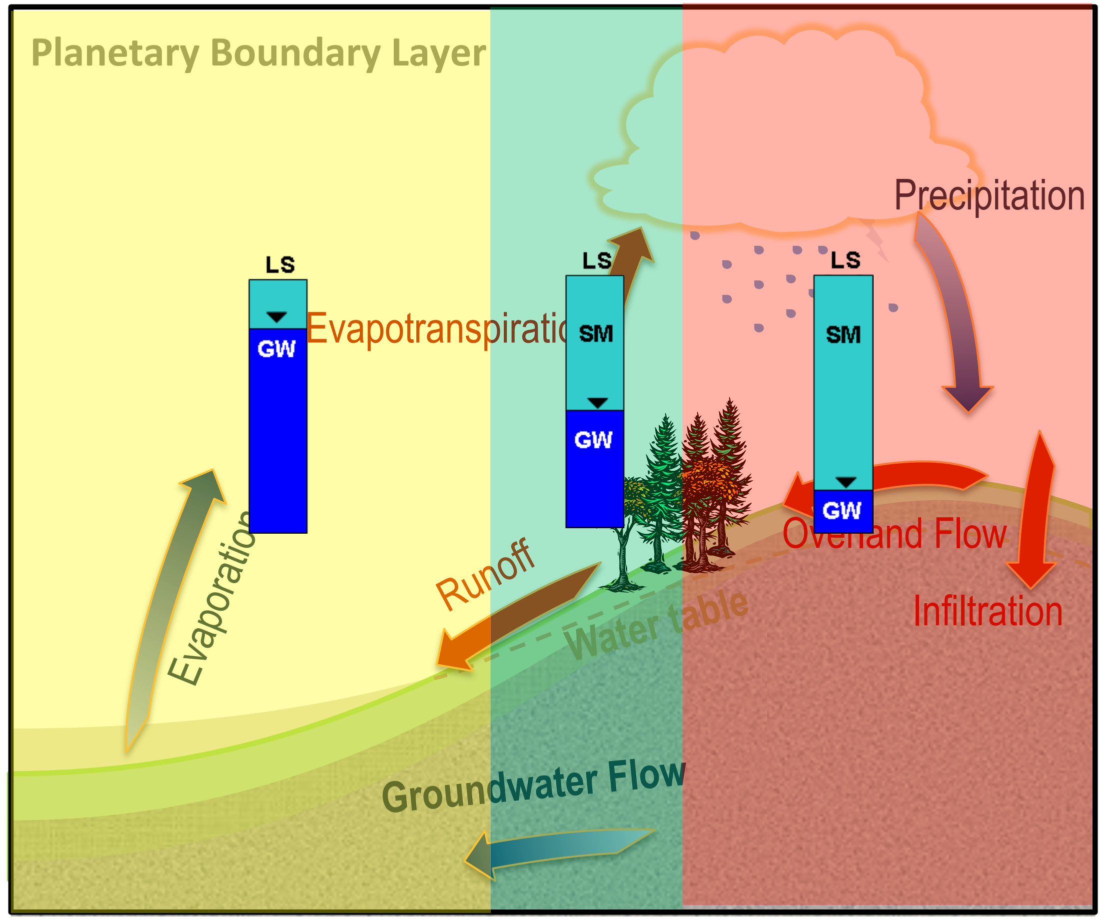
Land Surface Processes

Critical zone of coupling between LS energy fluxes and water table depth.



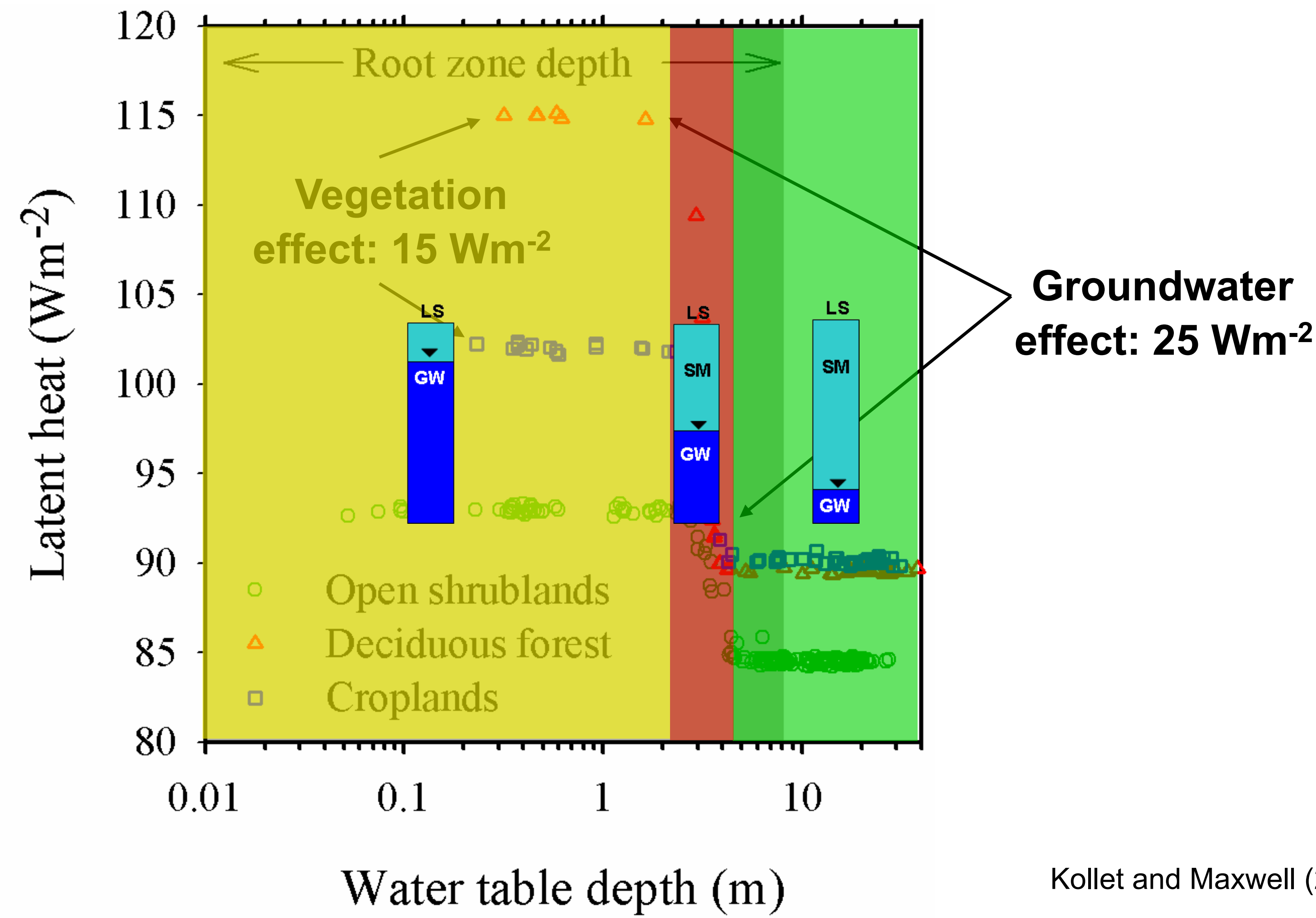
Land Surface Processes

We can think about this as three water table depths.



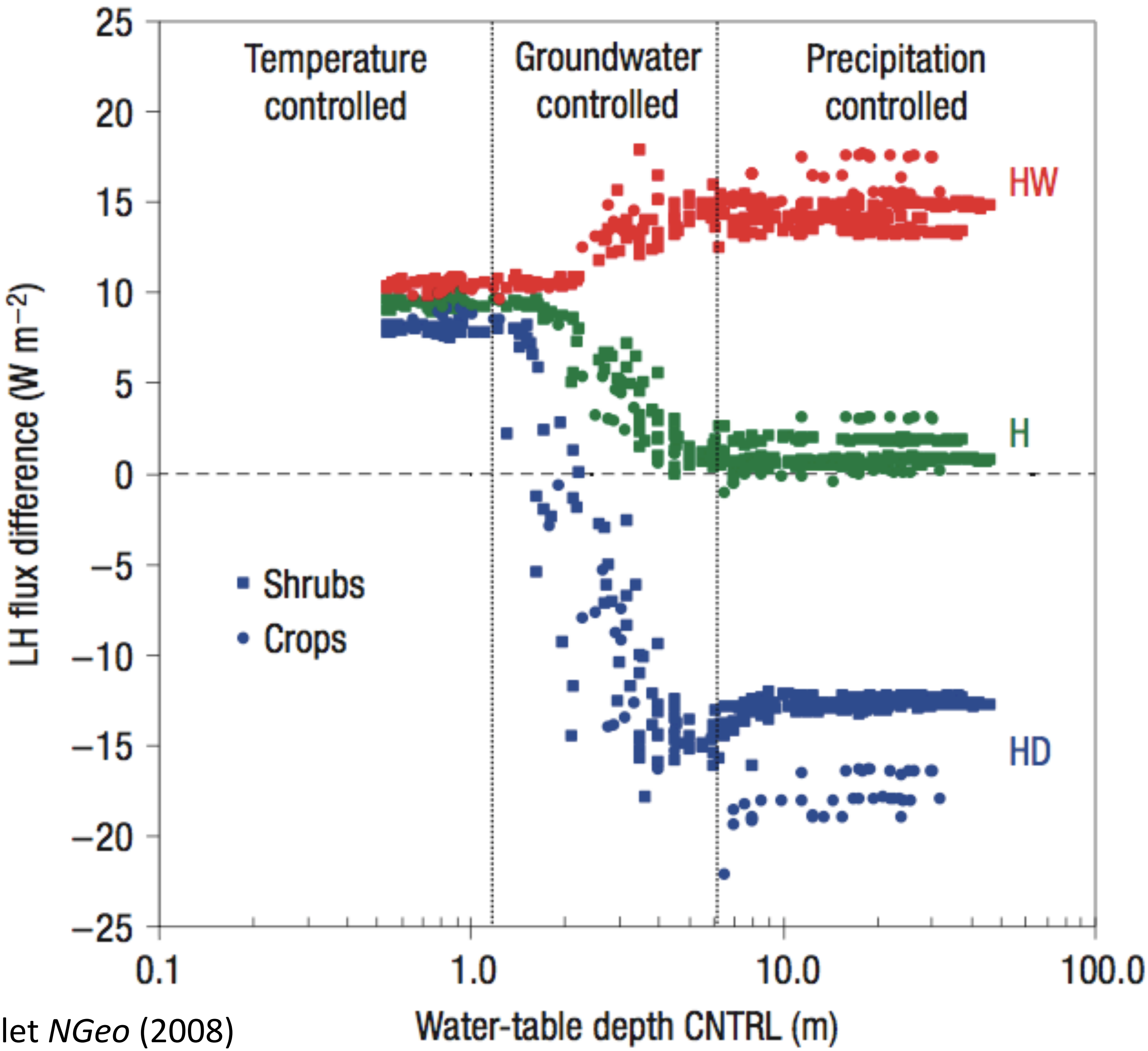
Kollet and Maxwell (2008)

Influence of Groundwater Dynamics on Energy Fluxes (yearly averaged)



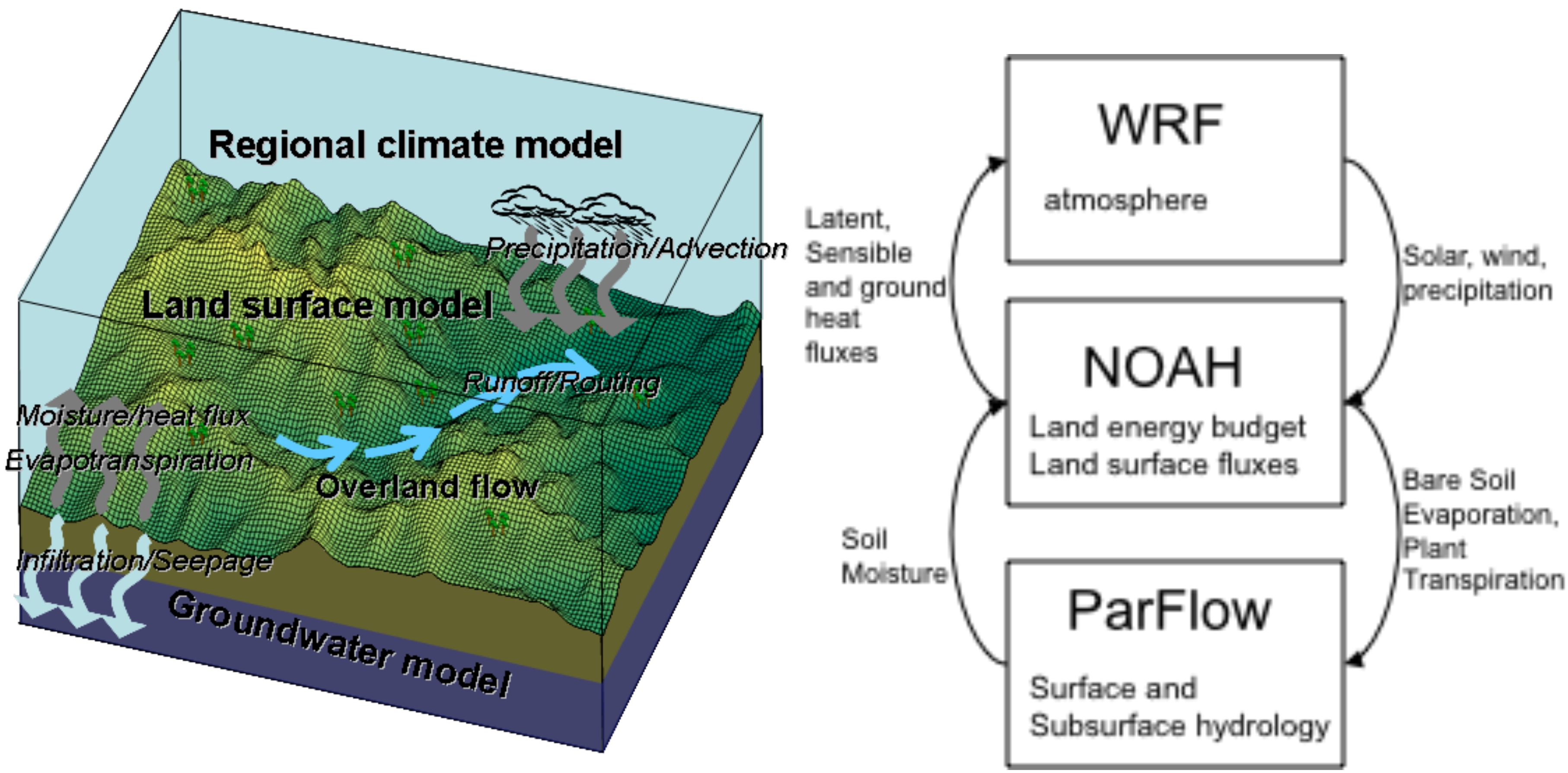
Kollet and Maxwell (2008)

Yearly-Averaged LH Flux Difference



Maxwell and Kollet *NGeo* (2008)

