# The construction of land models

Martyn Clark

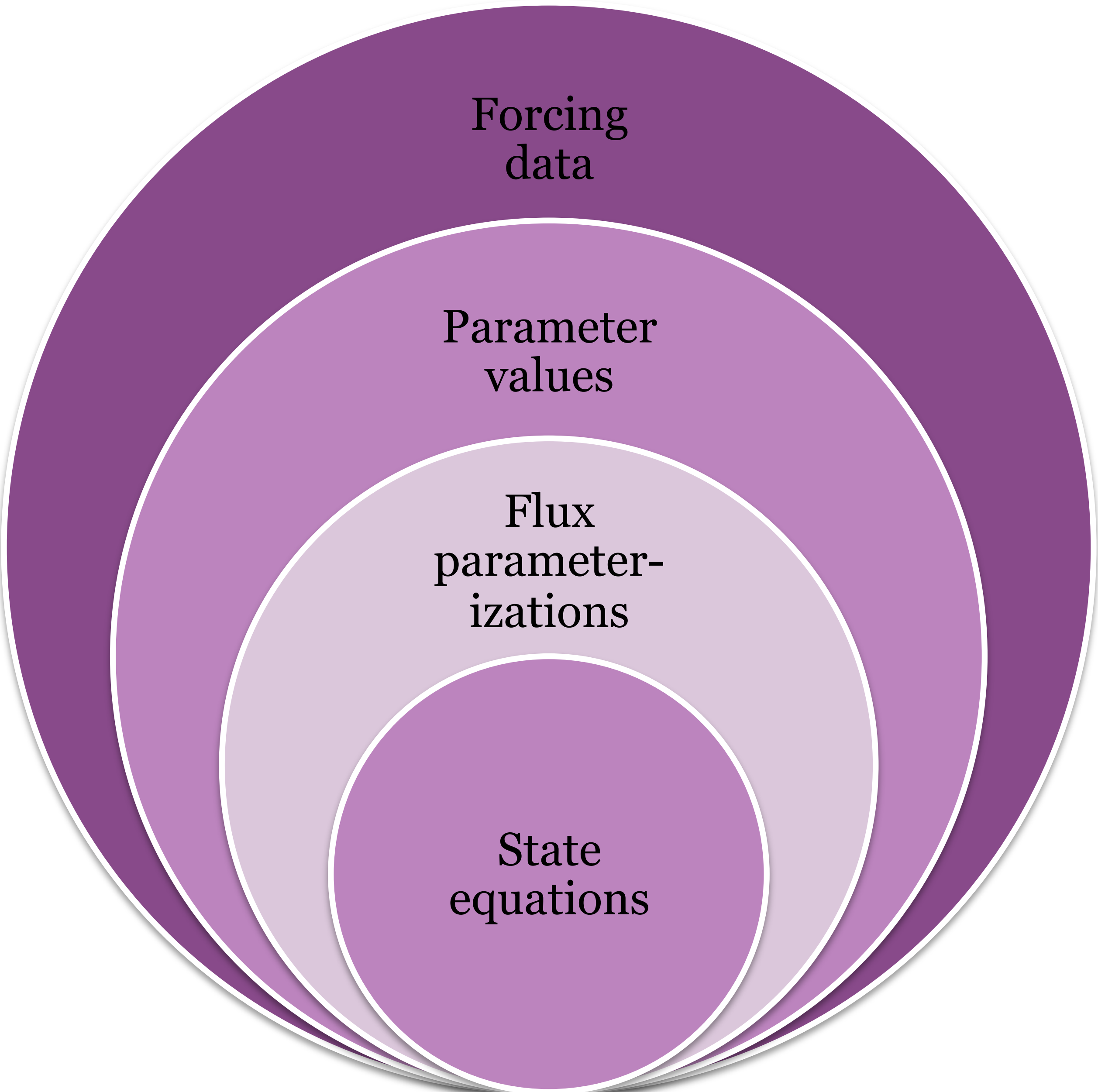
NCAR Research Applications Lab

**CLM Tutorial**
***NCAR, 16 September 2016***

# Outline

- The ingredients of a model
- Solving model equations (temporal integration of state equations)
- Impact of numerical solution on model simulations
- A modular approach to model construction

# The necessary ingredients of a model



Forcing data

Parameter values

Flux parameterizations

State equations

# States and flux parameterizations

## State variables

- Represent storage (mass, energy, momentum, etc.)
- Evolve over time: state at time t is a function of states at previous times

## Flux parameterizations

- Represent exchange/transport
- Rate of flow of a property per unit area
- Only depend on quantities at time t

*Rate of change of a state is determined by fluxes at the boundaries of a model control volume*

## Parameter values

- The (typically time-invariant) constants within flux parameterizations

# The necessary ingredients of a model

*Model forcing data, model state variables, flux parameterizations, model parameters, and the numerical solution*

- Example 1: A temperature-index snow model
  - The state equation

$$\frac{dS}{dt} = a - m$$

State variable
(also known as prognostic variable)

Fluxes

State variable:
$S$ = Snow storage (mm)

Fluxes:
$a$ = Snow accumulation (mm/day)
$m$ = Snow melt (mm/day)

  - Flux parameterizations and model parameters

$$a = \begin{cases} p & T_a < T_f \\ 0 & T_a \ge T_f \end{cases}$$

Forcing data

$$m = \begin{cases} 0 & T_a < T_f \\ \kappa\left(T_a - T_f\right) & T_a \ge T_f \end{cases}$$

Model parameter

Forcing data

Physical constant
(can also be treated as a model parameter)

Model forcing:
$p$ = Precipitation rate (mm/day)
$T_a$ = Air temperature (K)

Parameters:
$\kappa$ = Melt factor (mm/day/K)

Physical constants:
$T_f$ = Freezing point (K)

  - Numerical solution
    - Simple in this case, since fluxes do not depend on state variables

# The necessary ingredients of a model

*Model forcing data, model state variables, flux parameterizations, model parameters, and the numerical solution*

- Example 2: A conceptual hydrology model

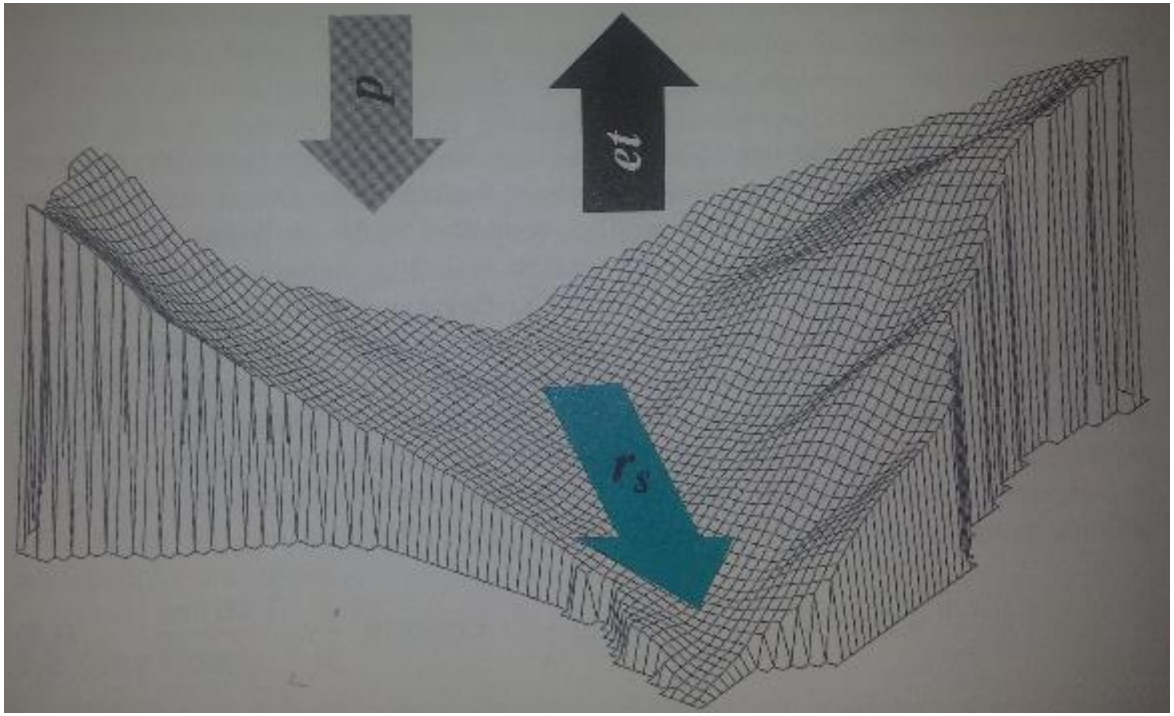


Figure from Hornberger et al. (1998) "*Elements of Physical Hydrology*" The Johns Hopkins University Press, 302pp.

- State equation

$$\frac{dS}{dt} = p - e_t - r_s$$

# The necessary ingredients of a model

*Model forcing data, model state variables, flux parameterizations, model parameters, and the numerical solution*

- Example 2: A conceptual hydrology model
  - The state equation

$$\frac{dS}{dt} = p - e_t - q_b$$

State variable

Forcing data

Fluxes

  - Flux parameterizations

State variable

$$e_t = \begin{cases} e_p \left( \dfrac{S}{S_{ps}} \right) & S < S_{ps} \\ e_p & S \geq S_{ps} \end{cases}$$

Model parameter

State variable

Forcing data

$$q_b = k_s \left( \frac{S}{S_{\max}} \right)^c$$

Model parameter

Model parameter

Model parameter

  - Numerical solution
    - Care must be taken: model fluxes depend on state variables (numerical daemons)

<u>State variable:</u>

$S$ = Soil storage (mm)

<u>Model forcing:</u>

$p$ = Precipitation rate (mm/day)

<u>Model fluxes:</u>

$e_t$ = Evapotranspiration (mm/day)

$q_b$ = Baseflow (mm/day

<u>Model forcing:</u>

$e_p$ = Potential ET rate (mm/day)

<u>Parameters:</u>

$S_{ps}$ = Plant stress storage (mm)

$S_{max}$ = Maximum storage (mm)

$k_s$ = Hydraulic conductivity (mm/day)

$c$ = Baseflow exponent (-)

# Outline

- The ingredients of a model
- Solving model equations (temporal integration of state equations)
- Impact of numerical solution on model simulations
- A modular approach to model construction

# The exact solution of an ODE system

- The ODE system for a simple land model can be written as

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

- The exact solution of the average flux over the interval $t^n$ (start of the time step) to $t^{n+1}$ (end of the time step) is

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

- Given an estimate of the average flux, the model state variables can be temporally integrated as

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

- *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*

# Let’s start with a skydiving example

- A famous land modeler (weight = 90 kg) has decided to go skydiving, and has asked you to determine how fast they will fall.
- The land modeler thinks that it is acceptable for you to use Newton’s second law of motion considering only the gravitational force ($F_{grav}$) and the force due to air resistance ($F_{res}$) . That is,

$$m\frac{dv}{dt} = F_{grav} + F_{res}$$

where $m$ = mass (kg) and $v$ is the fall velocity (m $s^{-1}$).

