Upscaling Threshold Nonlinearities in Distributed Surface Water Models

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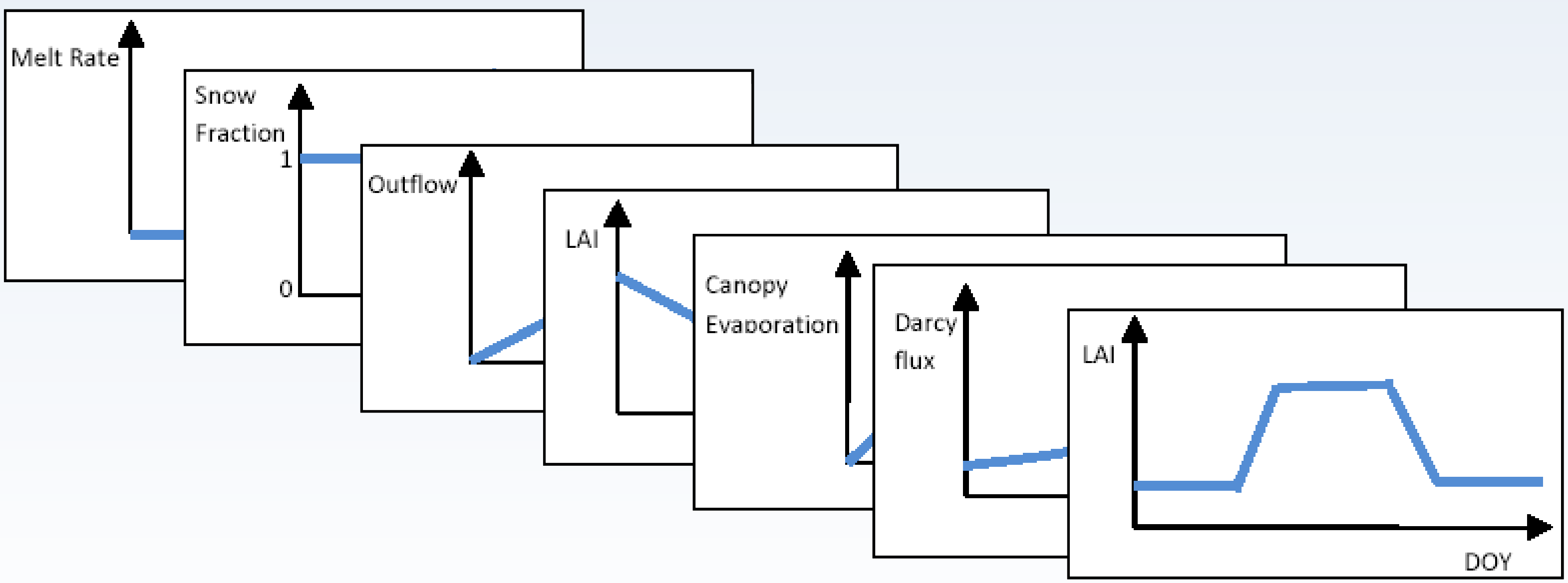
Problem Statement