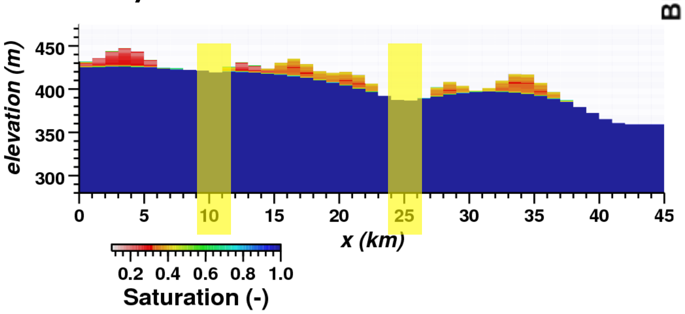
We have also developed "bedrock-to-atmosphere" models to explicitly integrate all these systems



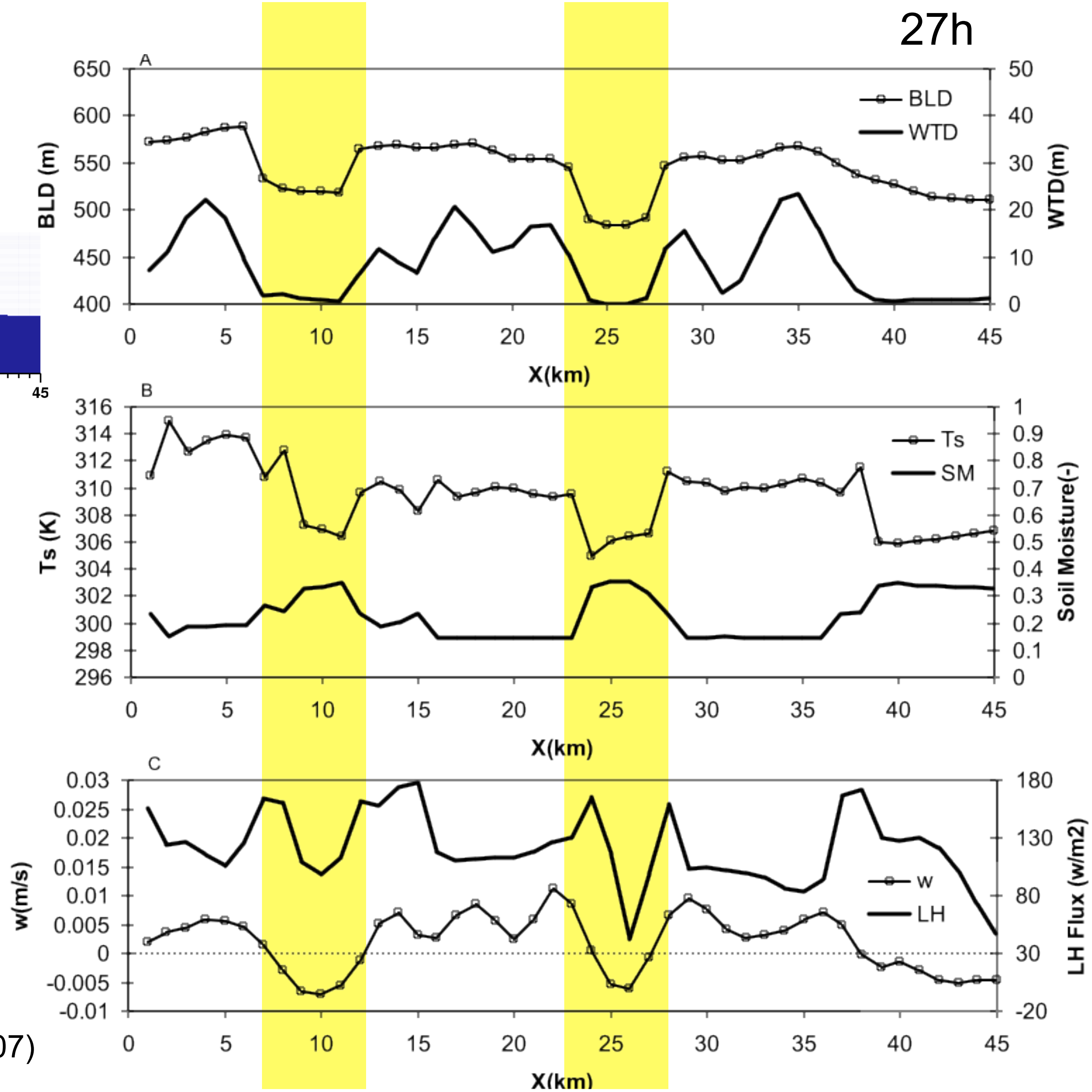
Maxwell, Lundquist et al *MWR* 2010; Maxwell, Chow, Kollet *AWR* 2007

Groundwater effects the lower atmosphere

- Cross-section at y=15km



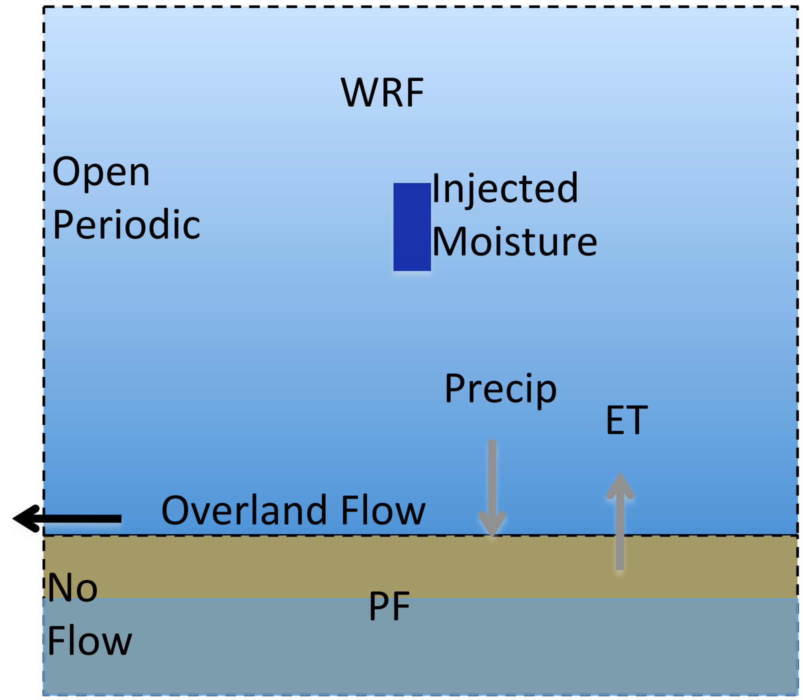
- Shallow WT=wetter
- Wetter=cooler
- Temperature variations=wind variations
- Wind variations=BL variations



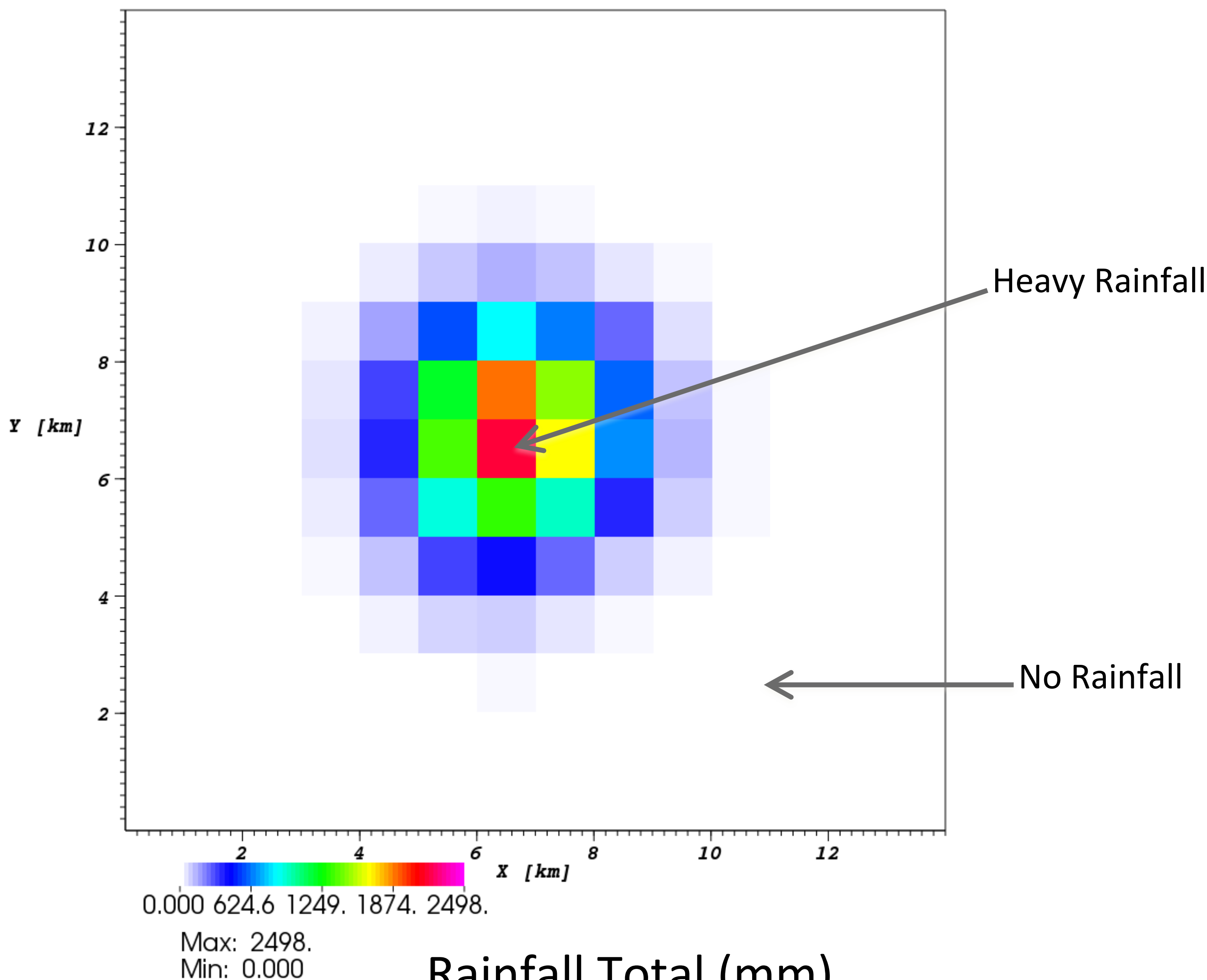
Maxwell, Chow and Kollet, AWR (2007)

Idealized PF.WRF Test Case

- Test coupling, physics, and water balance
- Idealized domain, rectangular atmosphere and subsurface
- Moderate slope, coupled overland flow
- Injected moisture to ensure lots of rainfall



Maxwell, *et al MWR* 2011

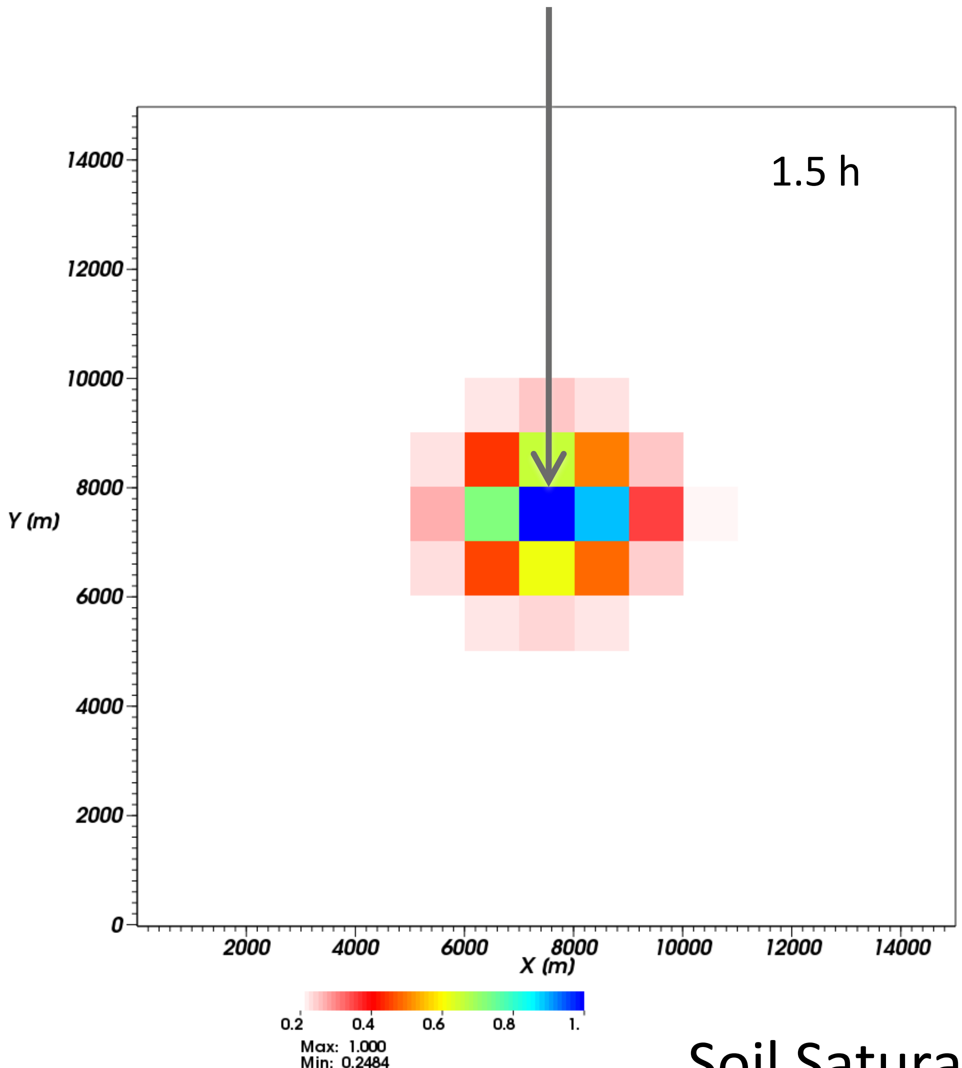


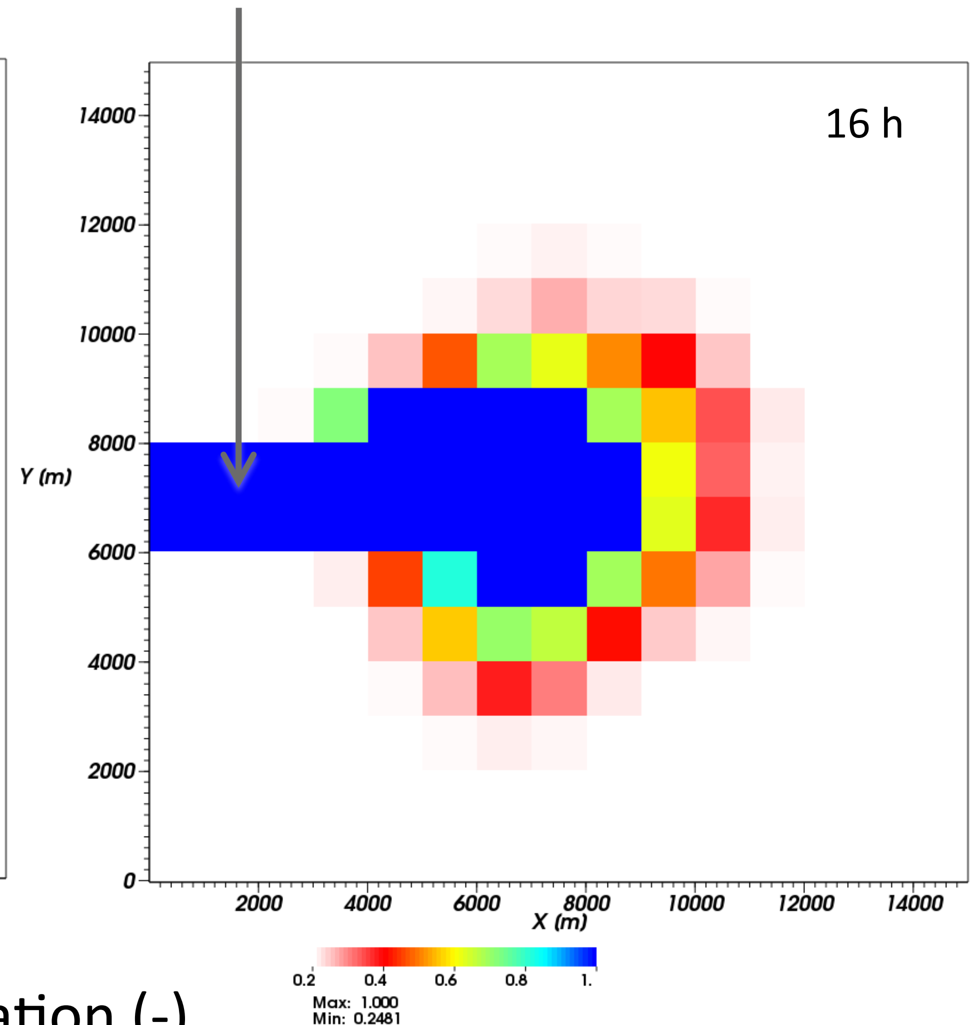
Rainfall Total (mm)