- Further, the land modeler is quite happy for you to use the empirical representations

$$F_{grav} = mg$$

$$F_{res} = -kv$$

where $k$ is a proportionality constant (assume $k$ = 15 kg $s^{-1}$ for freefall and 250 kg $s^{-1}$ for landing) and $g$ is the gravitational acceleration (9.81 m $s^{-2}$).

- *Based on an initial velocity of zero (the land modeler is hopping out of a hovering helicopter), temporally integrate the ODE for a 3 minute period using the explicit Euler method with 10 second time steps.*

# The parachute problem (freefall)

- ODE:

$$m\frac{dv}{dt} = mg - kv$$

- Constants:
  - $m$ = mass of the hydrologist (90 kg)
  - $g$ = gravitational acceleration (9.81 m $s^{-2}$)
  - $k$ = proportionality constant for freefall (15 kg $s^{-1}$)
- Hence

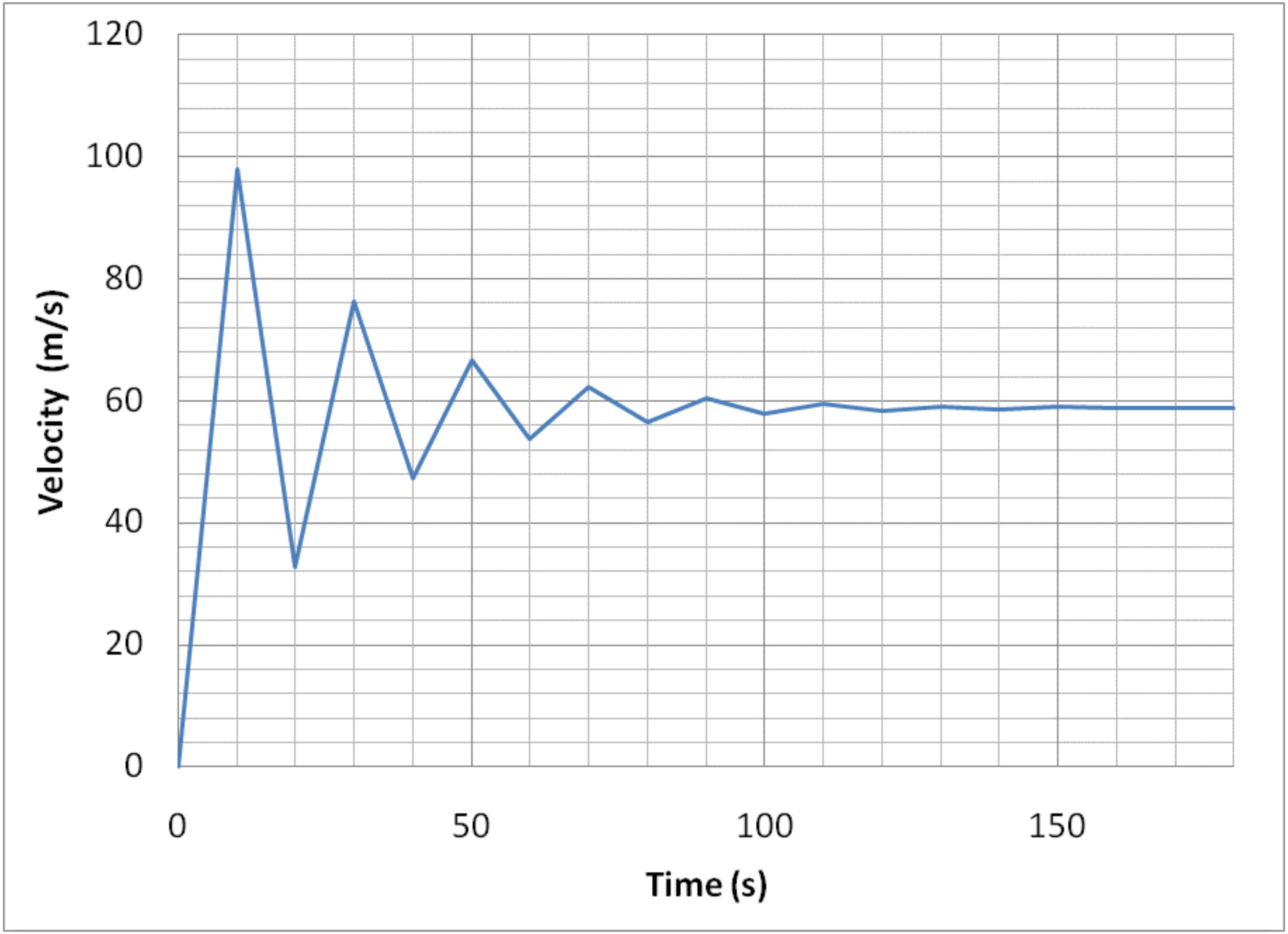
$$\frac{dv}{dt} = g(v)$$

- Numerical approximation: explicit Euler

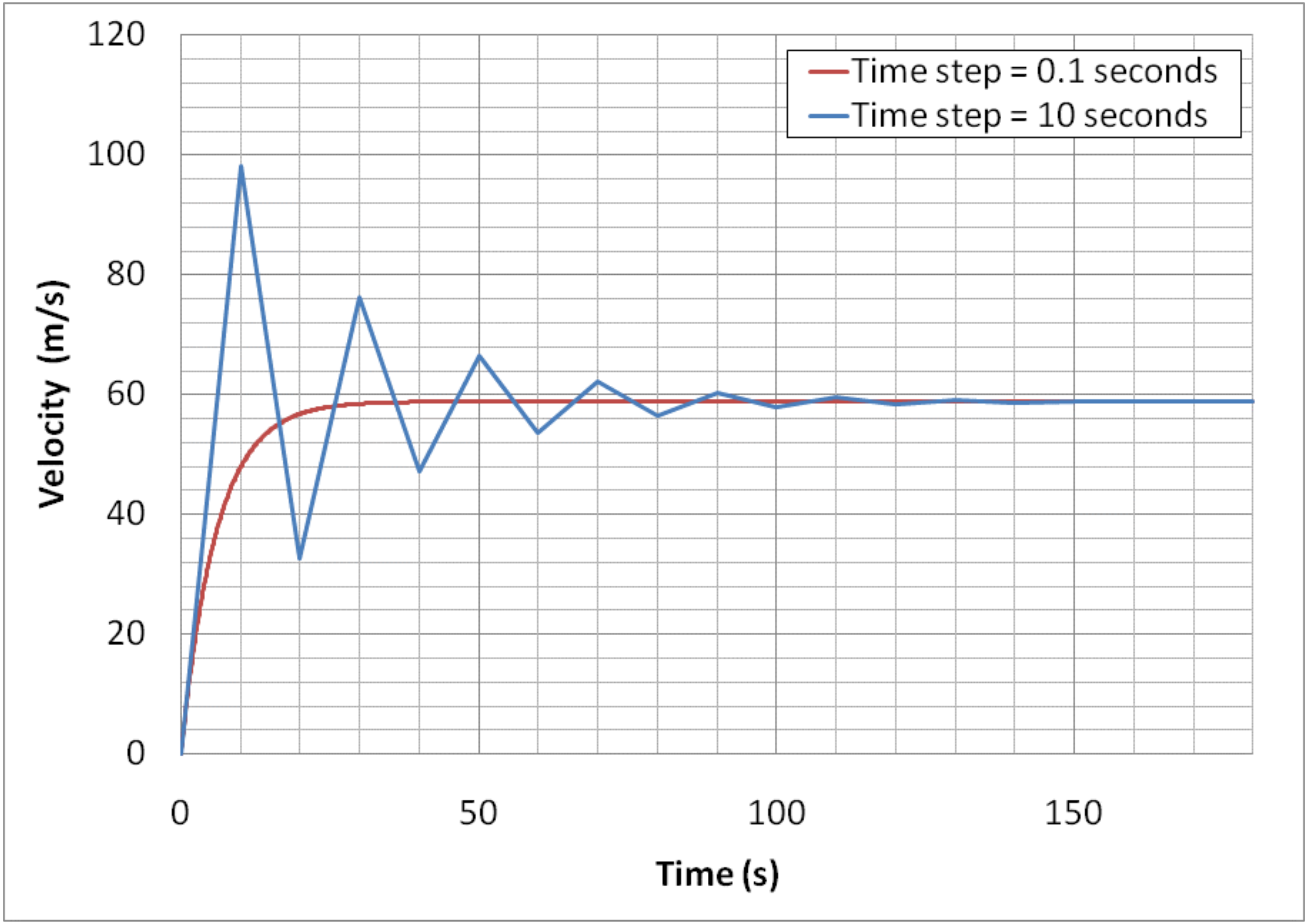
$$v^{n+1} = v^n + g(v^n)\Delta t$$

- Length of time step: $\Delta t$ = 10 seconds
- Initial velocity = zero m $s^{-1}$ (hovering helicopter)