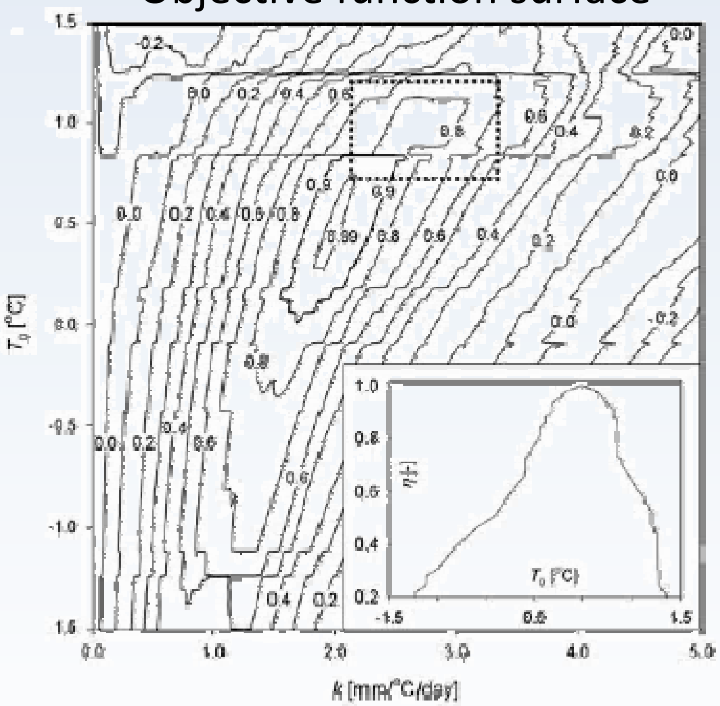
- Threshold non-linearities are ubiquitous in numerical surface water models
  - Rate processes and/or state-dependent parameters represented using discontinuous “jump” or “step” functions



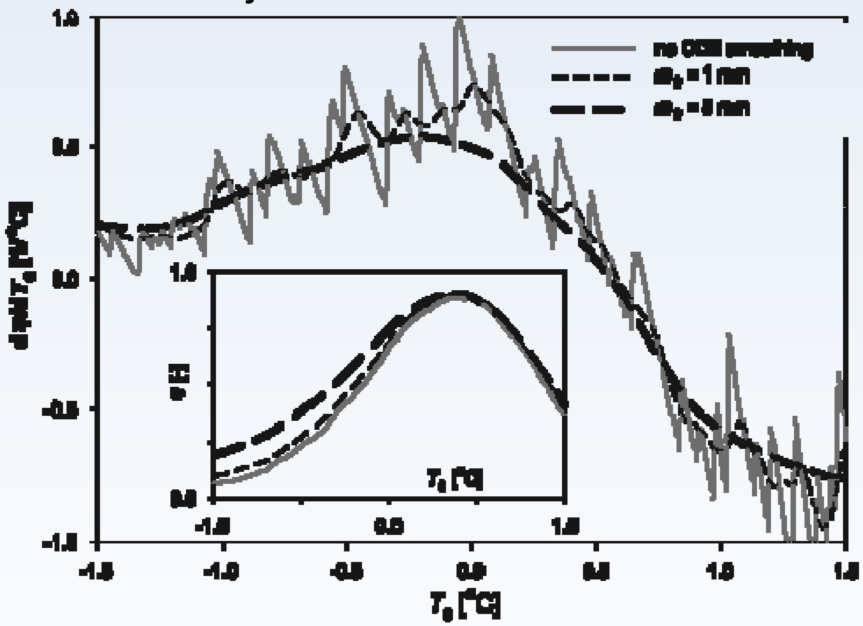
Problem Statement

- It has been demonstrated that threshold non-linearities induce numerical instability and reduce calibration performance (Kavetski & Kuczera, 2007)