Maxwell, *et al MWR* 2011

Early Times Saturation Follows Rainfall

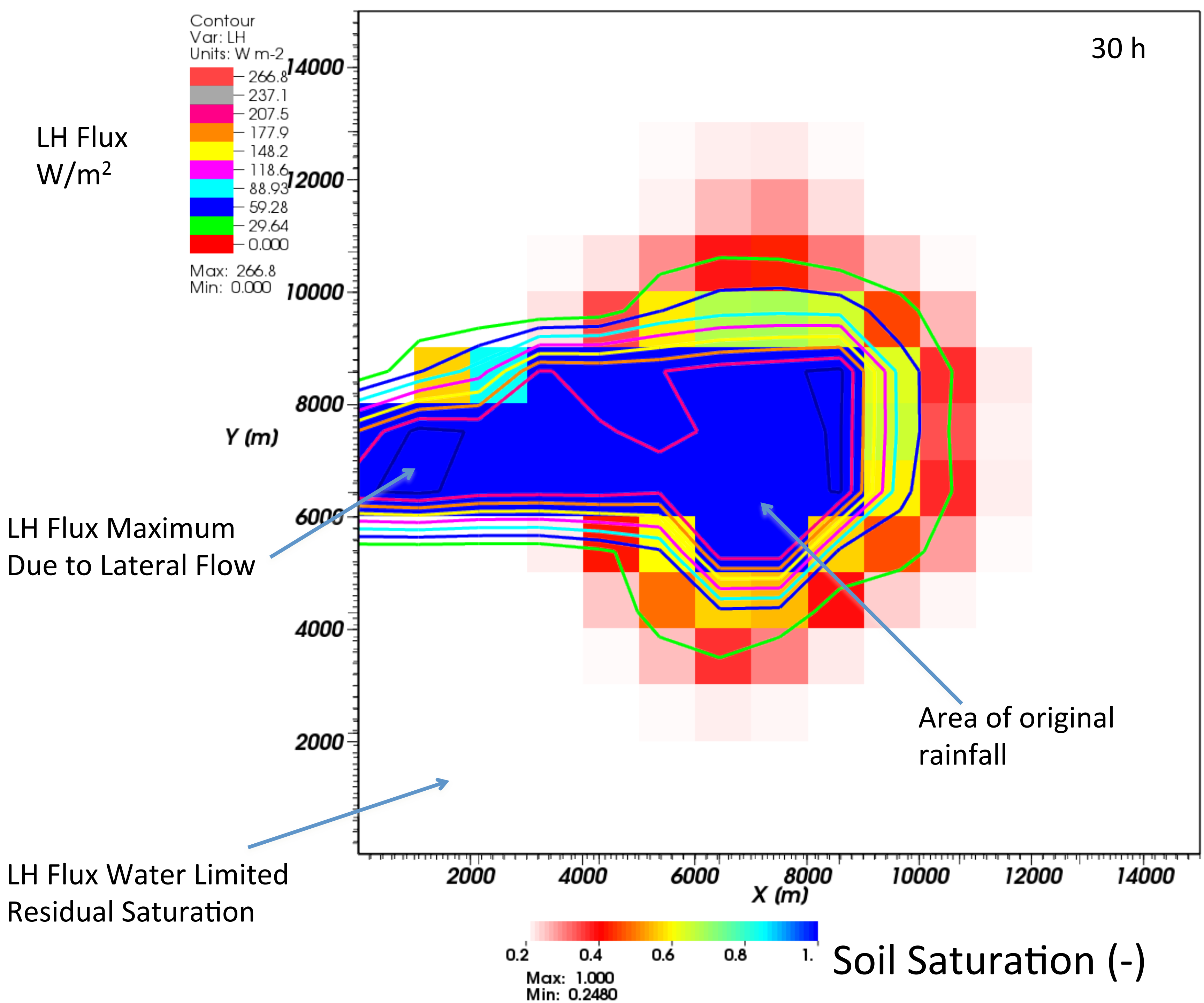
Later Times Overland Flow Generated by Saturation Excess





Soil Saturation (-)

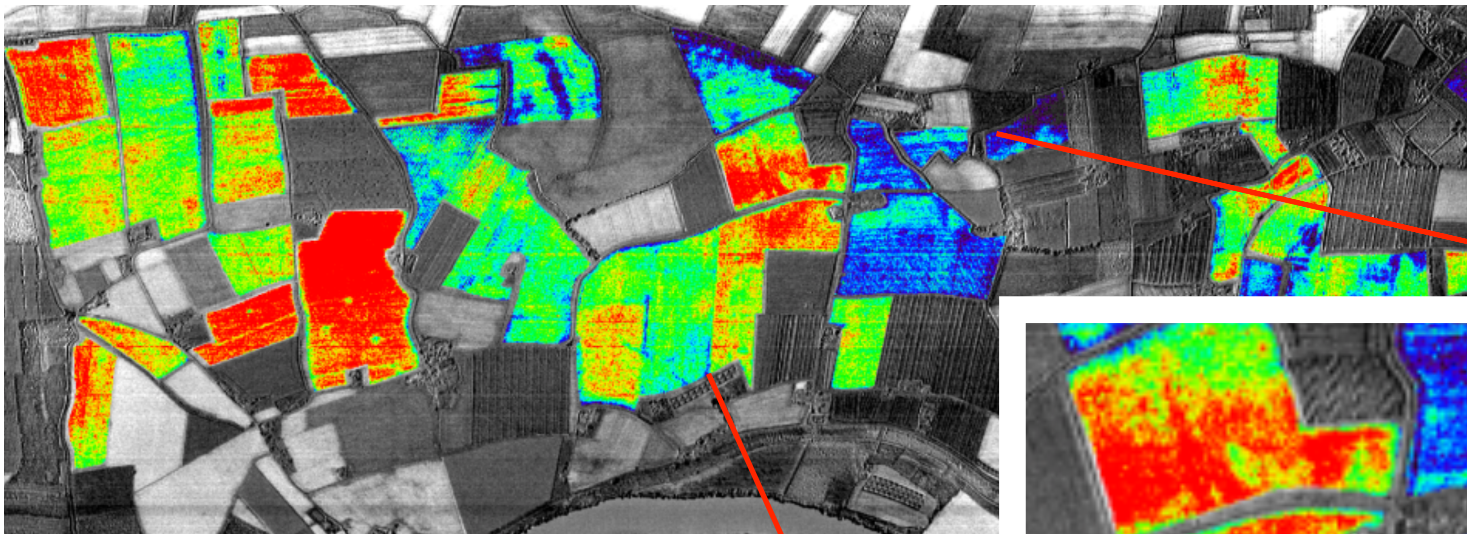
Maxwell, *et al MWR* 2011



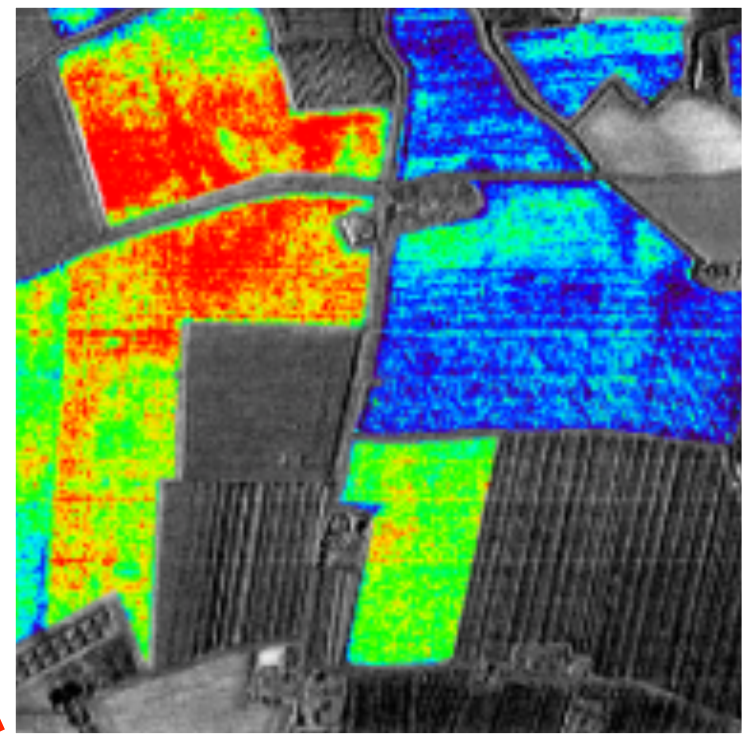
LH Flux
W/m²
Contour
Var: LH
Units: W m-2
266.8
237.1
207.5
177.9
148.2
118.6
88.93
59.28
29.64
0.000
Max: 266.8
Min: 0.000
30 h
Y (m)
X (m)
LH Flux Maximum
Due to Lateral Flow
Area of original
rainfall
LH Flux Water Limited
Residual Saturation
0.2
0.4
0.6
0.8
1.
Max: 1.000
Min: 0.2480
Soil Saturation (-)

Small-Scale Example: remotely sensed photosynthetic activity as a measure for ET

Agricultural test site of the Research Center TR32 close to Jülich, Germany



Rascher, Crewell et al., (2009)



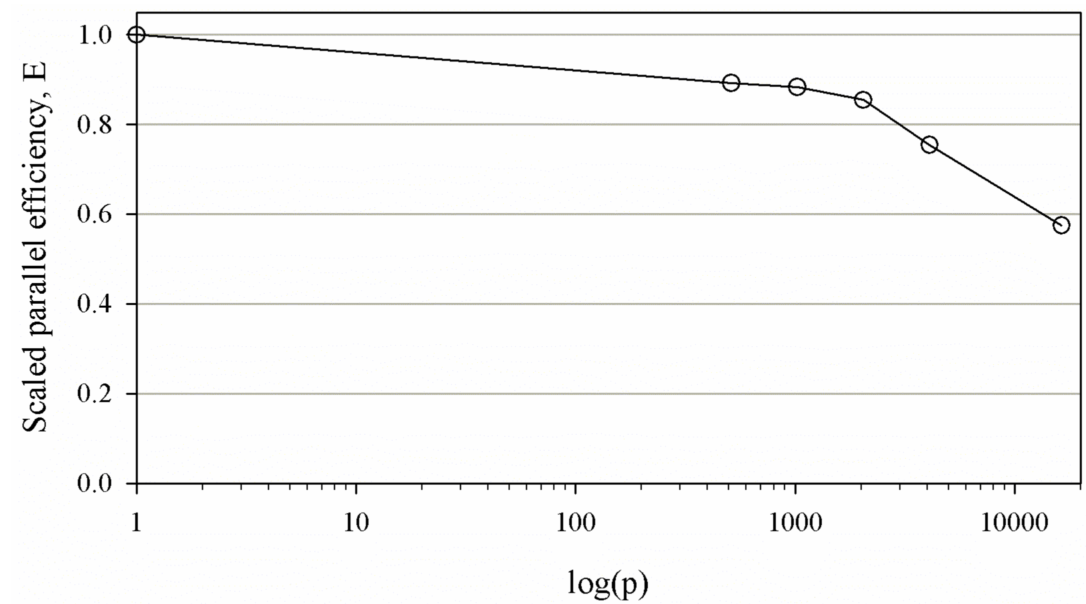
We encounter variance at all scales

AND

have to deal with coupled nonlinear physics.