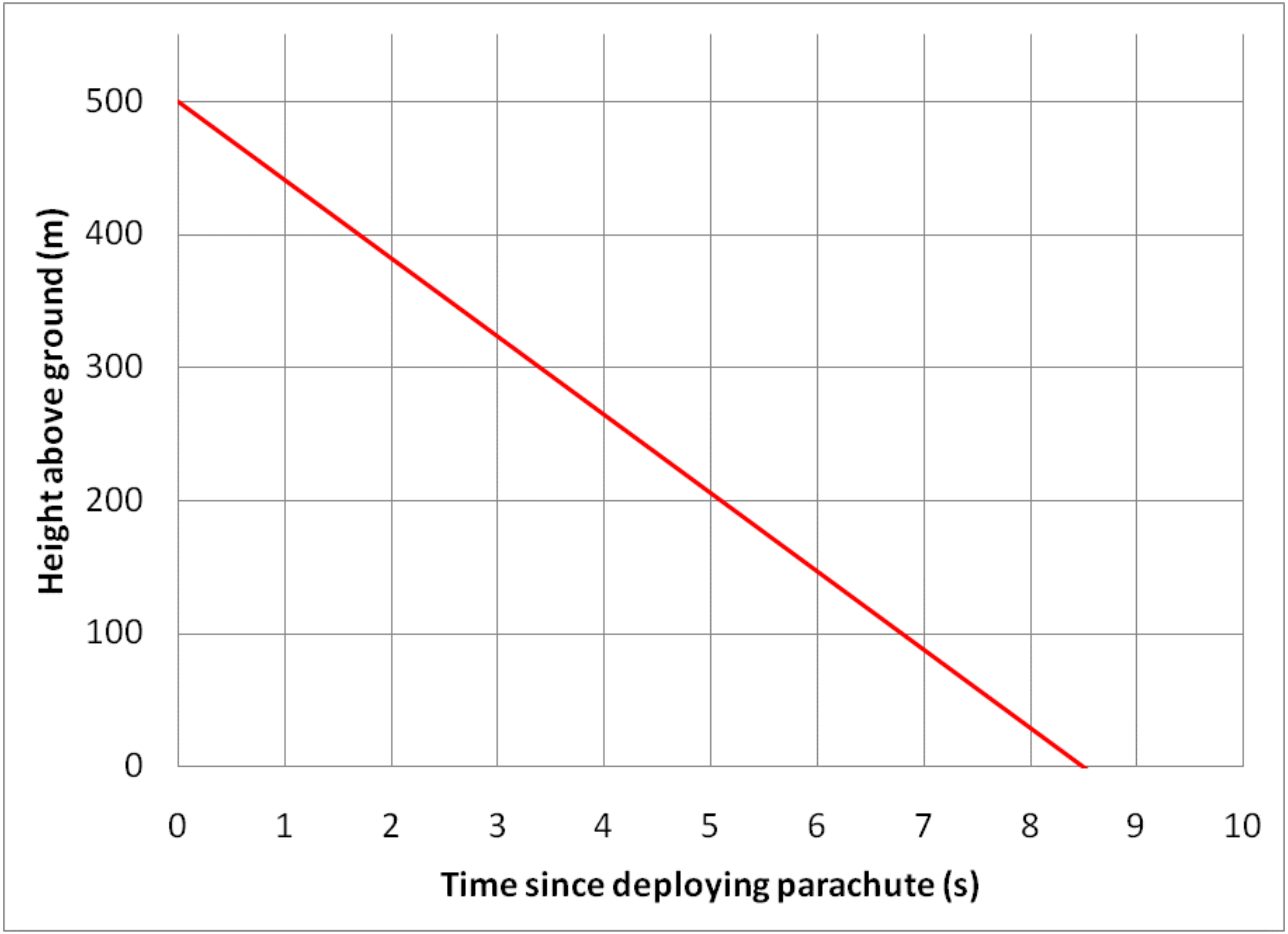
# …and, the end result…



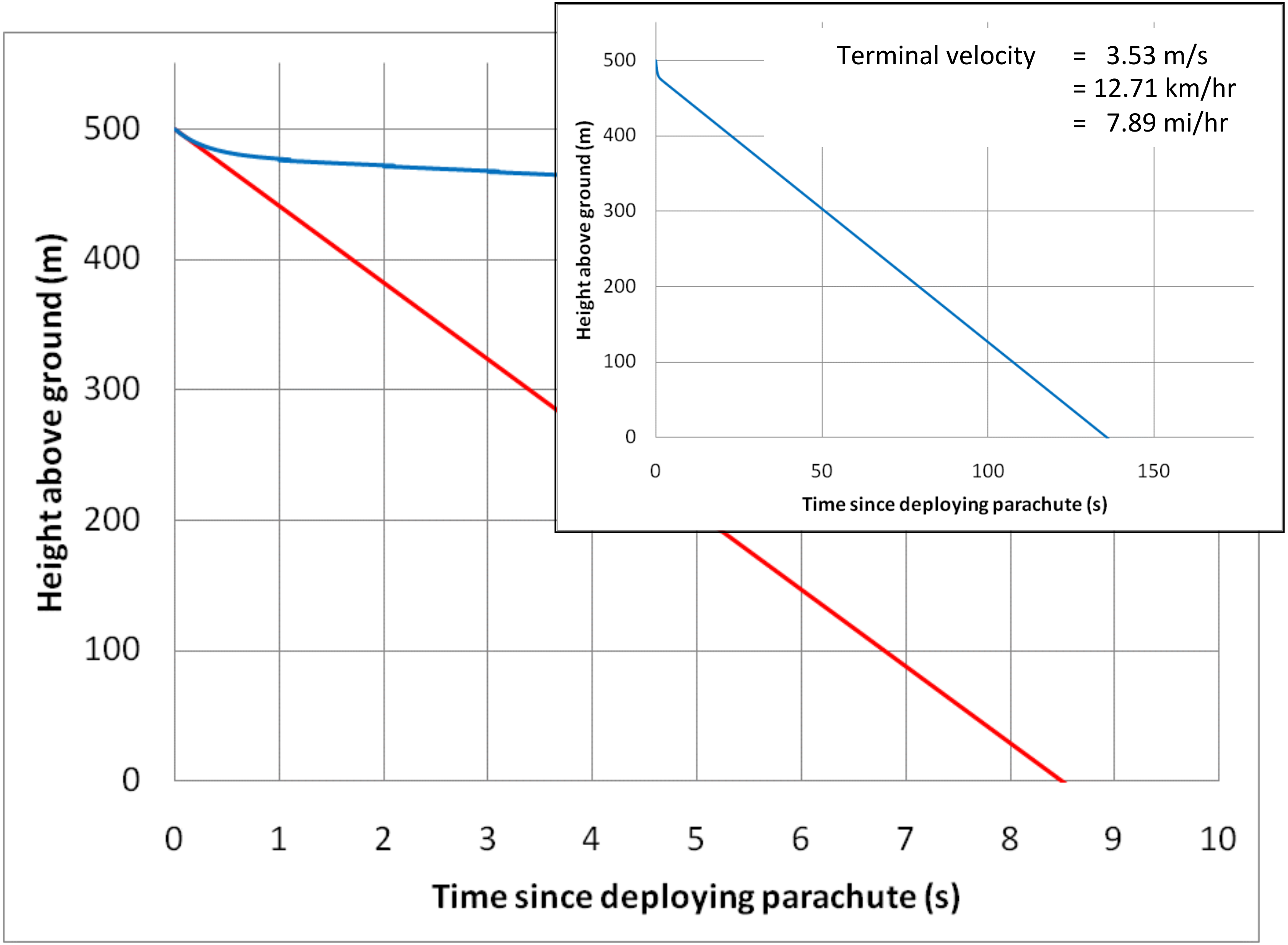
# …but now with 0.1 second time steps



# Landing example…

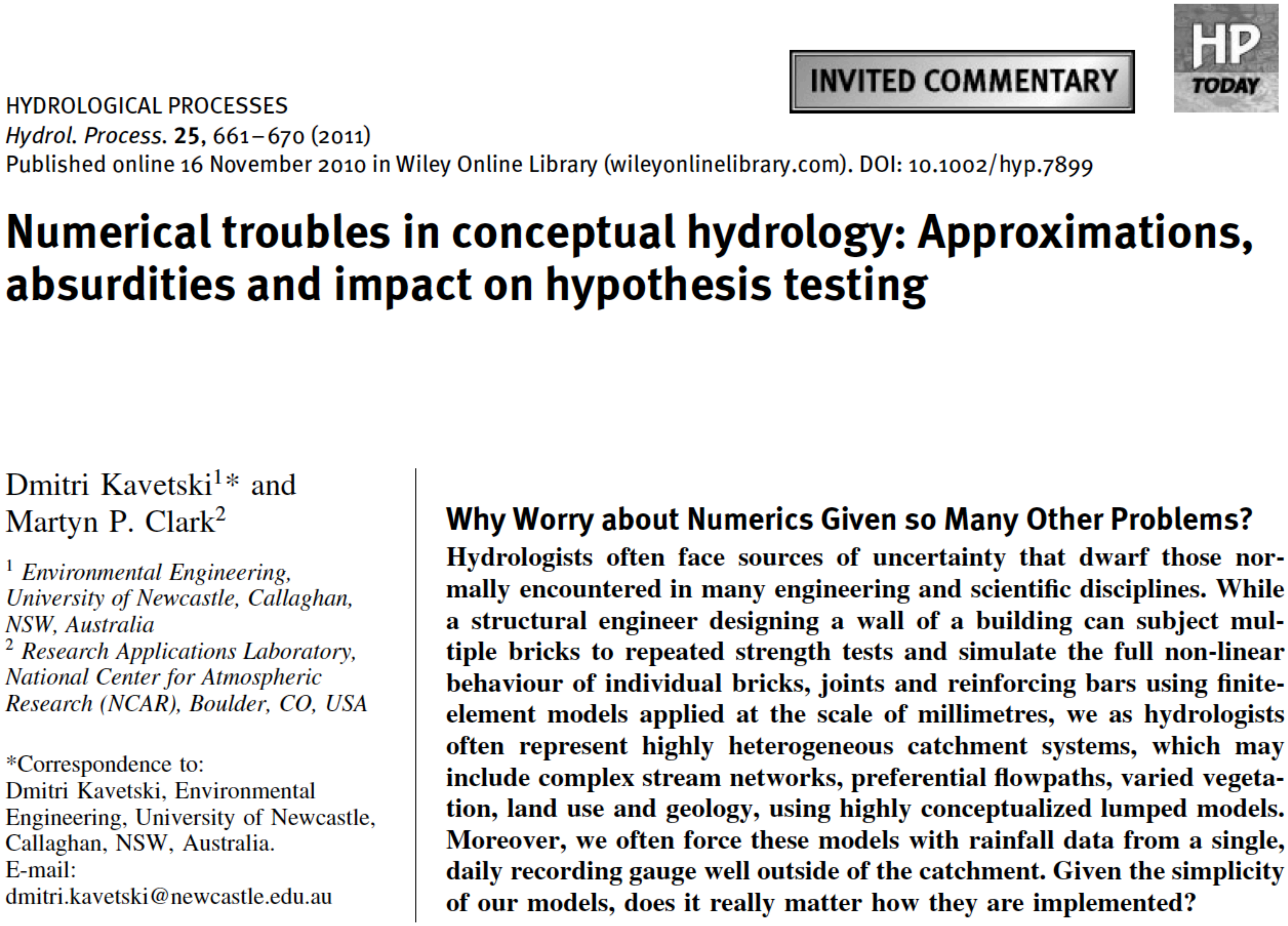


# Once again, short steps save the day…



Terminal velocity = 3.53 m/s
= 12.71 km/hr
= 7.89 mi/hr

# Application to land modeling…



INVITED COMMENTARY

HP TODAY

HYDROLOGICAL PROCESSES
*Hydrol. Process.* **25**, 661–670 (2011)
Published online 16 November 2010 in Wiley Online Library (wileyonlinelibrary.com). DOI: 10.1002/hyp.7899

## Numerical troubles in conceptual hydrology: Approximations, absurdities and impact on hypothesis testing

Dmitri Kavetski[1]* and
Martyn P. Clark[2]

[1] *Environmental Engineering, University of Newcastle, Callaghan, NSW, Australia*
[2] *Research Applications Laboratory, National Center for Atmospheric Research (NCAR), Boulder, CO, USA*

*Correspondence to:
Dmitri Kavetski, Environmental Engineering, University of Newcastle, Callaghan, NSW, Australia.
E-mail:
dmitri.kavetski@newcastle.edu.au

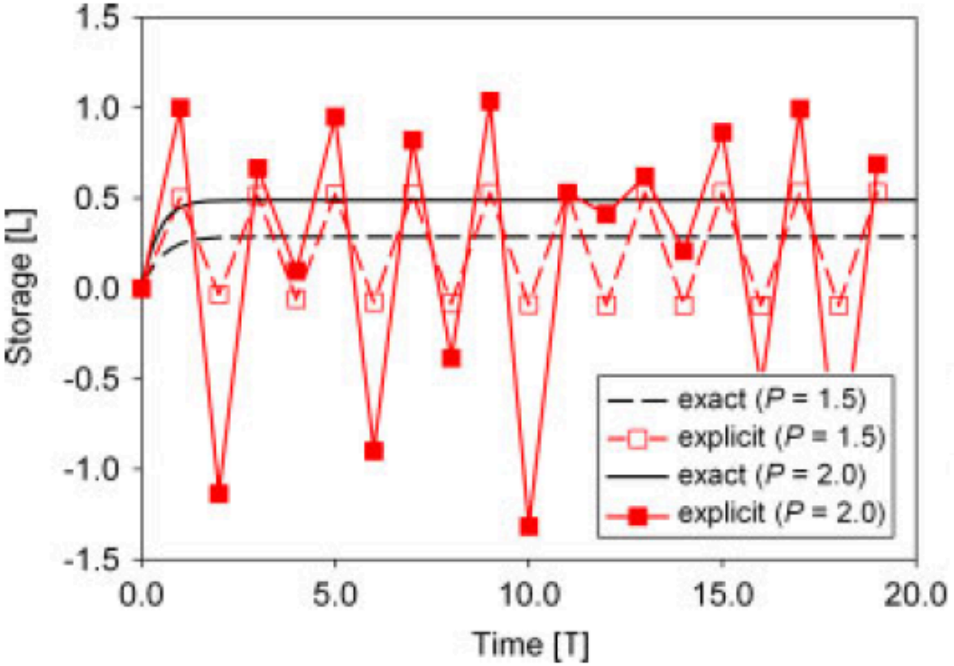
### Why Worry about Numerics Given so Many Other Problems?