Objective function surface



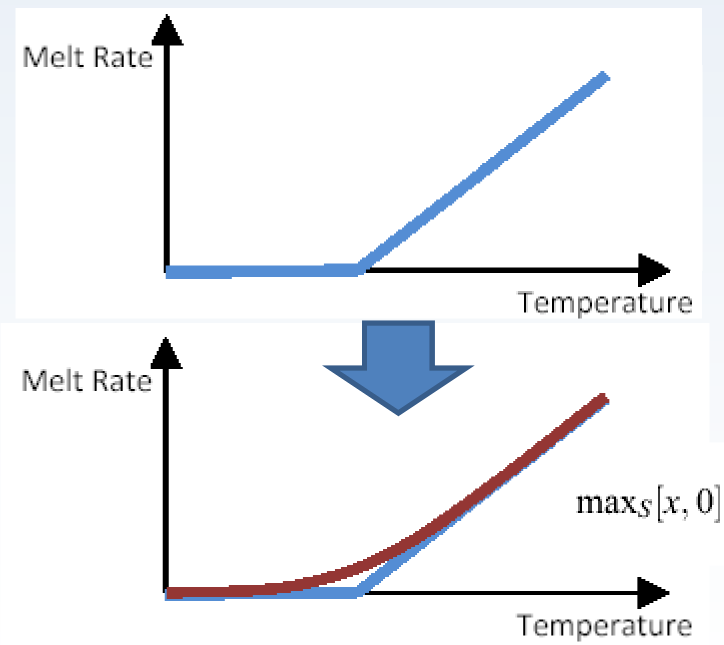
Objective Function Gradient



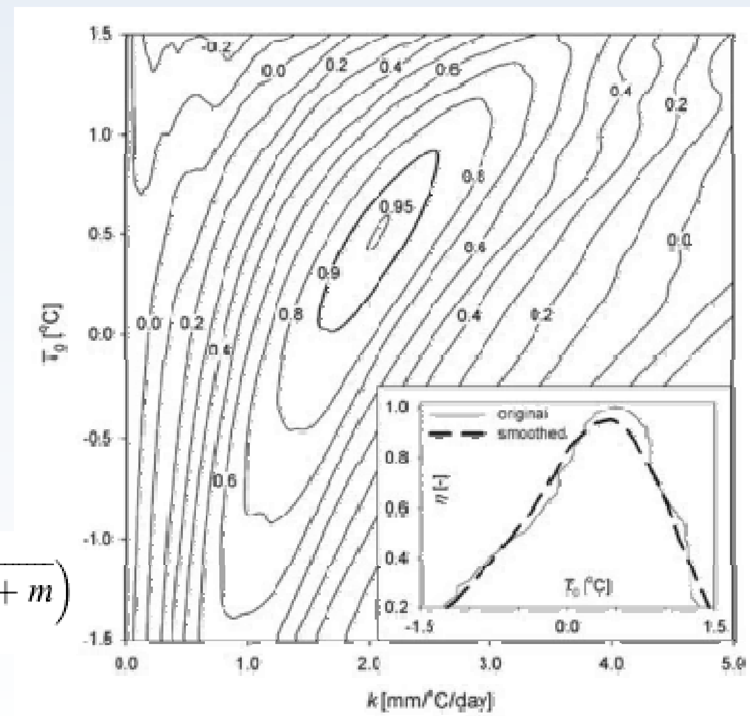
Kavetski, D., and G. Kuczera (2007), Model smoothing strategies to remove microscale discontinuities and spurious secondary optima in objective functions in hydrological calibration, *Water Resour. Res.*, 43, W03411, doi:10.1029/2006WR005195

Numerical Smoothing

- Kavetski & Kuczera (2007) proposed the use of smoothing functions to handle rate discontinuities
  - The goal was to alleviate non-linear artifacts while still respecting the essence of relationships between rate processes and state variables



$$\max_S[x, 0] = \frac{1}{2}\left(x + \sqrt{x^2 + m}\right)$$



Numerical Smoothing

- Benefits:
  - Demonstrated improvement in the objective function structure, and therefore the estimability of model parameters and parameter uncertainties
    - Faster calibration
    - Removal of secondary optima / multimodality
  - More well-behaved models with fewer stability and convergence issues
  - Easy to implement – simple functions
- Detriments:
  - **These smoothing functions were purely numerical in nature and had *no physical basis***

Smoothing: Another approach

- Many surface water component ODEs may be written in the following form:

$$\frac{d\overline{\phi}}{dt} = \sum \pm \overline{M}(t, \vec{\overline{\phi}})$$

- We will here assume that the processes, M, are upscaled from a point process with threshold discontinuities
- By making assumptions about the sub-computational scale variability in parameters, variables, and/or forcing functions we often can estimate effective (mean) rate processes ***analytically***
- ***These mean rate processes are smoother than their point-scale equivalents***