We can use HPC to directly upscale

- ParFlow has been scaled to JUGENE, a 1 PFLOP, 294,912p supercomputer at FZJ
- Simulations using a fully-coupled, fully-3D, nonlinear problem show good scaled parallel efficiency to very large number of processors



Good scaled parallel efficiency to 16,384 processors for a simulation of 8B compute cells

Kollet, Maxwell et al *WRR* 2010

We are able to simulate variance over orders of magnitude; example: influence of heterogeneity on evapotranspiration, *ET*

Correlated Gaussian heterogeneity in K_{sat}

Grass cover

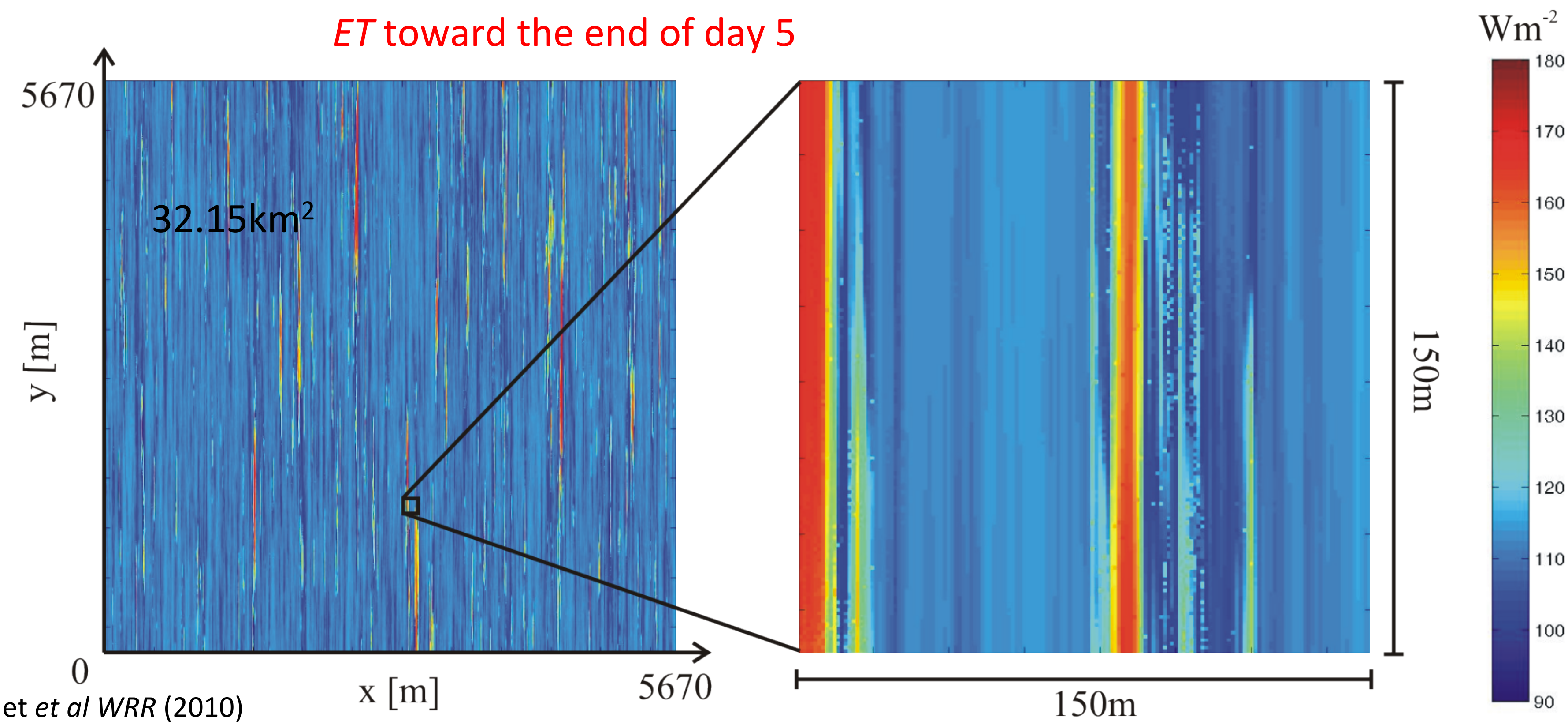
$\Delta x = \Delta y = 1m, \quad \Delta z = 0.025m$

Total number of grid cells

7,962,624,000

Total number of processors

16,384



Kollet *et al WRR* (2010)

My 'Talks' Used to end here: Future Directions

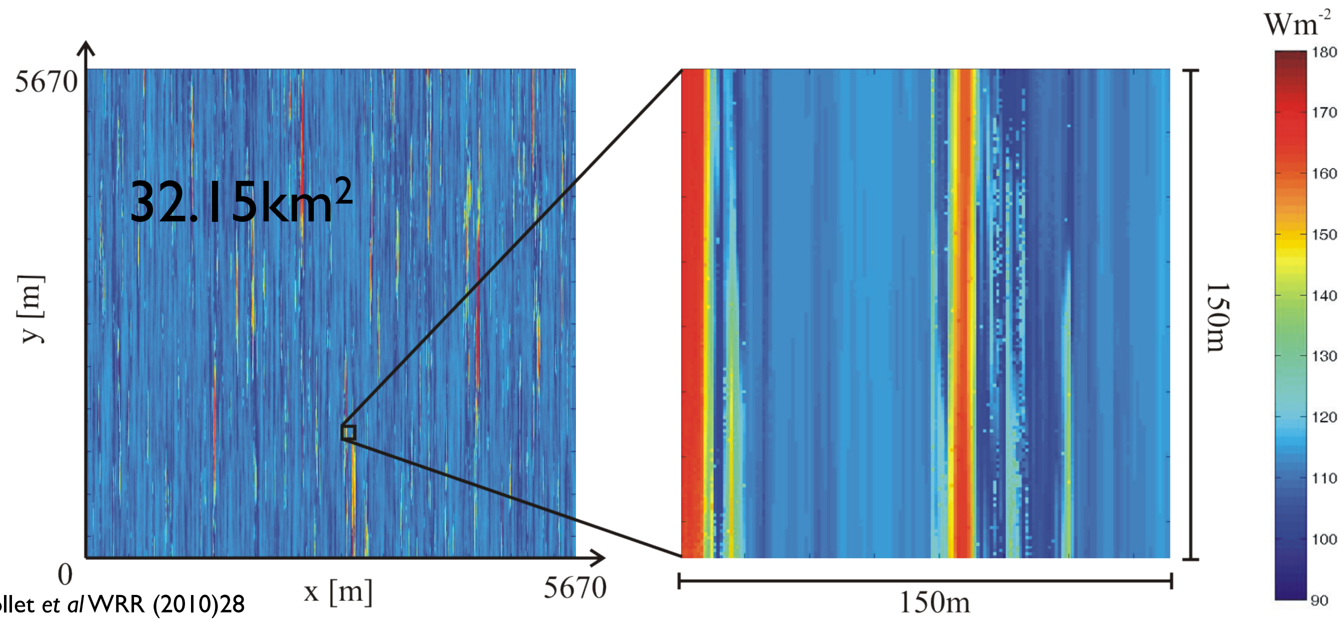
Parting thought: given HPC and great scaling of these codes, we can run multi-year, integrated simulations.

- Watersheds at *high resolution* (10-100 km^2 @ *m x cm*)
- Continental-scale at *high resolution* (10-100M km^2 <*km* x <*m*)

Why aren't we?

Correlated Gaussian heterogeneity in K_{sat}
Grass cover
$\Delta x = \Delta y = 1\text{m}, \quad \Delta z = 0.025\text{m}$

<u>Total number of grid cells</u>
7,962,624,000
<u>Total number of processors</u>
16,384



Kollet *et al* WRR (2010)28

This is not a unique idea

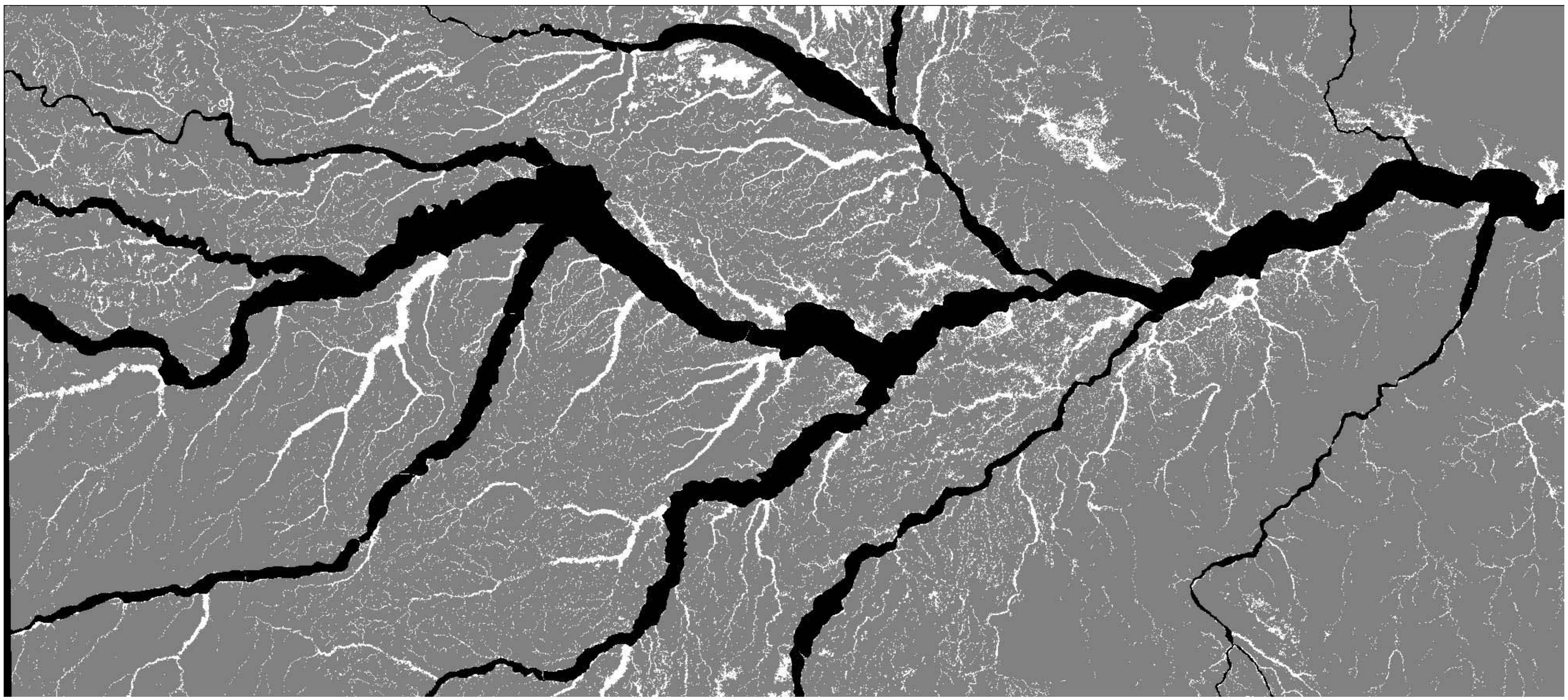


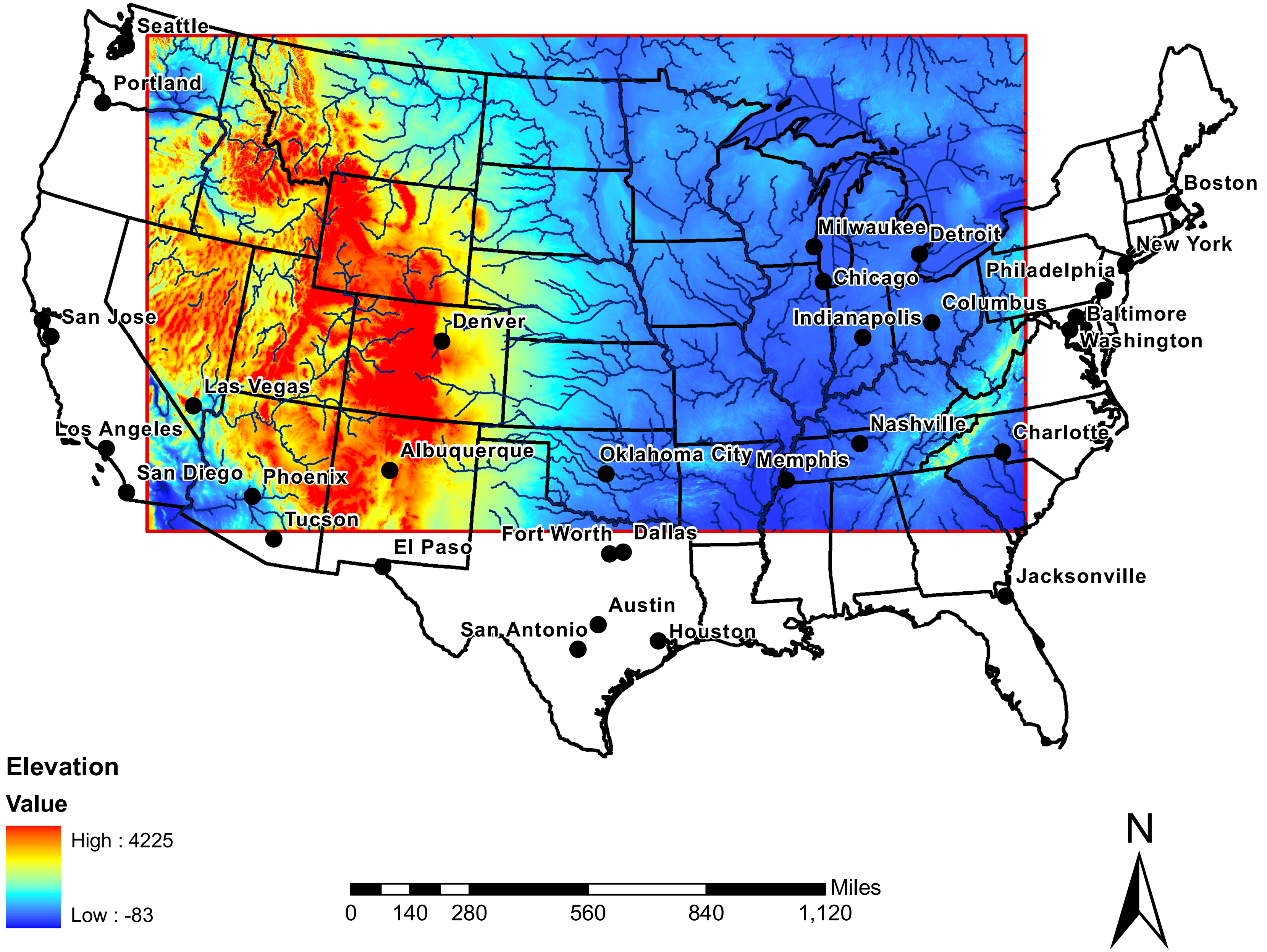
Figure 2. Complex, fine-scale inundation areas of the Amazon River and its tributaries control the CO_2 outgassing during the wet season. The spatial resolutions of current LSMs are unable to accurately simulate inundation dynamics because of limitations in resolution and parameterizations and therefore provide poor estimates of the outgassing. The quadrant extends from 72°W, 0°N to 54°W, 8°S. JERS imagery reprinted from *Hess et al.* [2003], with permission from Elsevier.