**Hydrologists often face sources of uncertainty that dwarf those normally encountered in many engineering and scientific disciplines. While a structural engineer designing a wall of a building can subject multiple bricks to repeated strength tests and simulate the full non-linear behaviour of individual bricks, joints and reinforcing bars using finite-element models applied at the scale of millimetres, we as hydrologists often represent highly heterogeneous catchment systems, which may include complex stream networks, preferential flowpaths, varied vegetation, land use and geology, using highly conceptualized lumped models. Moreover, we often force these models with rainfall data from a single, daily recording gauge well outside of the catchment. Given the simplicity of our models, does it really matter how they are implemented?**

# Application to land modeling…

*Surprisingly common model implementation…*

```
Srz = Srz_ini ! initialize store
DO i = 1, n   ! loop over time steps
  ! calculate outflow using parameters
  outflow(i) = b * exp(k * Srz)
  ! update storage
  Srz = Srz + inflow(i) − outflow(i)
END DO
```



# Implicit methods

- The average flux over the time step is approximated as the flux computed from the state at the end of the time step

$$\overline{\mathbf{g}}_{IE}^{n\to n+1} = \mathbf{g}\left(\mathbf{S}_{IE}^{n+1}\right)$$

- This is an implicit solution

$$\mathbf{S}_{IE}^{n+1} - \left[\mathbf{S}^{n} + \mathbf{g}\left(\mathbf{S}_{IE}^{n+1}\right)\Delta t\right] = 0$$

- often solved using Newton-Raphson procedure
  (scalar example)

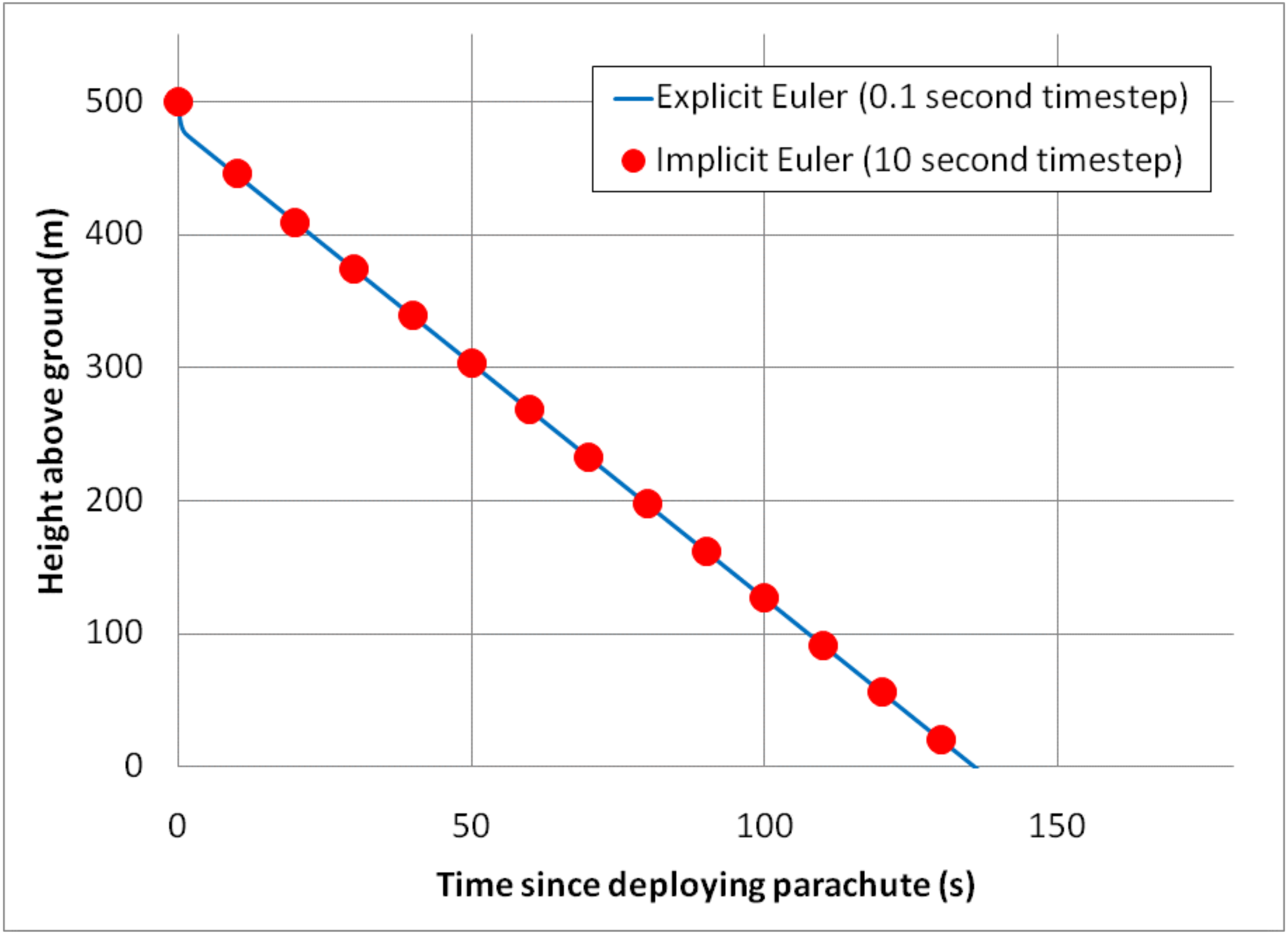
$$S^{n+1} = S^{n} + \left[g(S^{n}) + \left(\frac{dg}{dS}\right)^{n}\left(S^{n+1} - S^{n}\right)\right]\Delta t$$

$$\left[1 - \left(\frac{dg}{dS}\right)^{n}\Delta t\right]\left(S^{n+1} - S^{n}\right) = g(S^{n})\Delta t$$