Hypothesis

- Simple area-weighted process upscaling may be used to reduce the non-linearity of surface water models by (analytically) smoothing out discontinuities
- Smoothing Advantages:
  - Improves stability
  - Improves calibration performance
  - Easy to implement (once derived*)
  - Quickly calculated
- Upscaling Advantages:
  - Physically-based*
  - Recognizes and incorporates sub-HRU variability*
- Disadvantages:
  - Relies on assumptions about sub-computational-scale distributions

A simple example:
Degree-day snowmelt

- The simplest degree-day snow melt model (assumed to be valid at the point scale):

$$M(S,T) = \begin{cases} M_a \cdot (T - T_f) & \text{if } \boxed{T > T_f} \text{ and } \boxed{S > 0} \\ 0 & \text{otherwise} \end{cases}$$

Or, equivalently:

$$M(S,T) = M_a \cdot (T - T_f) \cdot H(T - T_f) \cdot H(S)$$

- Averaged melt rates may be calculated by assuming the frequency distributions of temperature and snow depth:

$$\overline{M} = \frac{1}{A}\int_A M(S,T)dA = \int_{-\infty}^{\infty} M f_M(M)dM = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} M(S,T) \cdot f_{ST}(S,T)dTdS$$

A simple example: Degree-day snowmelt

- T… …del (a…

Disclaimer:

The following research is not an endorsement of, nor an advertisement for, the standard or modified degree-day snow model as a representative of point-scale melt processes. The opinions shared here are not necessarily those of the University of Waterloo, and the authors recognize the superiority of alterative, physically-based snow models that may include a full energy balance, sublimation, radiative transfer, lateral transport, freezing/thawing, albedo, and/or canopy influences.

- A… …he fr… …th:

$$\overline{M} = \frac{1}{A}\int_A M(S,T)\,dA = \int_{-\infty} M f_M(M)\,dM = \int_{-\infty}\int_{-\infty} M(S,T)\cdot f_{ST}(S,T)\,dT\,dS$$

Upscaling

Temperature:
Normally distributed

$$f_T(T) = \frac{1}{\sqrt{\sigma_T 2\pi}} \exp\left(-\frac{(T-\overline{T})^2}{2\sigma_T^2}\right)$$

Snow depth:
3-parameter log-normally distributed

$$f_S(S) = \frac{1}{(S-S_0)\sigma_S\sqrt{2\pi}} \exp\left(-\frac{(\ln(S-S_0)-\ln(\overline{S}))^2}{2\sigma_S^2}\right)$$

$$\overline{M} = M_a \cdot \left[\left[\frac{1}{2}(\overline{T}-T_f)\,\text{erfc}\left(-\frac{(\overline{T}-T_f)}{\sqrt{2\sigma_T^2}}\right) + \frac{\sigma_T}{\sqrt{2\pi}} \exp\left(-\frac{(\overline{T}-T_f)^2}{2\sigma_T^2}\right)\right]\right] \left[\frac{1}{2}\,\text{erfc}\left(\frac{1}{\sqrt{2}\sigma_S} \ln\left(-\frac{S_0}{\overline{S}}\right)\right)\right]$$