1. Need for HyperResolution Modeling

[2] Hydrology as a scientific discipline traces its roots to

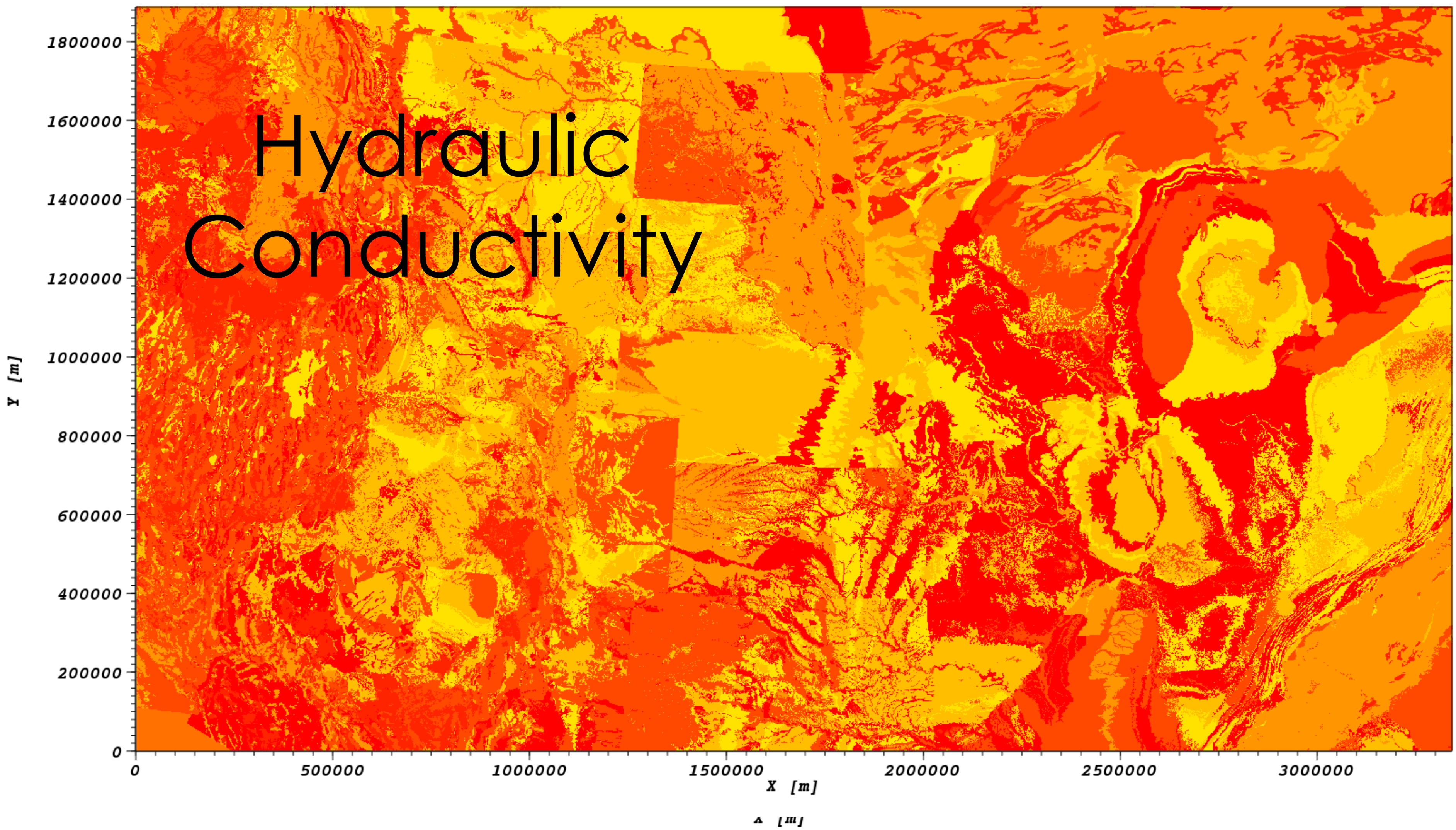
such as provision of safe drinking water to the industrial cities of the 19th century, development of the unit hydrograph method for predicting floods, and estimating evaporation

So this is what we decided to do



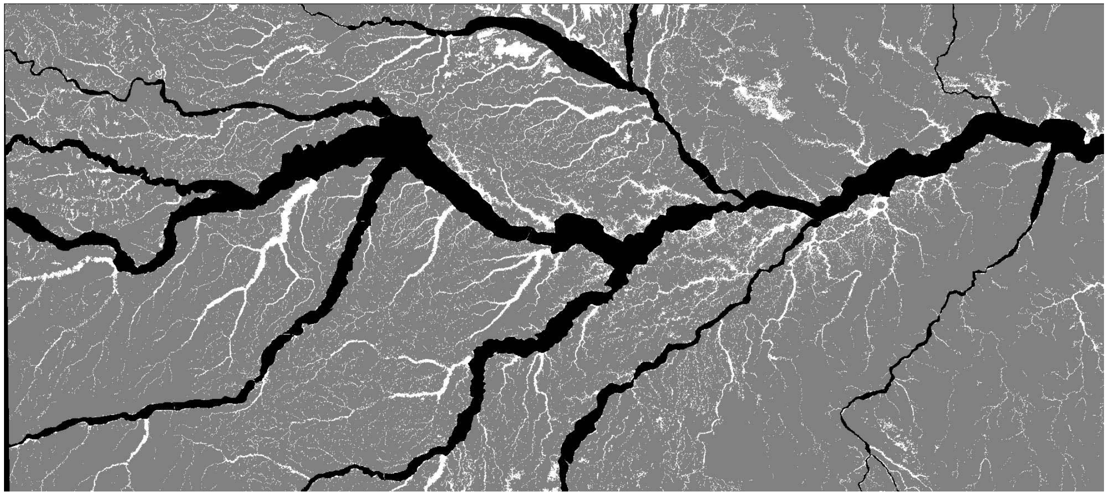
We built a 6.3M km^2 domain covering much of the CONUS

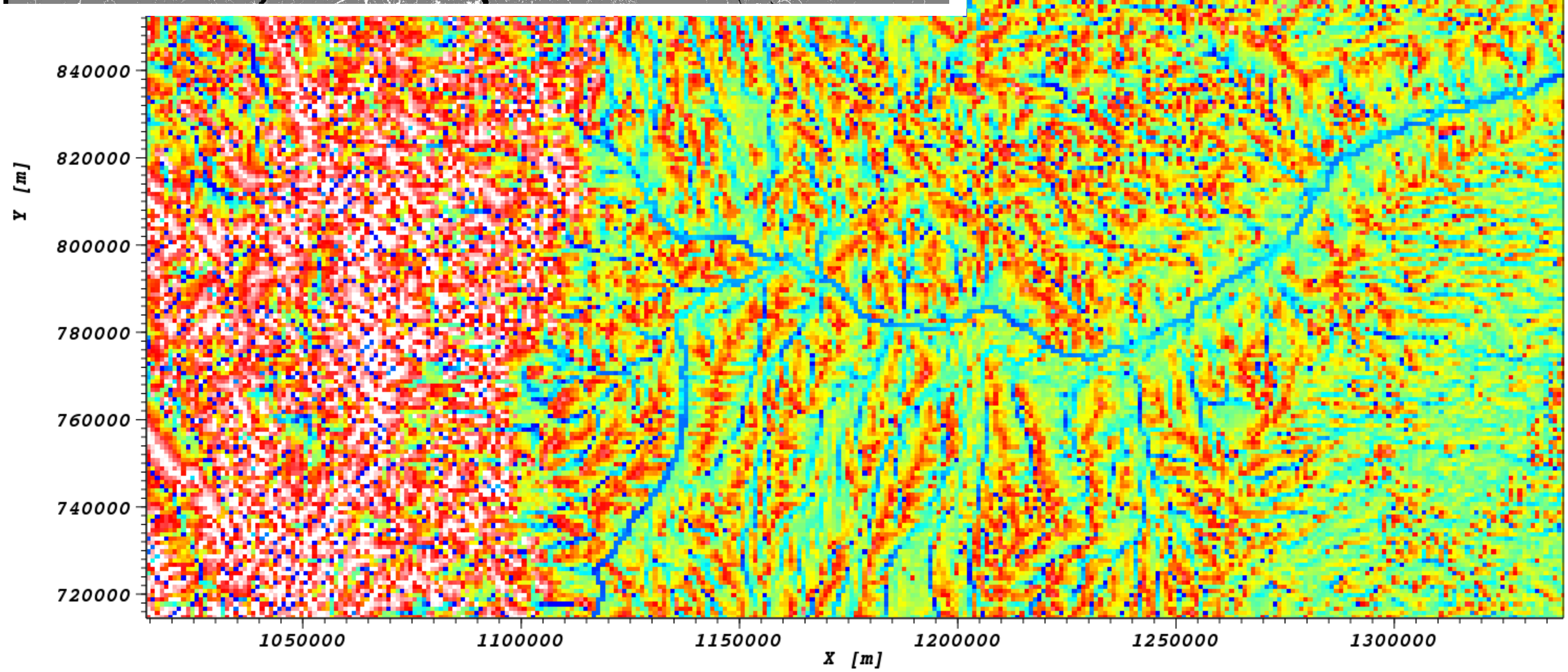
- 1 km lateral resolution
- .1 – 10m vertical resolution over 25 cells (200m depth)
- ~158M unknowns
- The Miss and CO watersheds
- Terrain from USGS HydroSheds dataset
- Subsurface properties from new Gleeson et al (GRL 2011) database and Statsgo
- Fully integrated, 3D Richards' EQ, Shallow Water Equations, Land Surface Processes

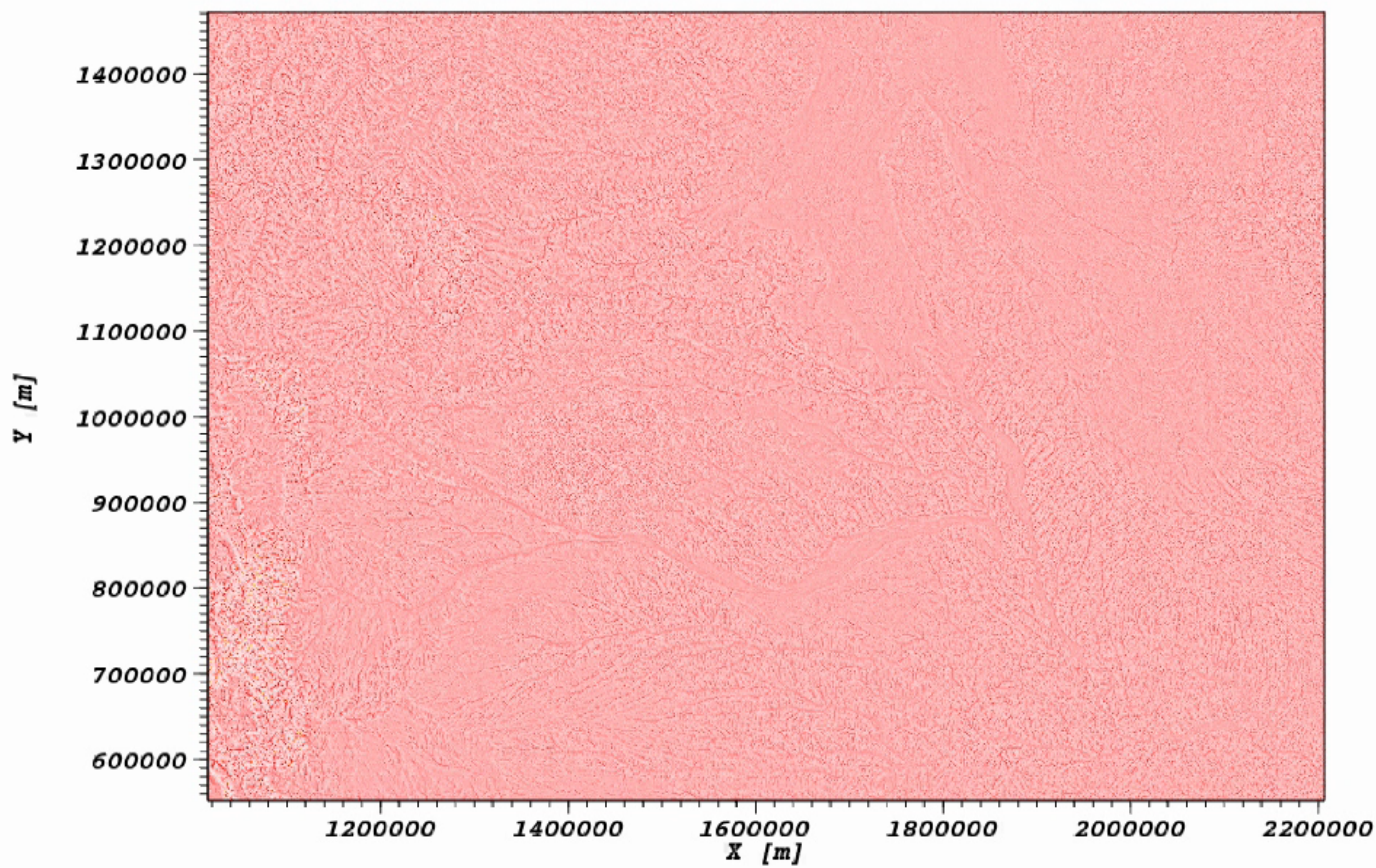


Gleeson et al GRL (2011)