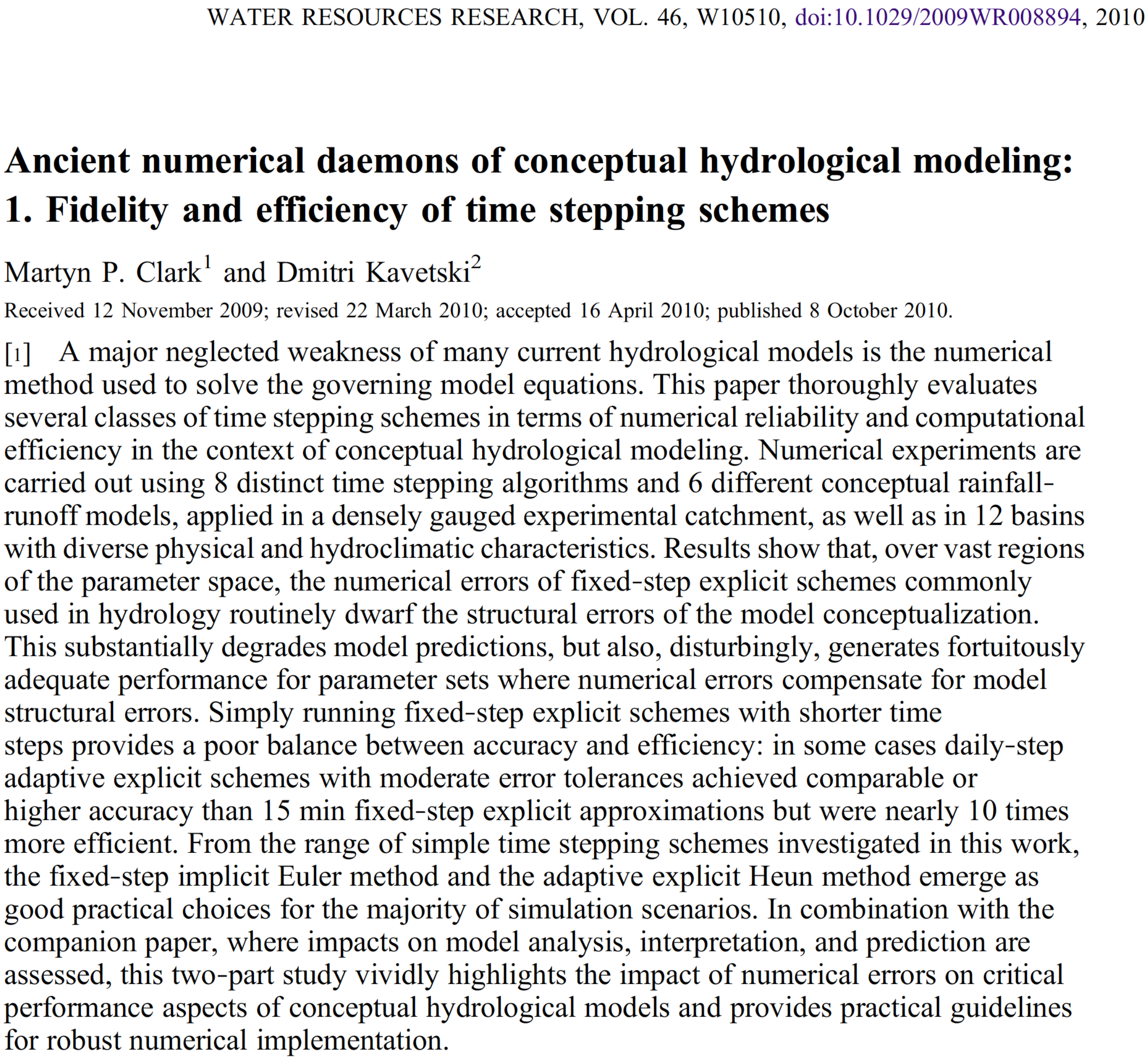
- Or.. for a state vector

$$\mathbf{J}\Delta\mathbf{S} = -\mathbf{r}$$

# Implicit solution of the parachute problem



# Application to land modeling…



WATER RESOURCES RESEARCH, VOL. 46, W10510, doi:10.1029/2009WR008894, 2010

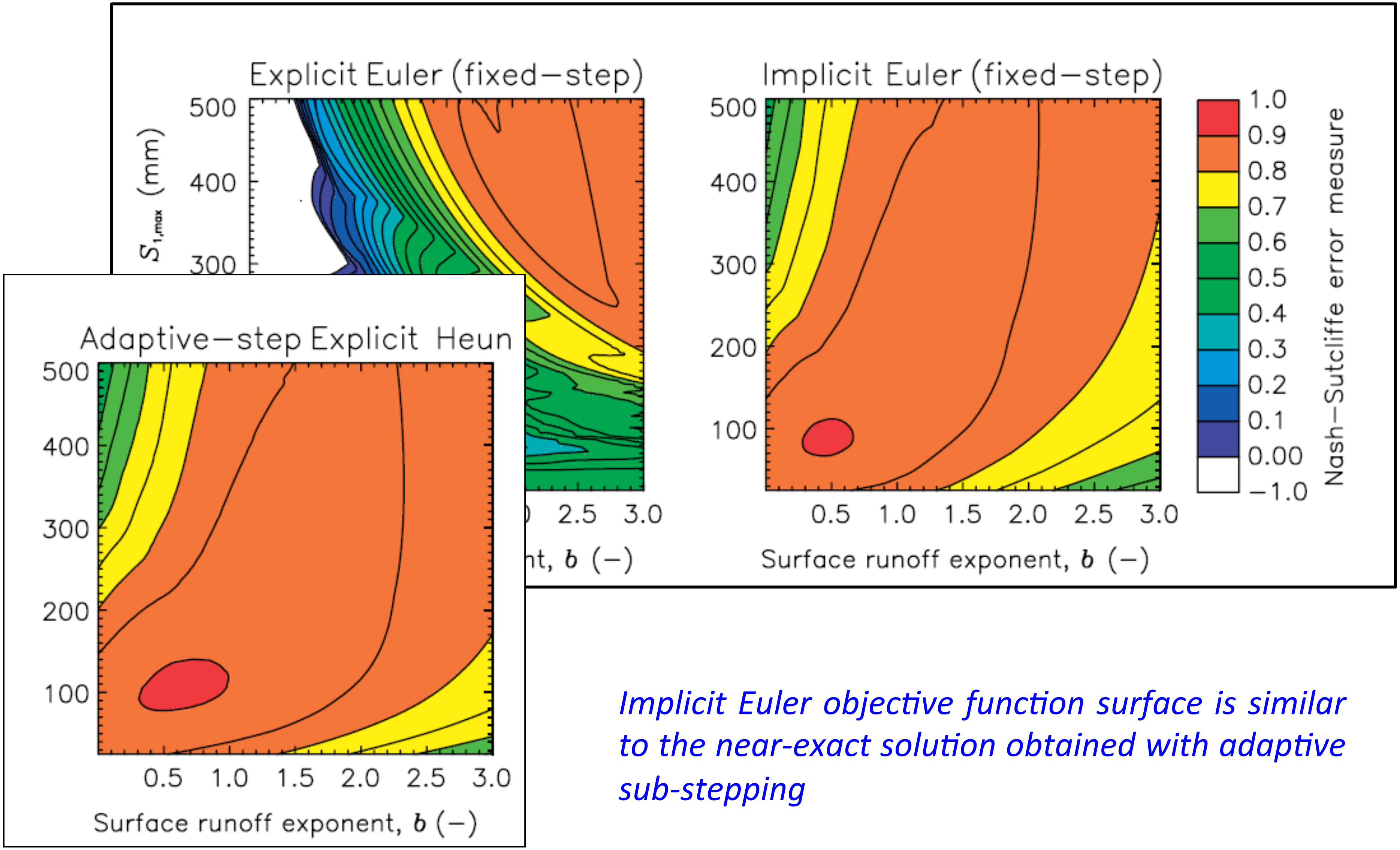
## Ancient numerical daemons of conceptual hydrological modeling: 1. Fidelity and efficiency of time stepping schemes

Martyn P. Clark[1] and Dmitri Kavetski[2]

Received 12 November 2009; revised 22 March 2010; accepted 16 April 2010; published 8 October 2010.

[1] A major neglected weakness of many current hydrological models is the numerical method used to solve the governing model equations. This paper thoroughly evaluates several classes of time stepping schemes in terms of numerical reliability and computational efficiency in the context of conceptual hydrological modeling. Numerical experiments are carried out using 8 distinct time stepping algorithms and 6 different conceptual rainfall-runoff models, applied in a densely gauged experimental catchment, as well as in 12 basins with diverse physical and hydroclimatic characteristics. Results show that, over vast regions of the parameter space, the numerical errors of fixed-step explicit schemes commonly used in hydrology routinely dwarf the structural errors of the model conceptualization. This substantially degrades model predictions, but also, disturbingly, generates fortuitously adequate performance for parameter sets where numerical errors compensate for model structural errors. Simply running fixed-step explicit schemes with shorter time steps provides a poor balance between accuracy and efficiency: in some cases daily-step adaptive explicit schemes with moderate error tolerances achieved comparable or higher accuracy than 15 min fixed-step explicit approximations but were nearly 10 times more efficient. From the range of simple time stepping schemes investigated in this work, the fixed-step implicit Euler method and the adaptive explicit Heun method emerge as good practical choices for the majority of simulation scenarios. In combination with the companion paper, where impacts on model analysis, interpretation, and prediction are assessed, this two-part study vividly highlights the impact of numerical errors on critical performance aspects of conceptual hydrological models and provides practical guidelines for robust numerical implementation.

# Impact on the objective function surface

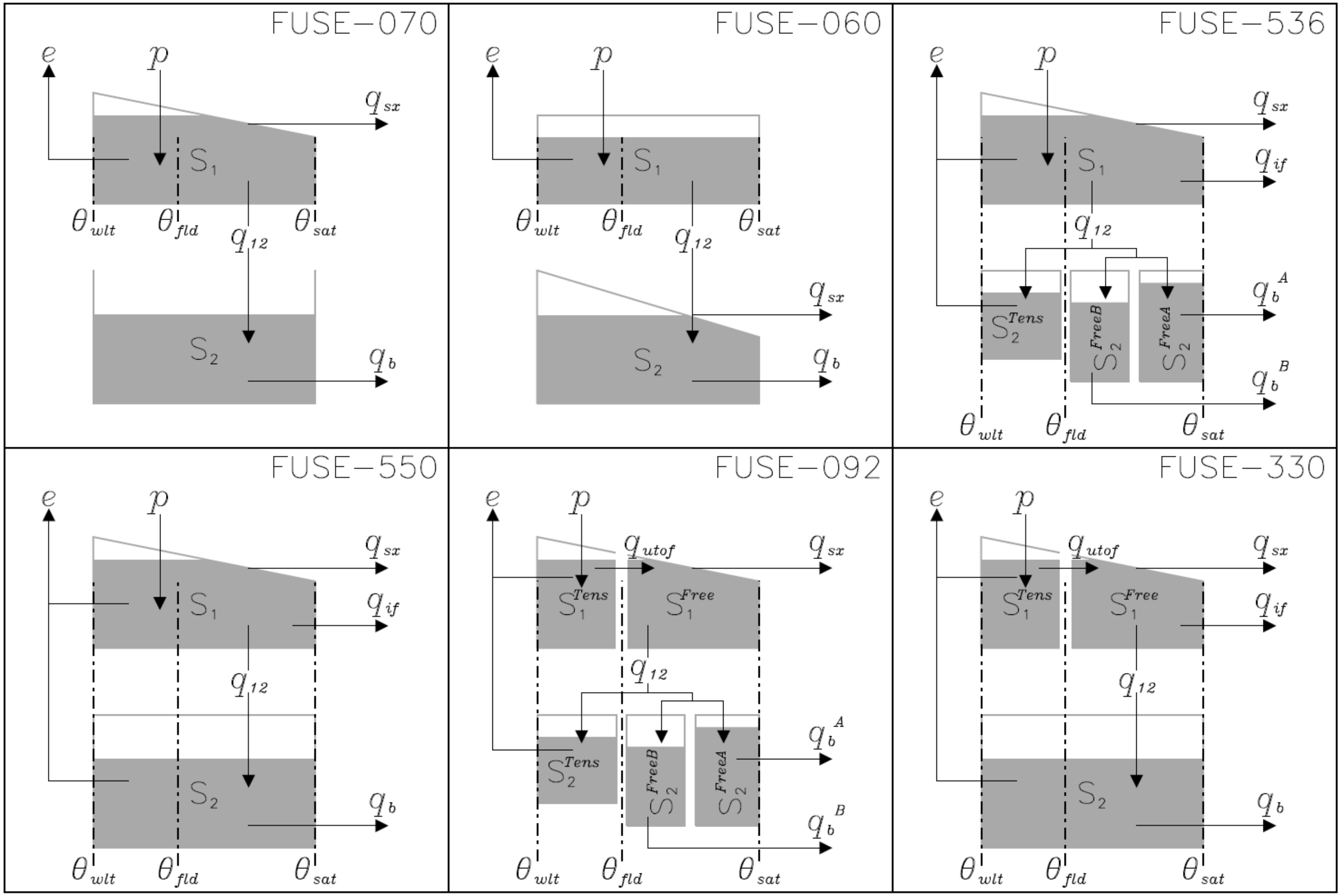


*Implicit Euler objective function surface is similar to the near-exact solution obtained with adaptive sub-stepping*