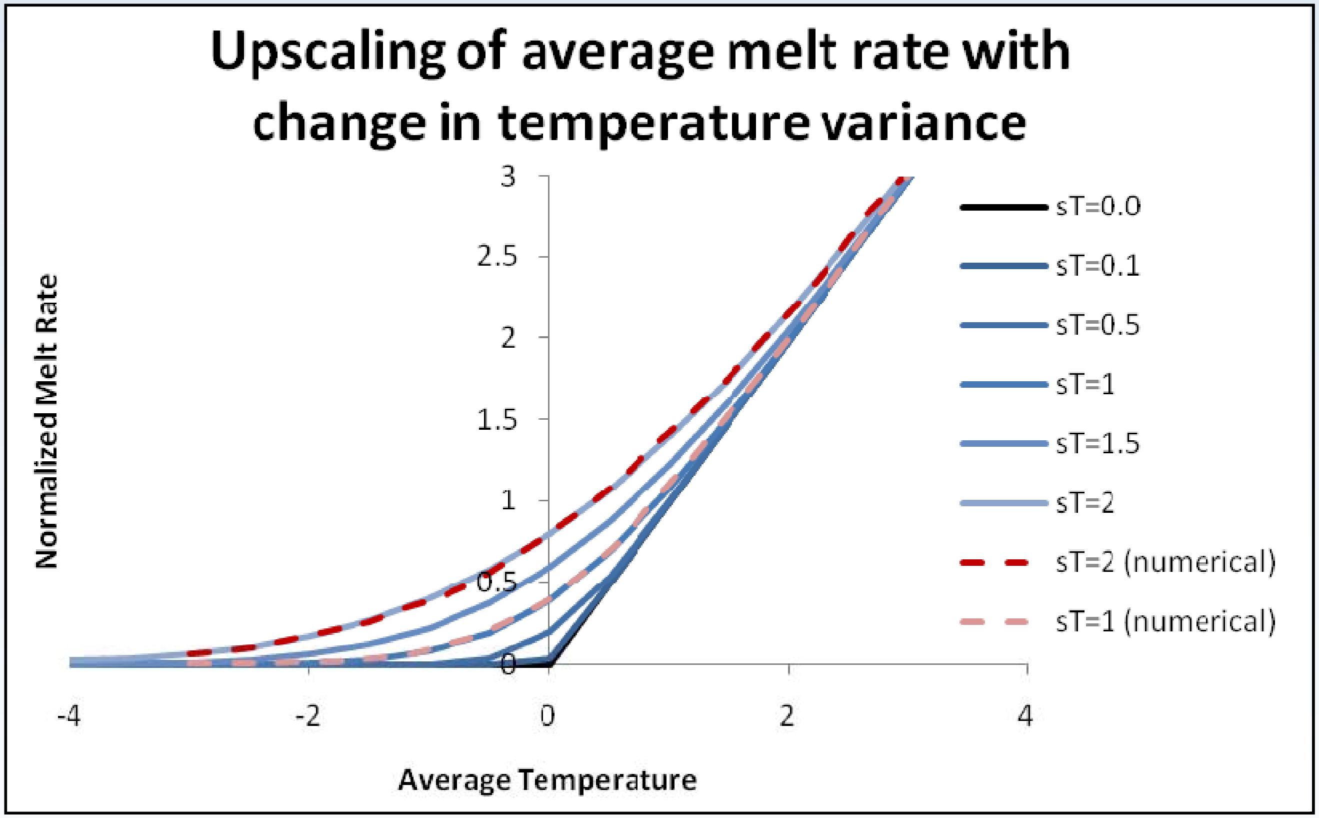
Percentage of snow-covered ground, F_S

Averaged melt rate over computational unit

A simple function of
- average temperature
- average snow depth
- distribution parameters

-Reverts to point scale when $\sigma_S=\sigma_T=0$

Smoothing Effect of Upscaling

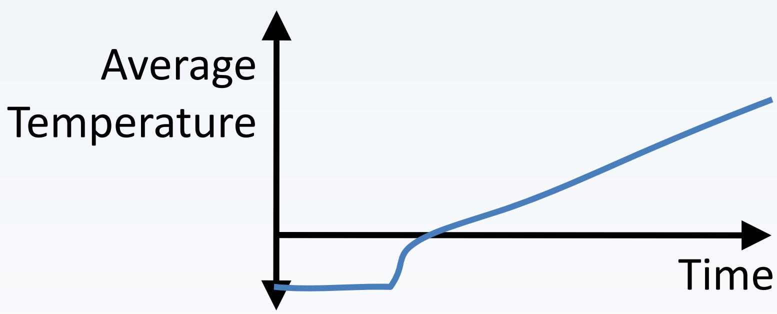


Testing

1 parcel
(traditional approach)