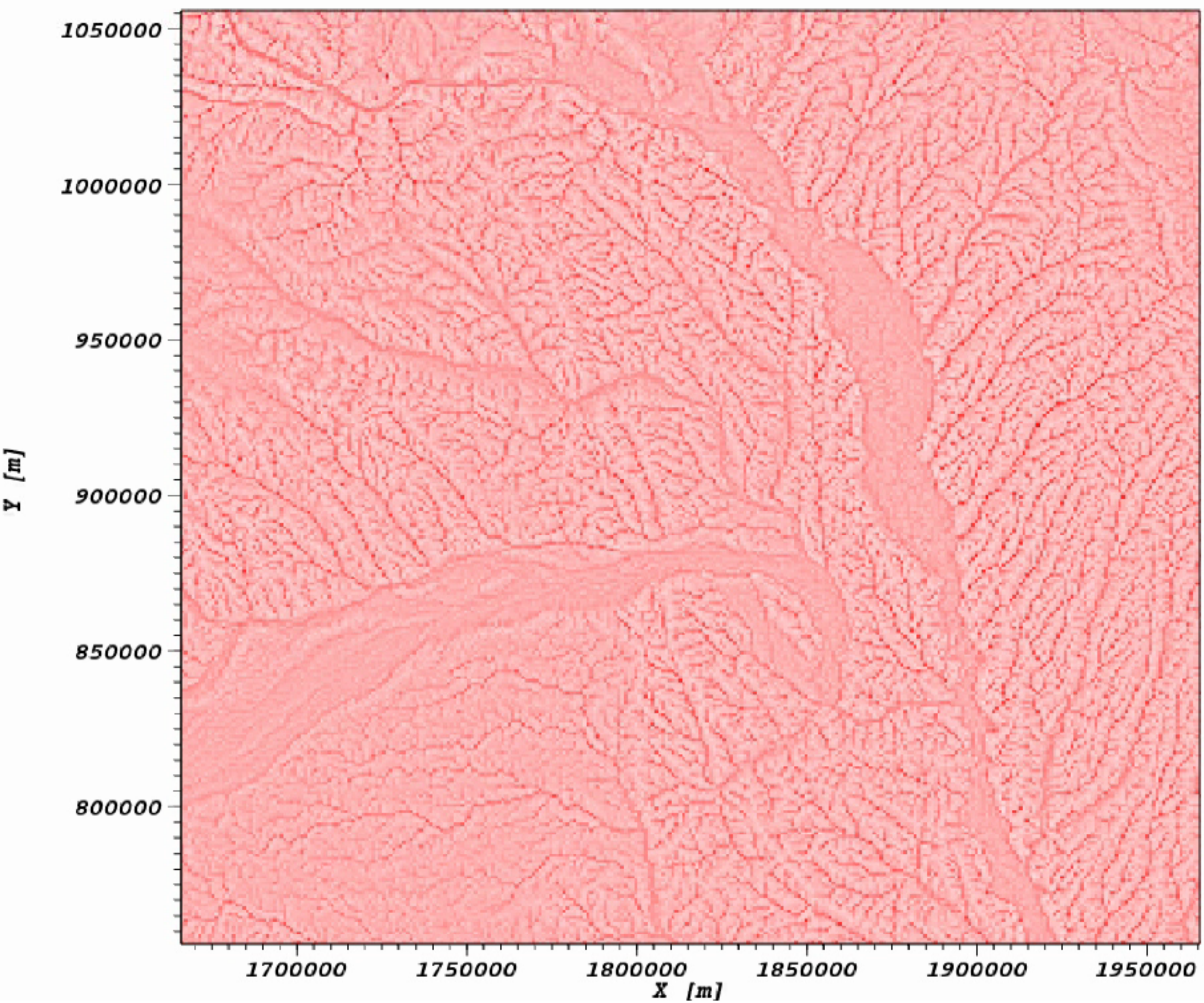
Preliminary Results Show Cross-Scale
r





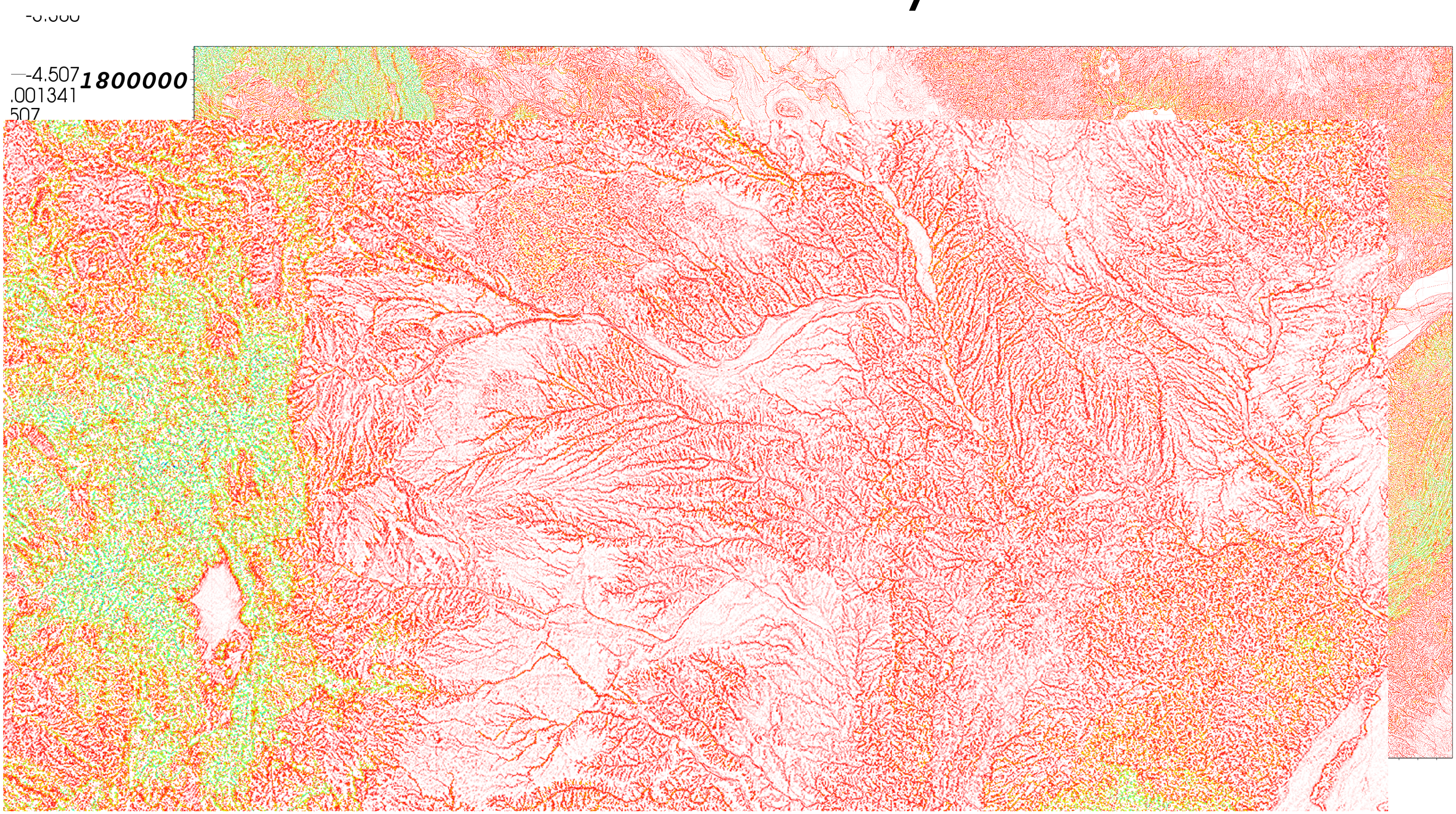


1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
Y [m]
1200000
1400000
1600000
1800000
2000000
2200000
X [m]

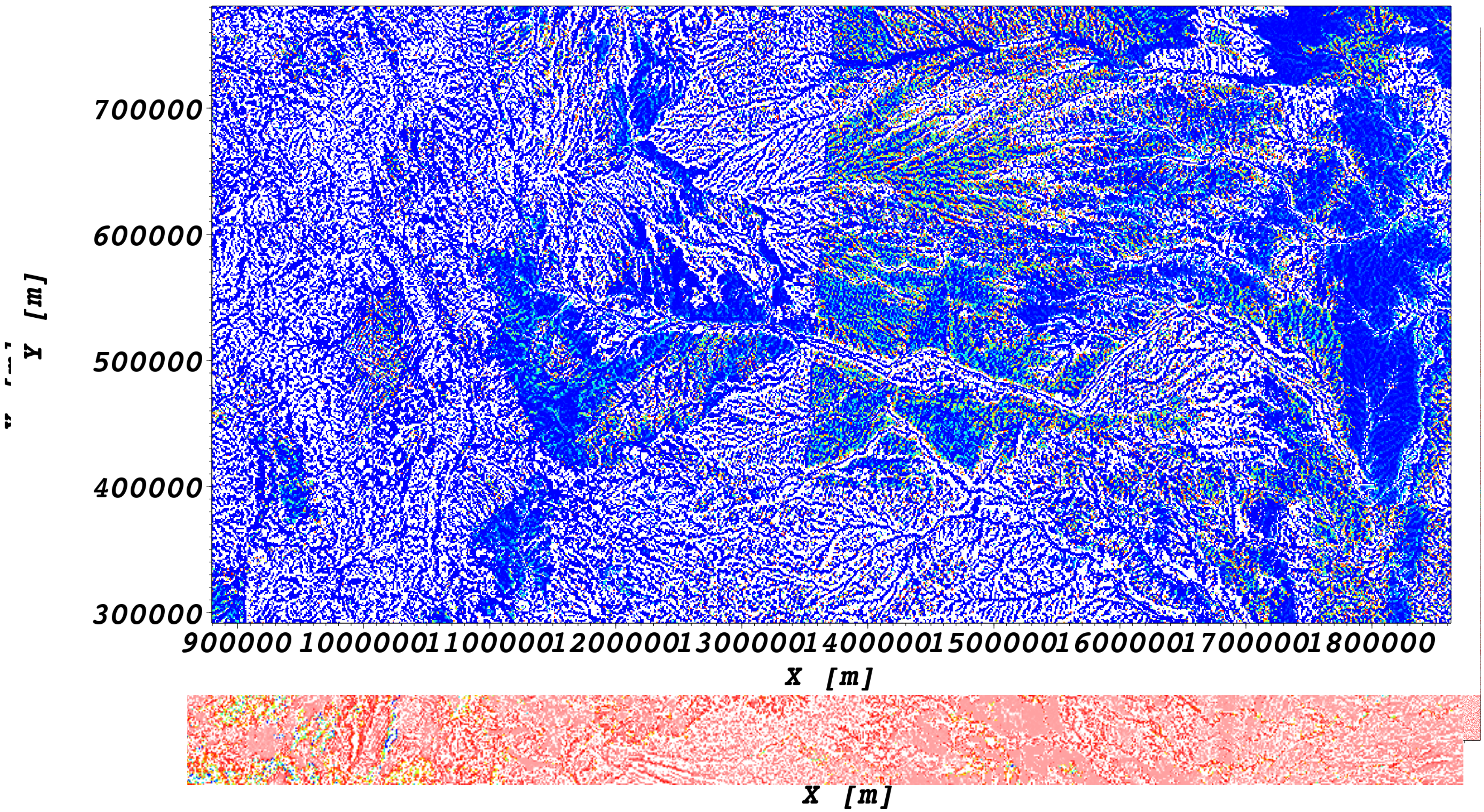


1050000
1000000
950000
900000
850000
800000
Y [m]
1700000
1750000
1800000
1850000
1900000
1950000
X [m]

Subsurface has a huge effect on return-flow dynamics



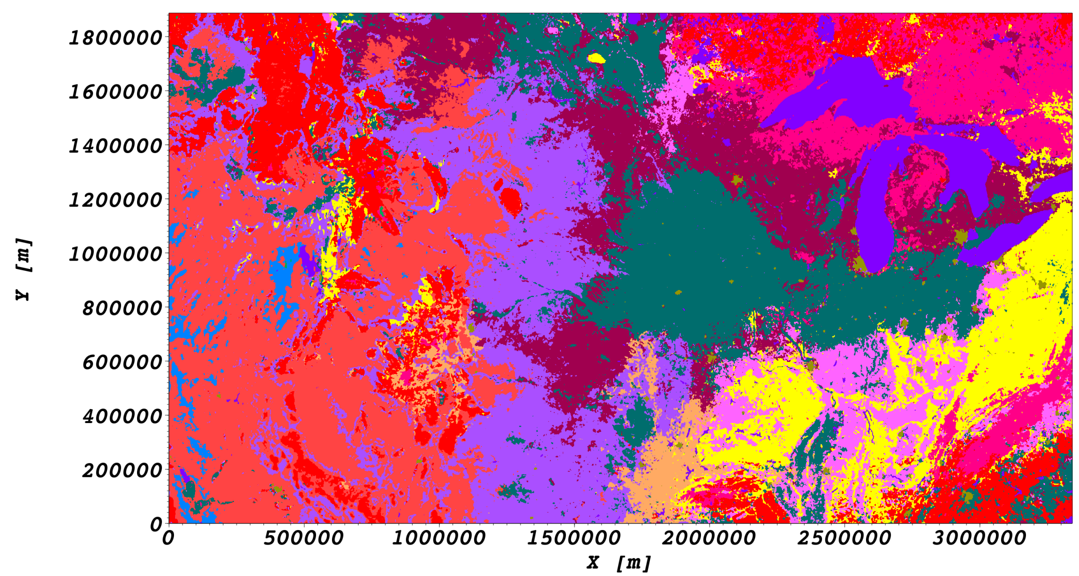
Homogeneous subsurface, terrain effects only



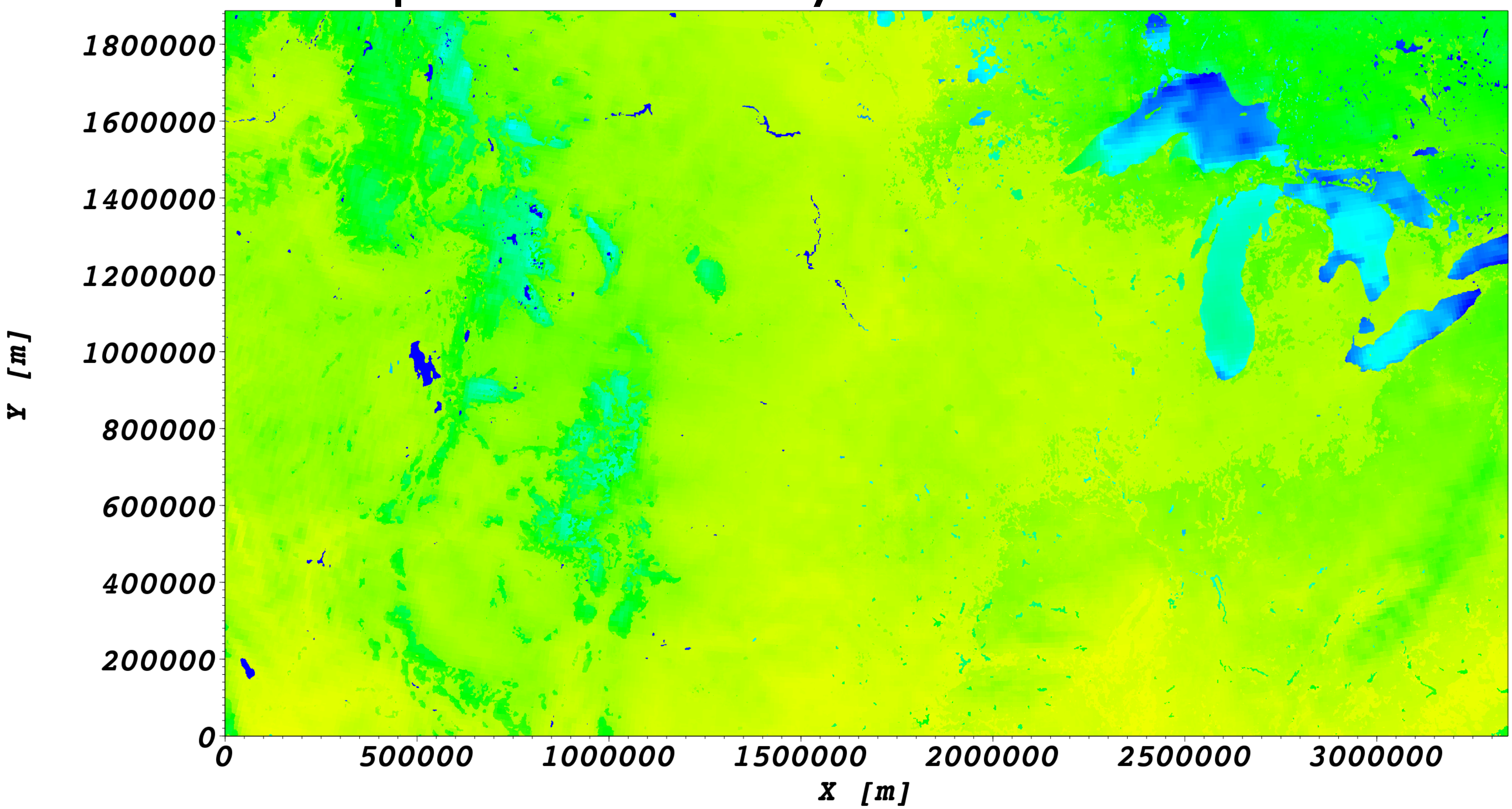
Heterogeneous subsurface, influence of ~7 OM parameter variability

Using PF.CLM we are running fully integrated simulations

- Full surface/subsurface
- Forced by spatially-distributed meteorology
- Transient, high temporal resolution