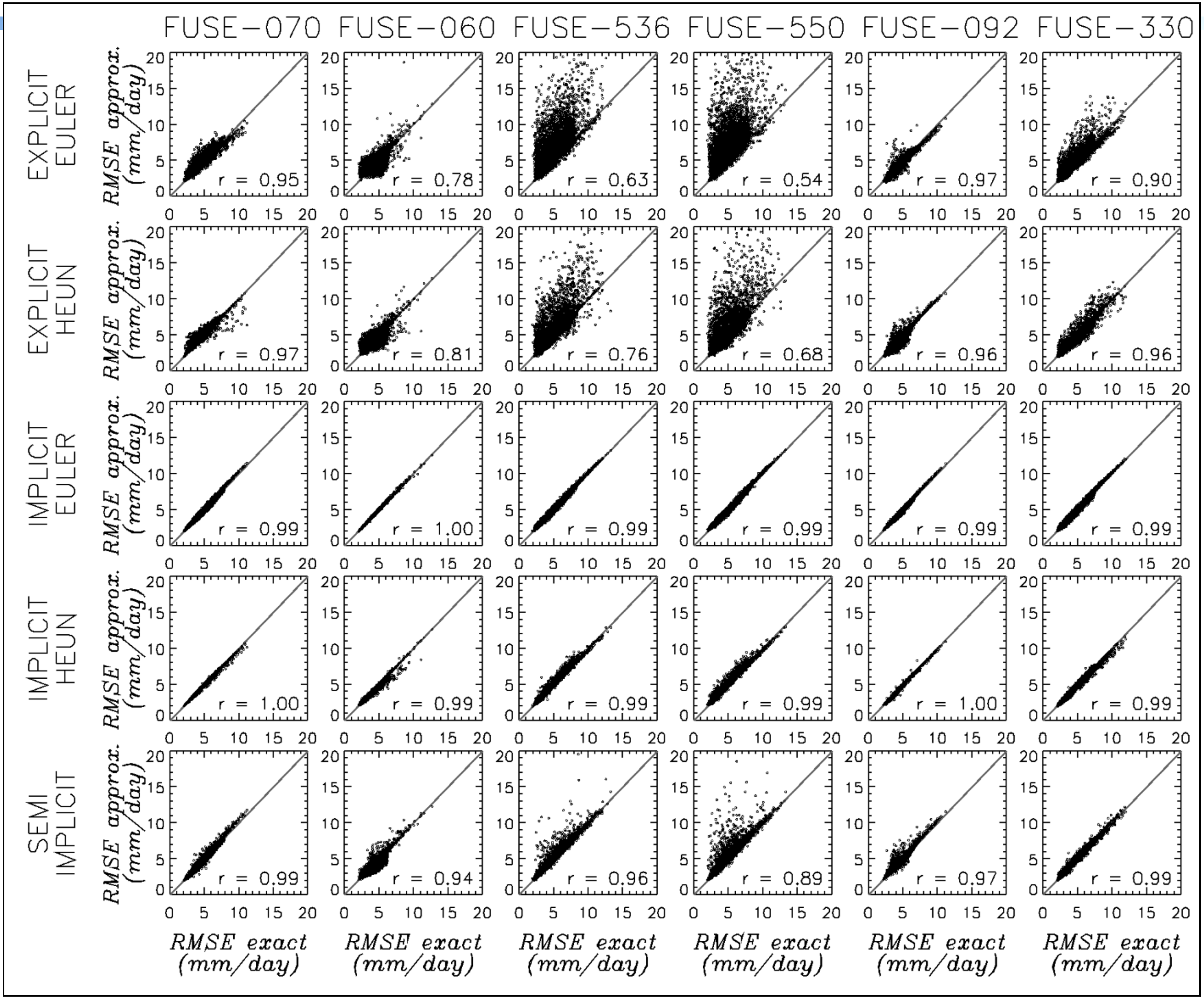
# Outline

- The ingredients of a model
- Solving model equations (temporal integration of state equations)
- Impact of numerical solution on model simulations
- A modular approach to model construction

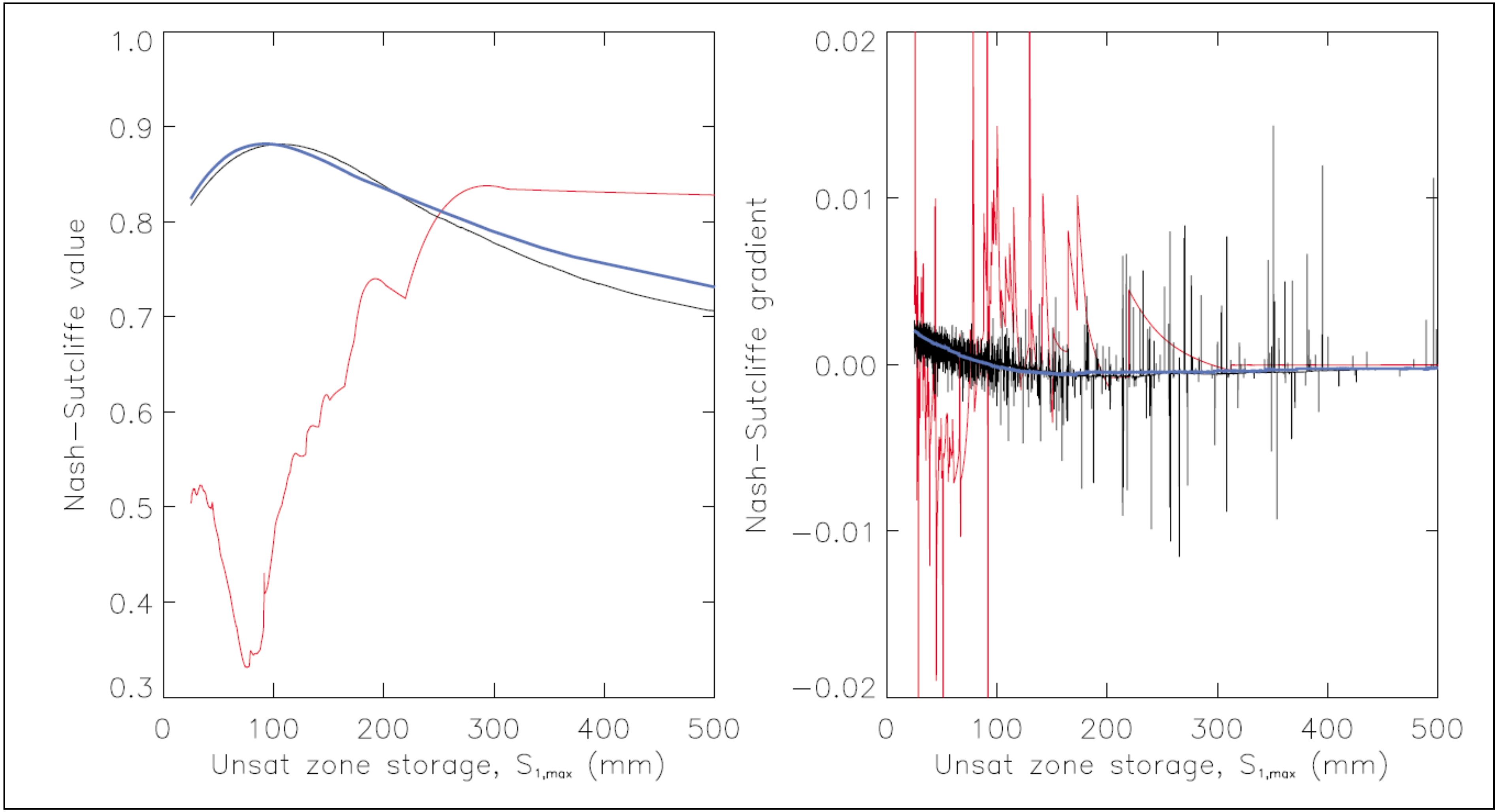
# Six simple "bucket-style" models



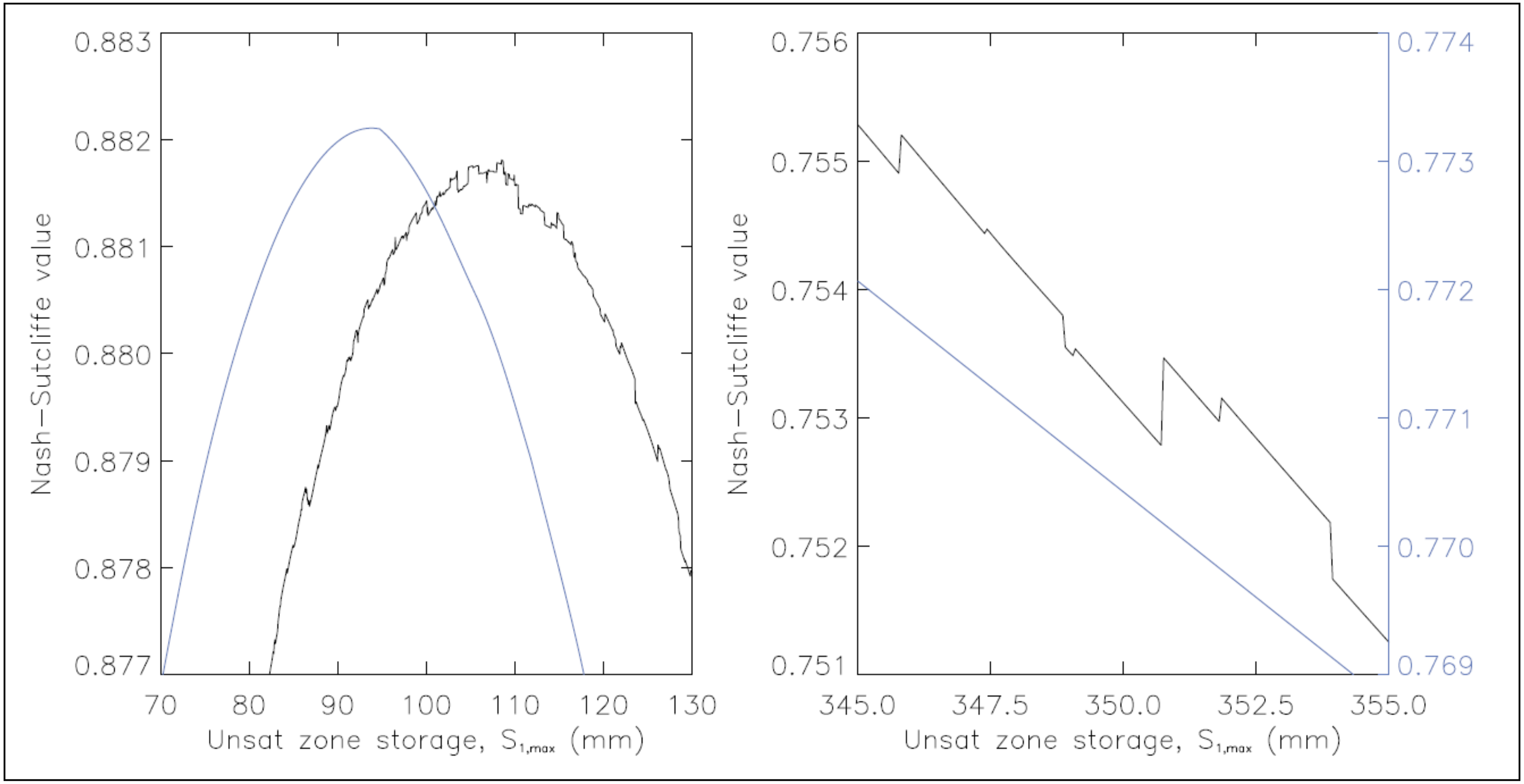
# Fidelity of fixed-step time stepping schemes