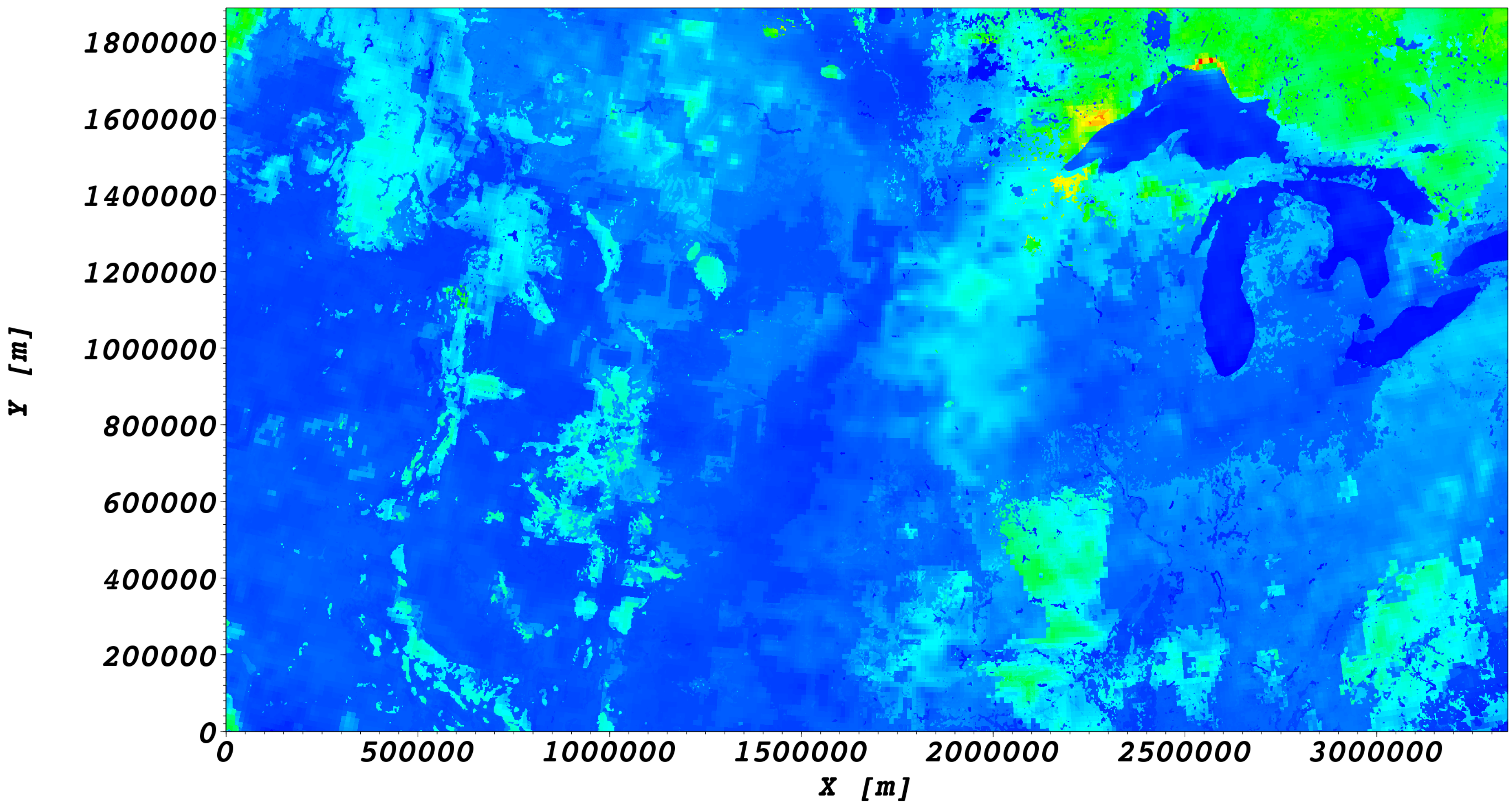


These fully-integrated simulations are already yielding interesting preliminary results



Ground Temperature

Latent Heat Flux shows effects of integrated system



Latent Heat Flux

Conclusions

- It is an exciting time for developing models of the hydrologic cycle
- The same feedbacks seen in the land-atmosphere literature may also be driven by groundwater
- We can tackle these ‘Grand-Challenge’ problems in Hydrology using integrated modeling and HPC

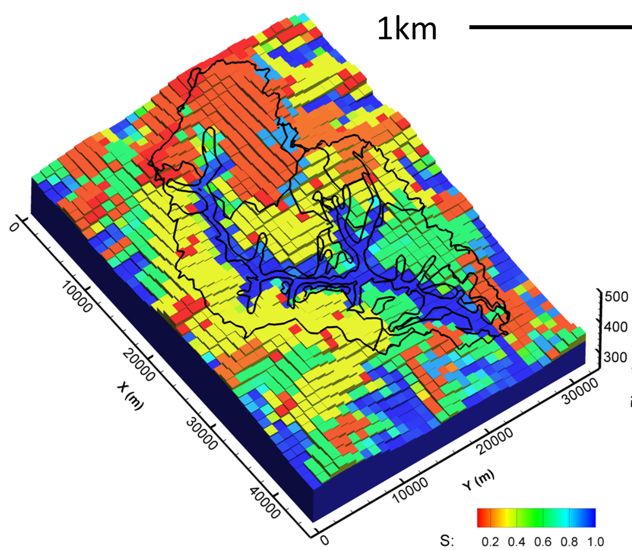
These models should help us address component interaction, topography, scaling to address *critical challenges in water quantity and quality*

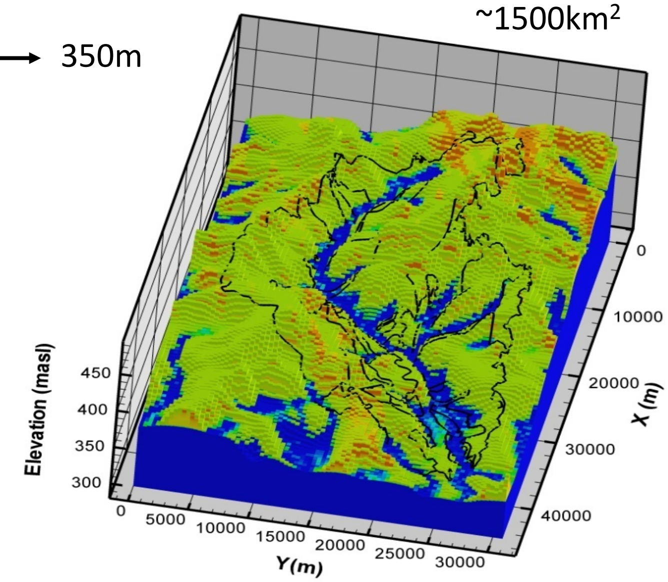
- Clearly dispersion, inputs critical for reactions are complicated, function of scale
- Need to understand roles of each component interaction if we really want to *predict*
- HPC and integrated models a useful tool in this process
- **Big challenges like climate change and cleanup need innovative solutions**

Increasing resolution results in more realistic soil moisture fields: Little Washita

1km → 350m

~1500km^2





Kollet & Maxwell, WRR (2008)

Can we go to higher resolution?

Integrated Flow Equations

Richards' EQ:

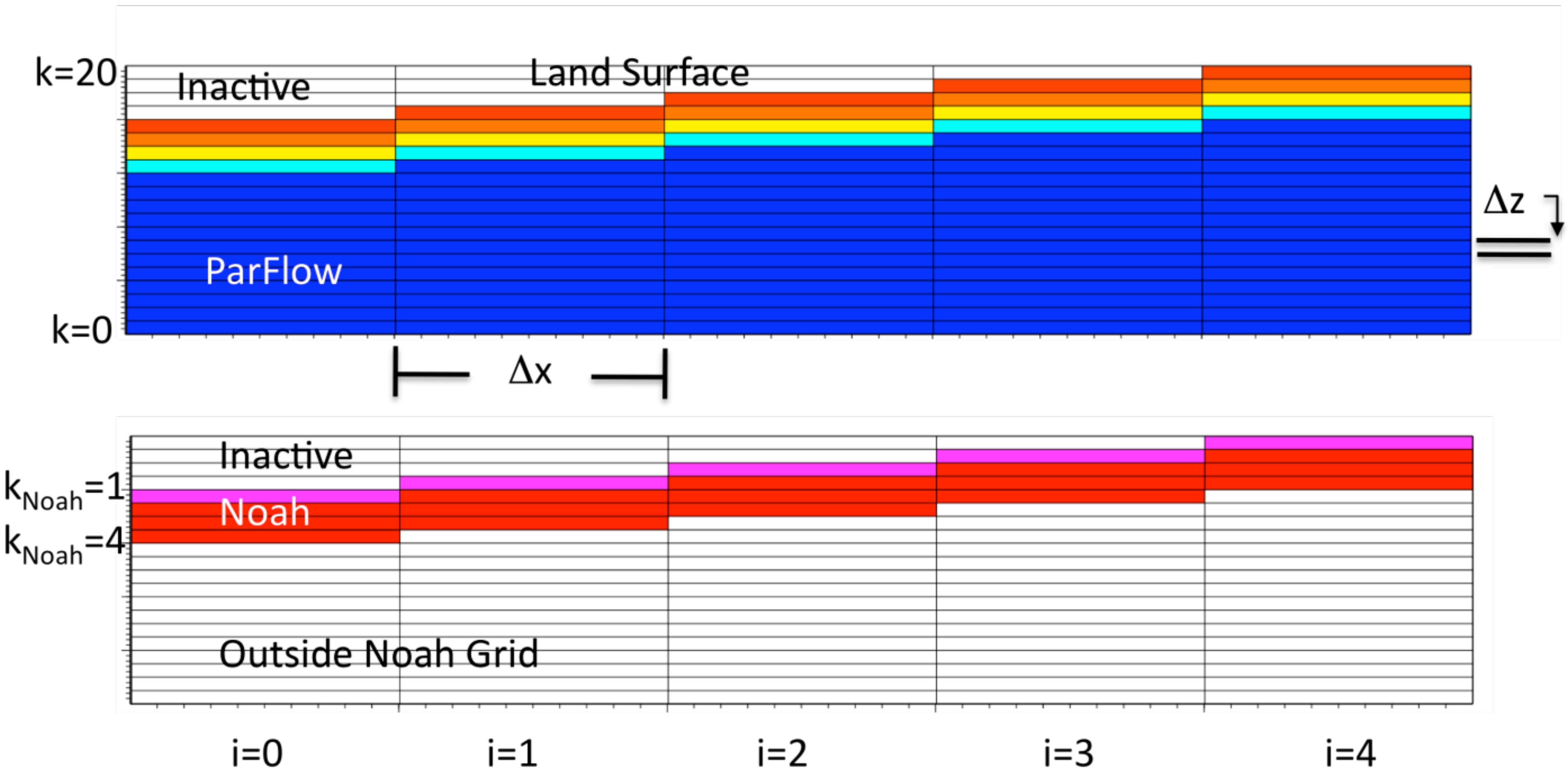
$$S_s S_w \frac{\partial h}{\partial t} + \phi \frac{\partial S_w(h)}{\partial t} = \nabla \cdot \mathbf{q} + \boxed{q_r(x,z)}$$

Overland Flow BC:

$$\mathbf{k} \cdot \left(-\mathbf{K}_s(\mathbf{x}) k_r \cdot \nabla(h - z)\right) = \frac{\partial \|h,0\|}{\partial t} - \nabla \cdot \|h,0\| \mathbf{v}^{sw} \boxed{+ q_r(\mathbf{x})}$$

Kollet and Maxwell *AWR*, 2006; Maxwell, Chow, Kollet, *AWR*, 2007; Maxwell, Lundquist, *et al MWR* 2011

Surface/Subsurface Grids and Geometries can be complicated.



Coupled Land Surface Processes

$$q_r(x) = P(x) - E(x)$$

Upper layer flux, Precip-Evap

$$E(x) = F^{fx}\left(1 - f_{veg}\right)E_{pot}$$

$$F = \left(\frac{\phi S_w - \phi S_{res}}{\phi - \phi S_{res}}\right)$$

Actual Evap is a moderated function of Potential Evap

$$q_r(x,z) = T(x,z)$$

Deeper soil layers, Transpiration

$$T(x,z) = G(z)C_{plant}f_{veg}E_{pot}$$

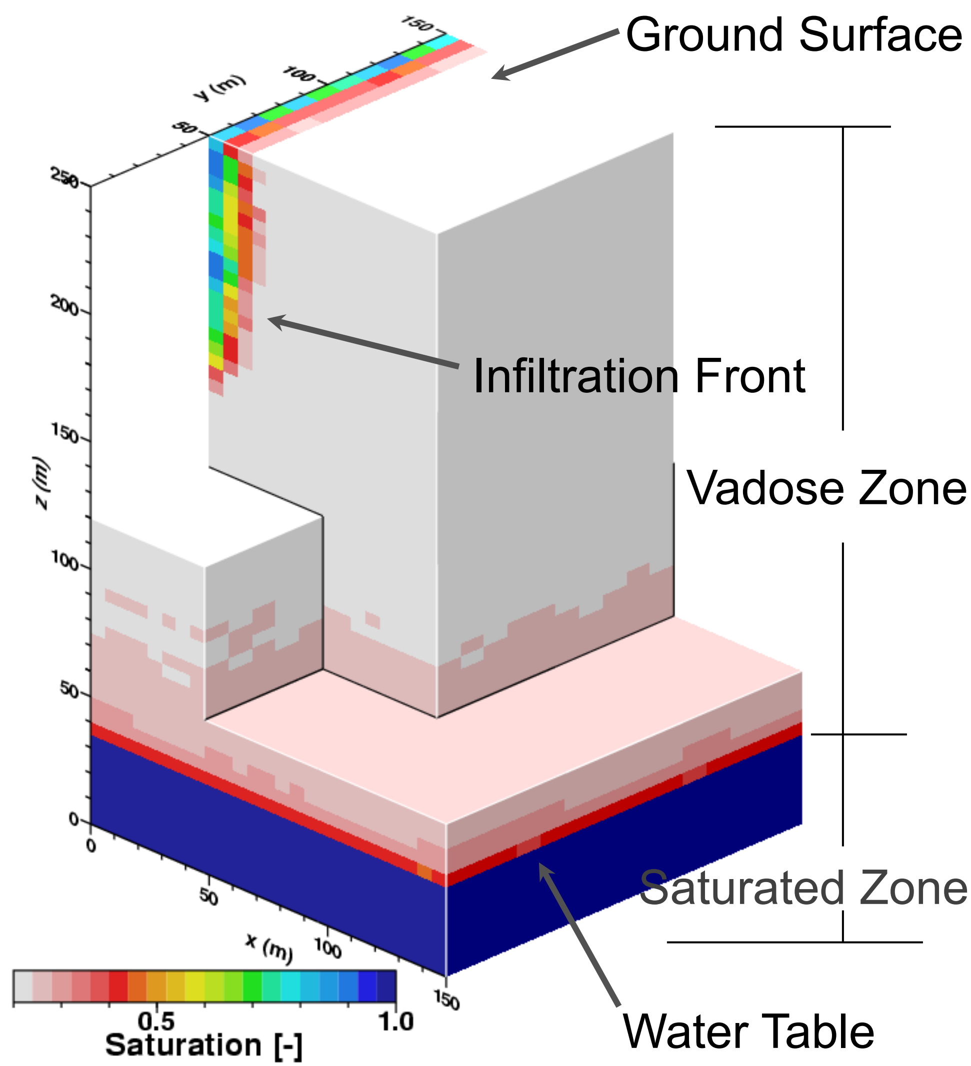
$$G(z) = \left.\frac{\left(\phi S_w^{k_{noah}} - \phi S_{wilt}\right)\Delta z^{k_{noah}}}{\left(\phi S_{ref} - \phi S_{wilt}\right)z_{n_{root}}}\right|_{k_{noah}=2}^{n_{root}}$$

Also calculated as function of potential

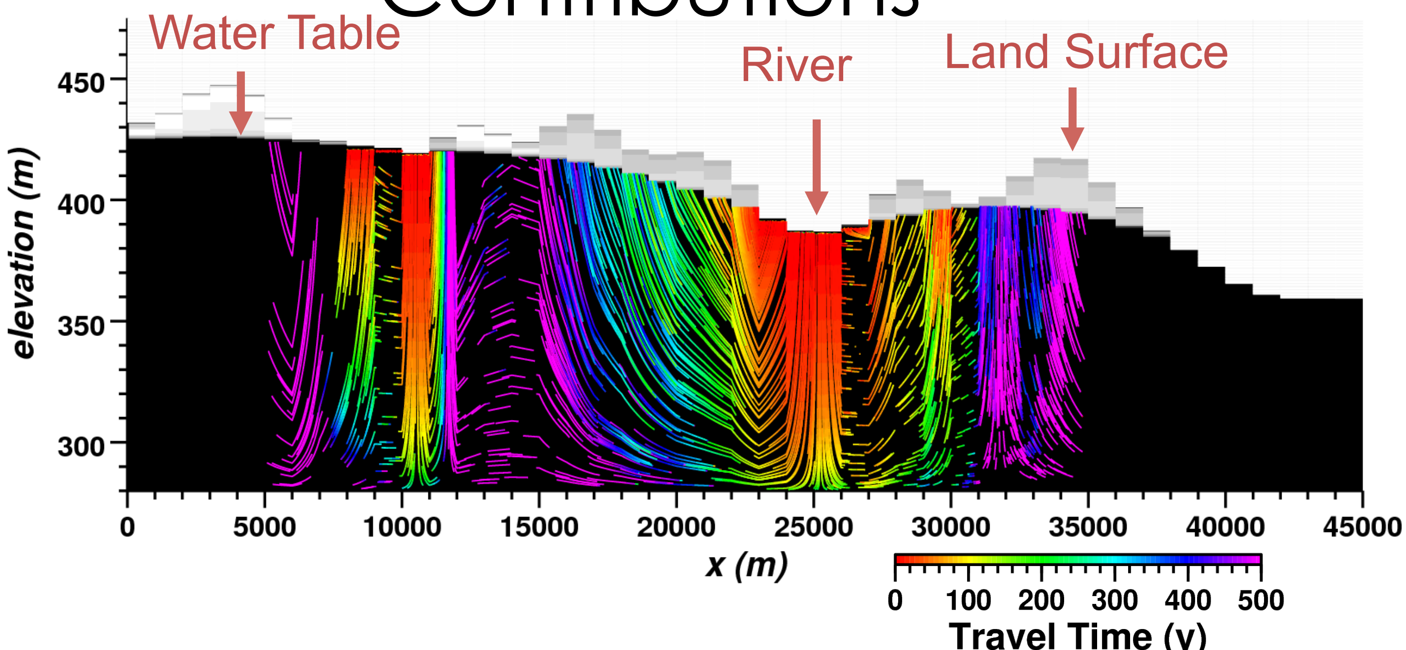
Maxwell, *et al MWR* 2011

ParFlow is a combination of:

- Physics
  - Integrated flow equations (Kollet and Maxwell, 2006)
  - Land surface processes (Maxwell and Miller, 2005)
- Solvers
  - Hypre linear solver (multigrid preconditioned conjugate gradient; Ashby and Falgout, 1996)
  - Kinsol nonlinear solver (Newton-Krylov; Jones and Woodward, 2001)
- Parallelism



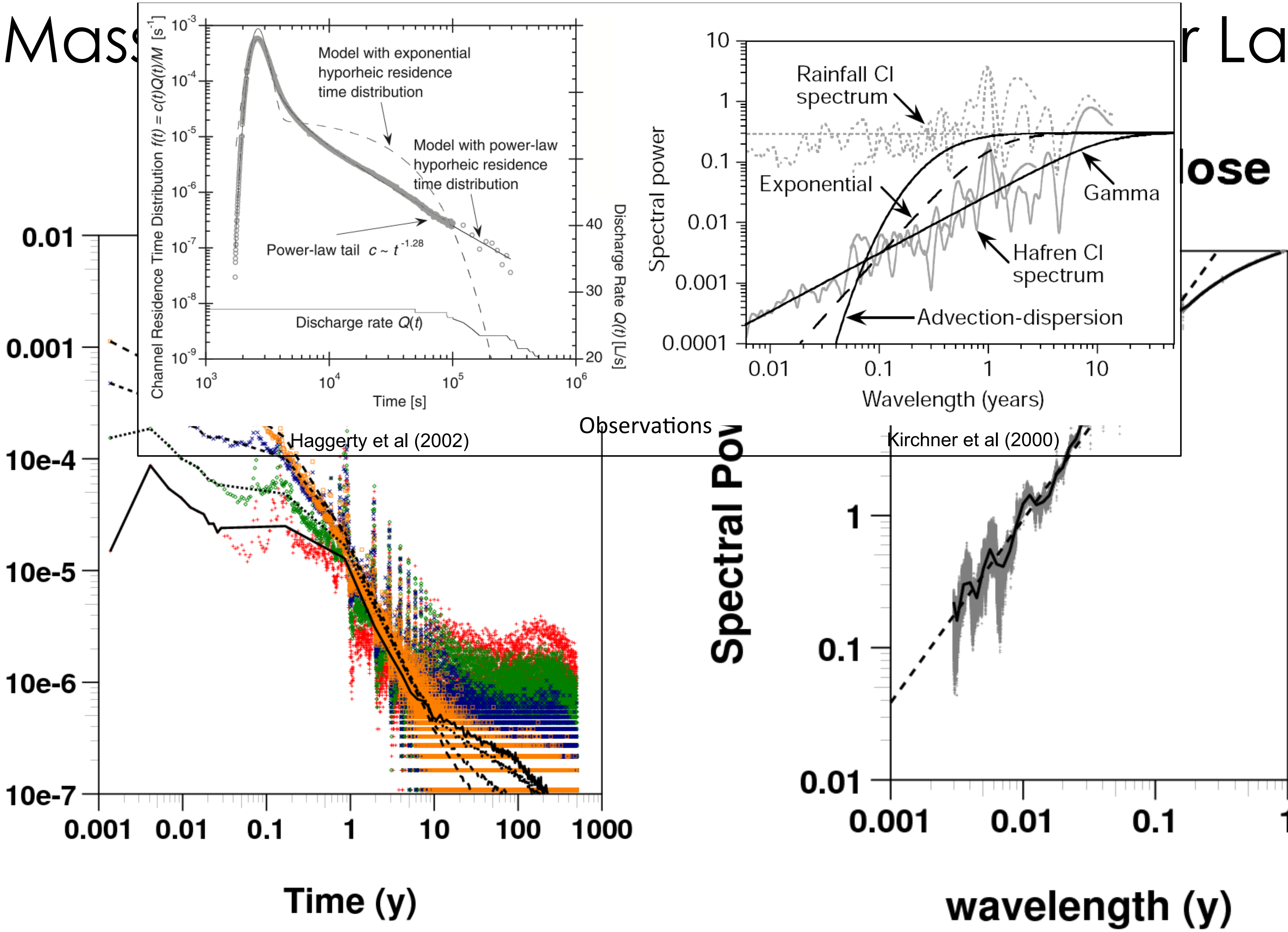
Understanding Residence Times: Spatiotemporal Scaling of Baseflow Contributions



- Particles initialized at bottom of riverbed
- Velocities reversed, simulation run for 500 water-years at 1d timestep
- Particle times to recorded at 1) water table and 2) land surface
- Range of dispersivities create macrodispersion as surrogate for heterogeneity
- Resulting PDF of travel times transformed using Lomb(1976)-Scargle (1982) technique

Kollet and Maxwell, GRL (2008)

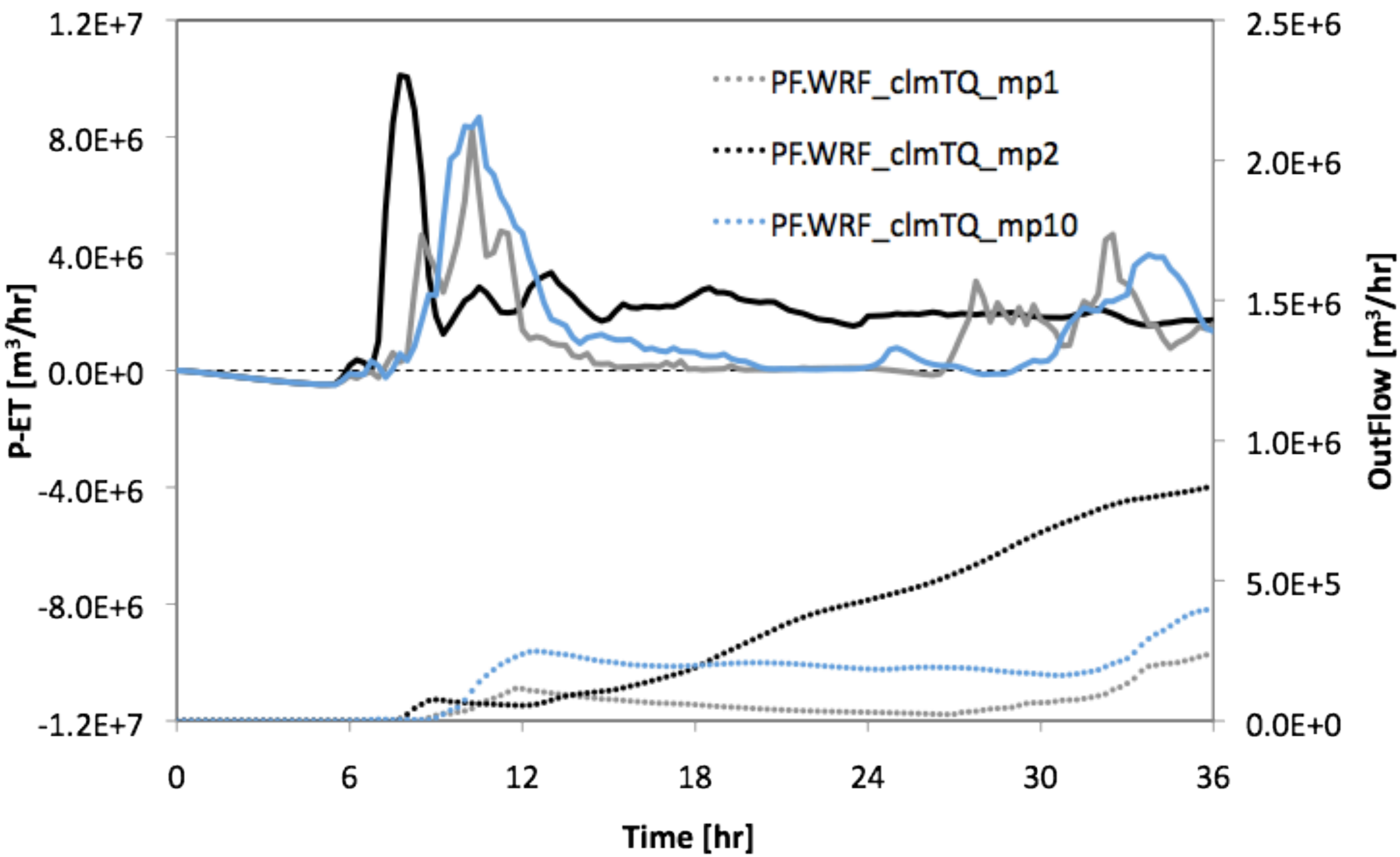
Mass… r Law



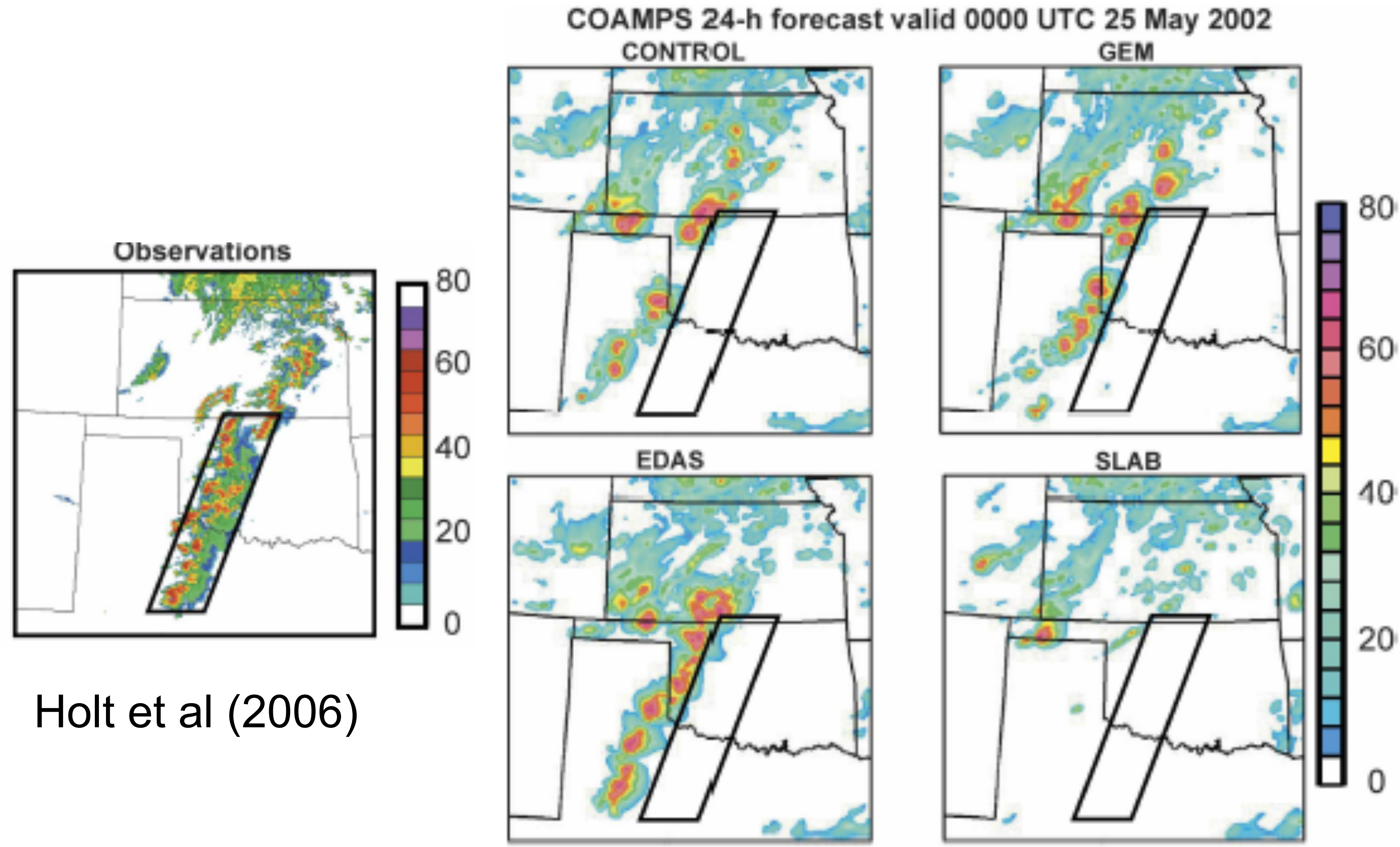
Spectral transform of distribution of arrival times demonstrates scaling in fully coupled model

Kollet and Maxwell, GRL (2008)

In PF.WRF we see different rainfall-runoff relationships per microphysics scheme



Soil moisture influences atmospheric processes (rain)



Holt et al (2006)

Questions to ponder:

- Are there spatiotemporal correlations between the land surface energy budget and subsurface storage?
- Do these feedbacks persist into the atmospheric boundary layer?
- Can we use the model to understand residence times, cycling and scaling of water parcels?
- How can HPC play a role in understanding land energy scaling?
- At what scales do we see these impacts on the atmosphere?