# More detail: objective function x-sections

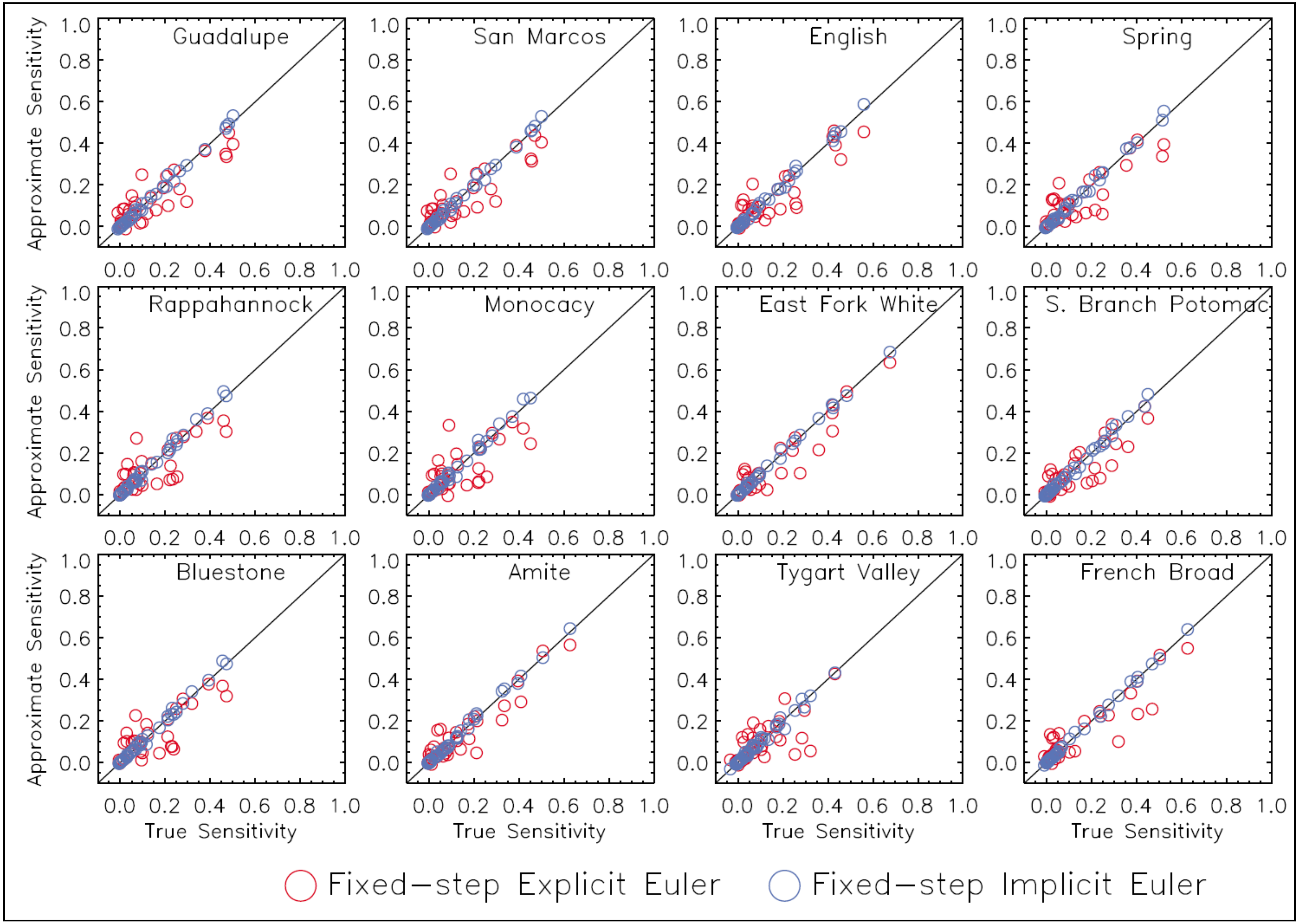


# Zooming in: micro-scale roughness



# Macro-scale roughness

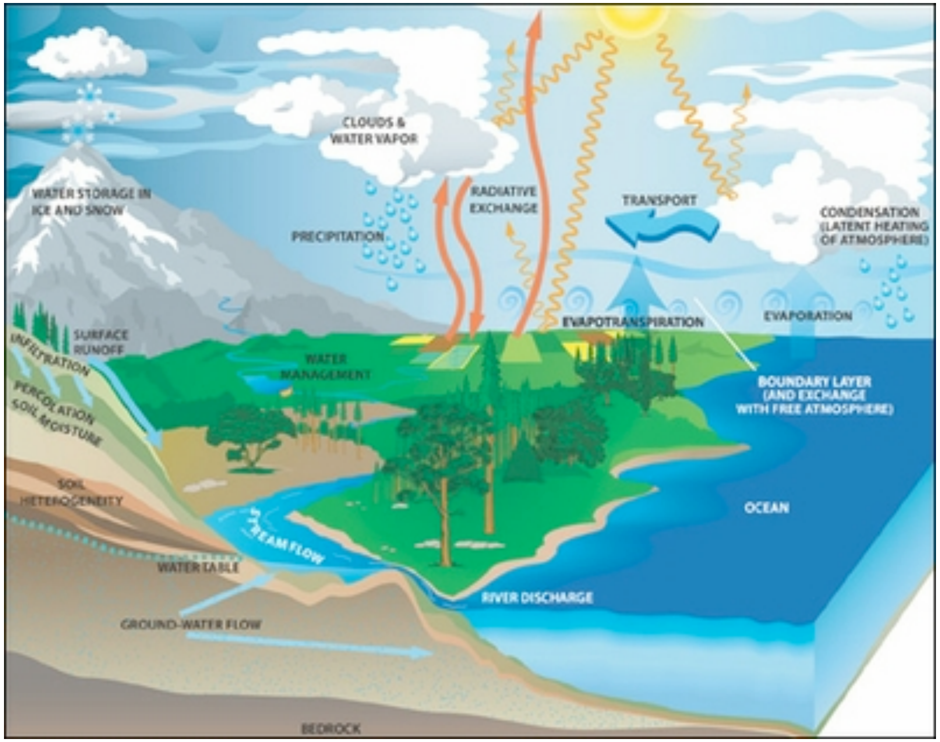
contaminates sensitivity analyses



# Outline

- The ingredients of a model
- Solving model equations (temporal integration of state equations)
- Impact of numerical solution on model simulations
- A modular approach to model construction

# Development of a unifying model framework



*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

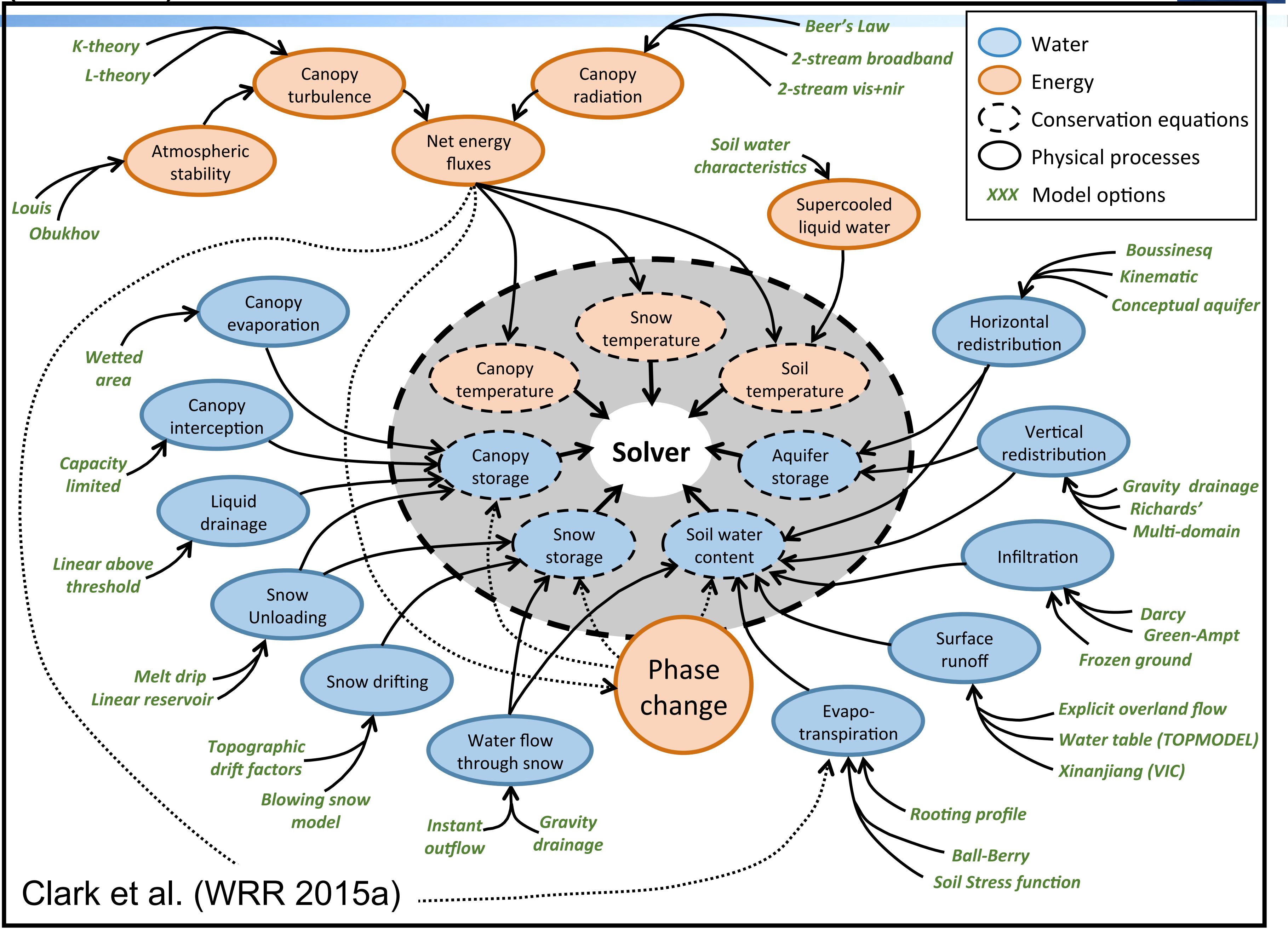
2. Differences among models relate to
   a) the spatial discretization of the model domain;
   b) the approaches used to parameterize individual fluxes (including model parameter values); and
   c) the methods used to solve the governing model equations.

## *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)

# The Structure for Unifying Multiple Modeling Alternatives (SUMMA)



Water

Energy

Conservation equations

Physical processes

*XXX* Model options

*K-theory*

*L-theory*

Canopy turbulence

Atmospheric stability

*Louis*

*Obukhov*

Net energy fluxes

Canopy radiation

*Beer's Law*

*2-stream broadband*

*2-stream vis+nir*

*Soil water characteristics*

Supercooled liquid water

*Boussinesq*

*Kinematic*

*Conceptual aquifer*

Horizontal redistribution

Canopy evaporation

*Wetted area*

Canopy interception

*Capacity limited*

Liquid drainage

*Linear above threshold*

Snow Unloading

*Melt drip*

*Linear reservoir*

Snow drifting

*Topographic drift factors*

*Blowing snow model*

Water flow through snow

*Instant outflow*

*Gravity drainage*

Snow temperature

Canopy temperature

Soil temperature

**Solver**

Canopy storage

Aquifer storage

Snow storage

Soil water content

Phase change

Vertical redistribution

*Gravity drainage*

*Richards'*

*Multi-domain*

Infiltration

*Darcy*

*Green-Ampt*

*Frozen ground*

Surface runoff

*Explicit overland flow*

*Water table (TOPMODEL)*

*Xinanjiang (VIC)*

Evapo-transpiration

*Rooting profile*

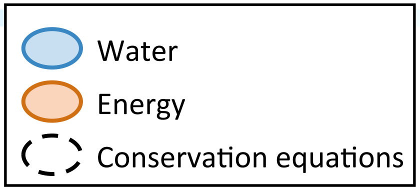
*Ball-Berry*

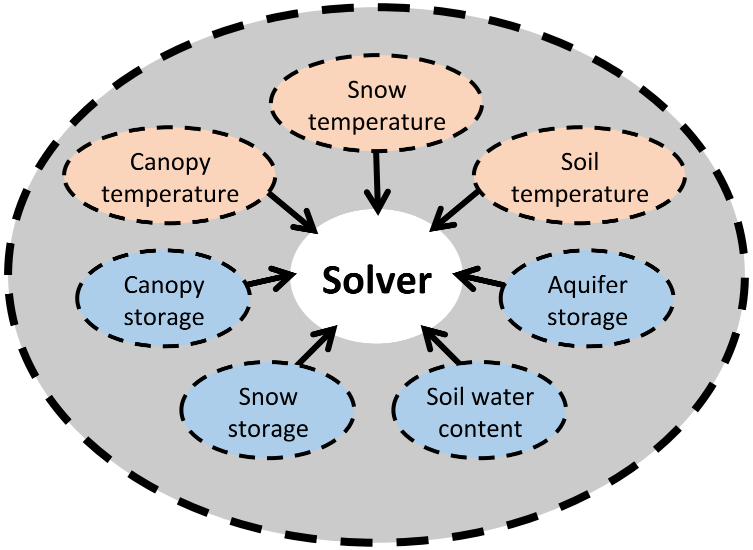
*Soil Stress function*

Clark et al. (WRR 2015a)

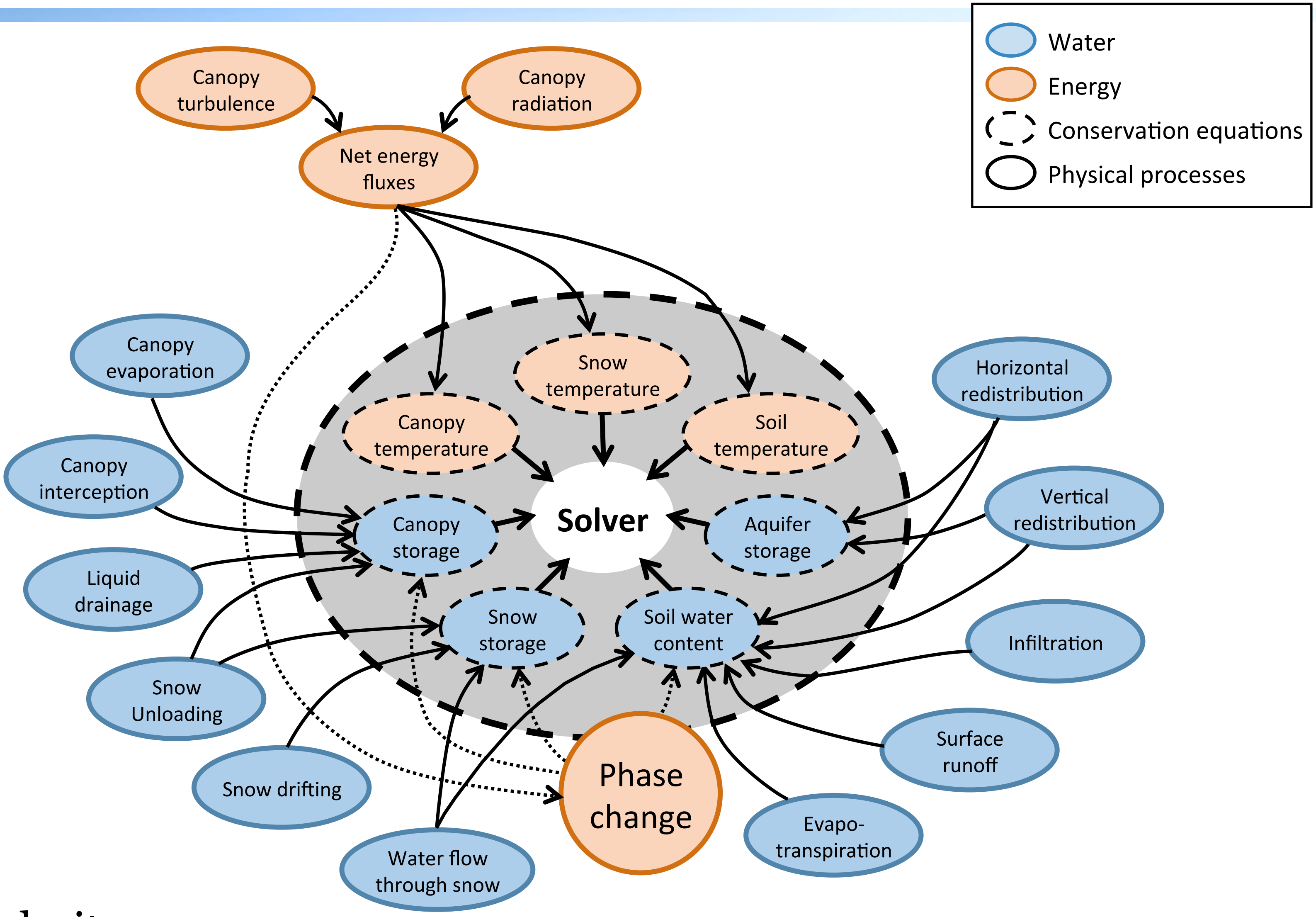
# Model construction

- Numerical solution
  - Traditional approach in land modeling: Operator splitting
  - SUMMA: Fully coupled implicit solution



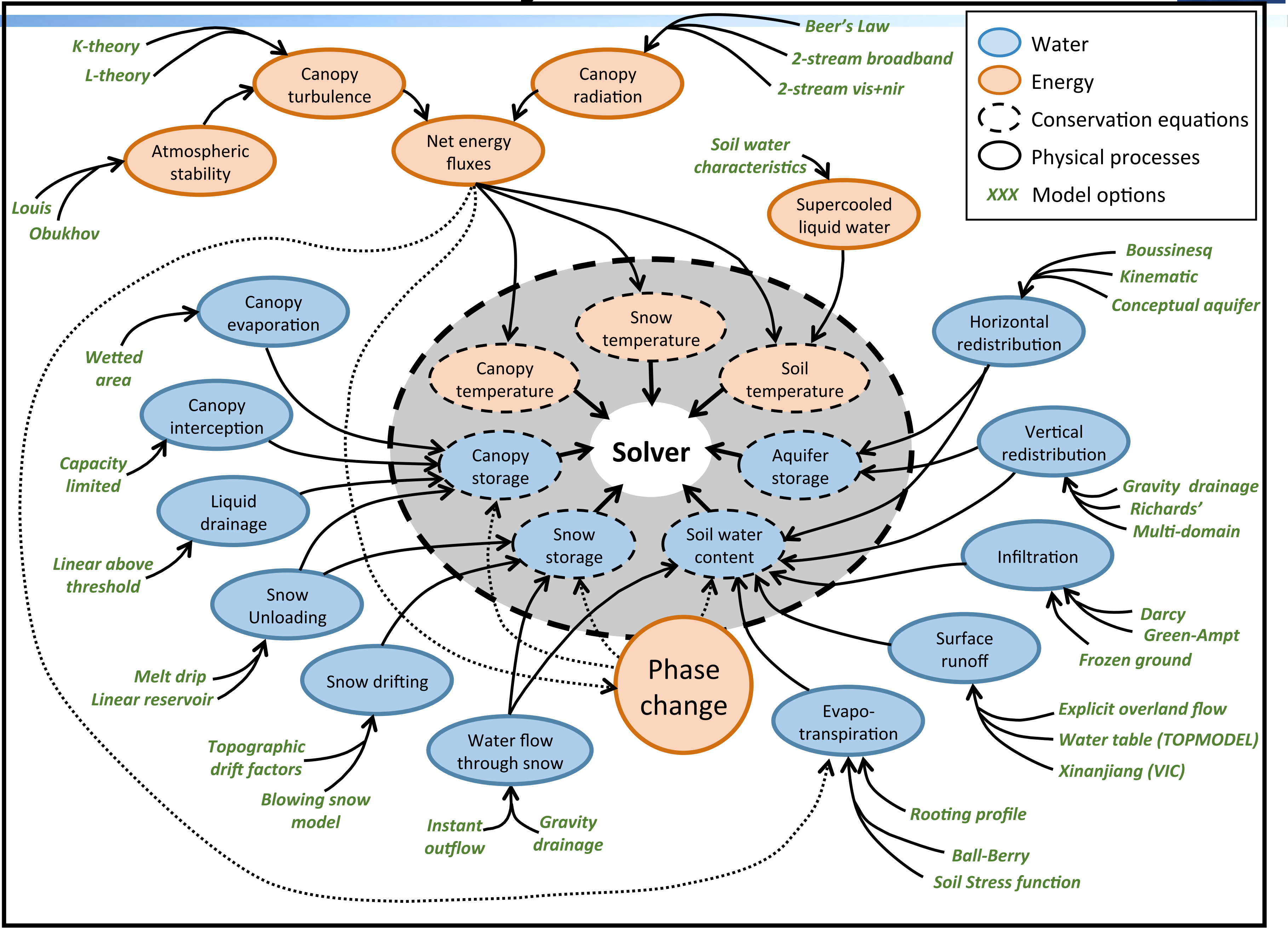


# Model construction



- Modularity
  - Modularity at the level of individual fluxes
  - Separation of physical processes and the numerical solution greatly simplifies adding new modeling options

# Process flexibility



K-theory

L-theory

Canopy turbulence

Canopy radiation

Beer's Law

2-stream broadband

2-stream vis+nir

Atmospheric stability

Louis

Obukhov

Net energy fluxes

Soil water characteristics

Supercooled liquid water

🔵 Water

🟠 Energy

◌ Conservation equations

○ Physical processes

*XXX* Model options

Boussinesq

Kinematic

Conceptual aquifer

Horizontal redistribution

Canopy evaporation

Wetted area

Snow temperature

Canopy temperature

Soil temperature

Canopy interception

Capacity limited

Canopy storage

**Solver**

Aquifer storage

Vertical redistribution

Gravity drainage

Richards'

Multi-domain

Liquid drainage

Linear above threshold

Snow storage

Soil water content

Infiltration

Darcy

Green-Ampt

Frozen ground

Snow Unloading

Melt drip

Linear reservoir

Snow drifting

Topographic drift factors

Blowing snow model

Phase change

Surface runoff

Explicit overland flow

Water table (TOPMODEL)

Xinanjiang (VIC)

Water flow through snow

Instant outflow

Gravity drainage

Evapo-transpiration

Rooting profile

Ball-Berry

Soil Stress function

# Modeling requirements

- Scientific requirements
  - Process flexibility
  - Spatial flexibility
  - Numerical flexibility
- User requirements
  - Can be configured to meet a broad range of requirements
  - Can be configured to minimize run time, and enable use of ensembles and extensive model analysis
  - Easy to modify
- Existing multiple hypothesis frameworks meet these requirements to varying degrees
  - JULES, CLM, Noah-MP, etc.

# Summary

- The numerical implementation matters
  - Numerical errors are not “overwhelmed” by other uncertainties
  - Numerical errors can contaminate almost every aspect of model analysis and prediction

- Relatively simple numerical solutions provide effective and efficient solutions in land models
  - Stability issues
  - Order of operations

- The next generation of land models should separate the physics from the numerical implementation, and provide modularity at the level of individual processes (easier for the community to engage).

# QUESTIONS??