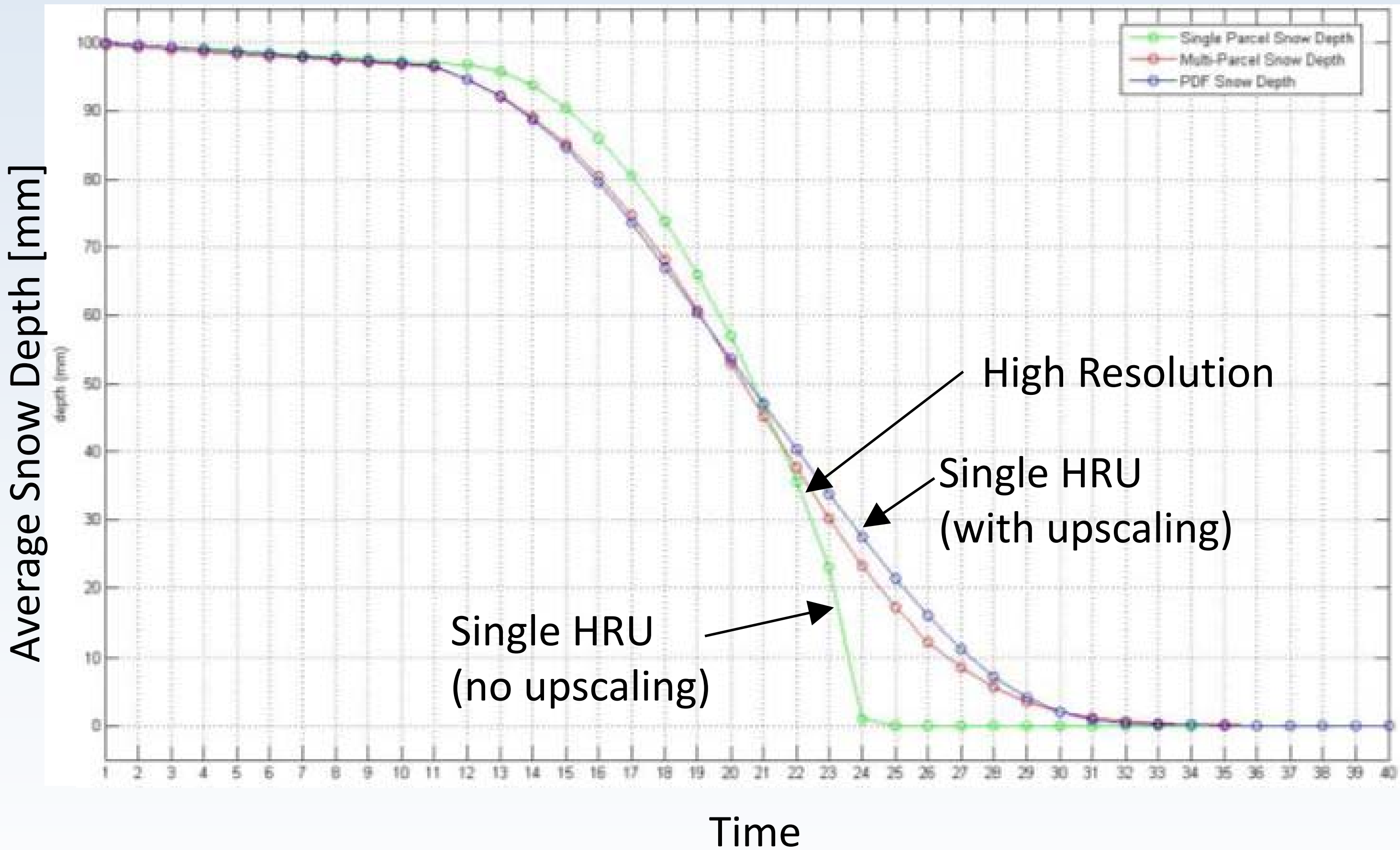
1 parcel
(upscaled approach)

10,000 parcels
Lognormal depth



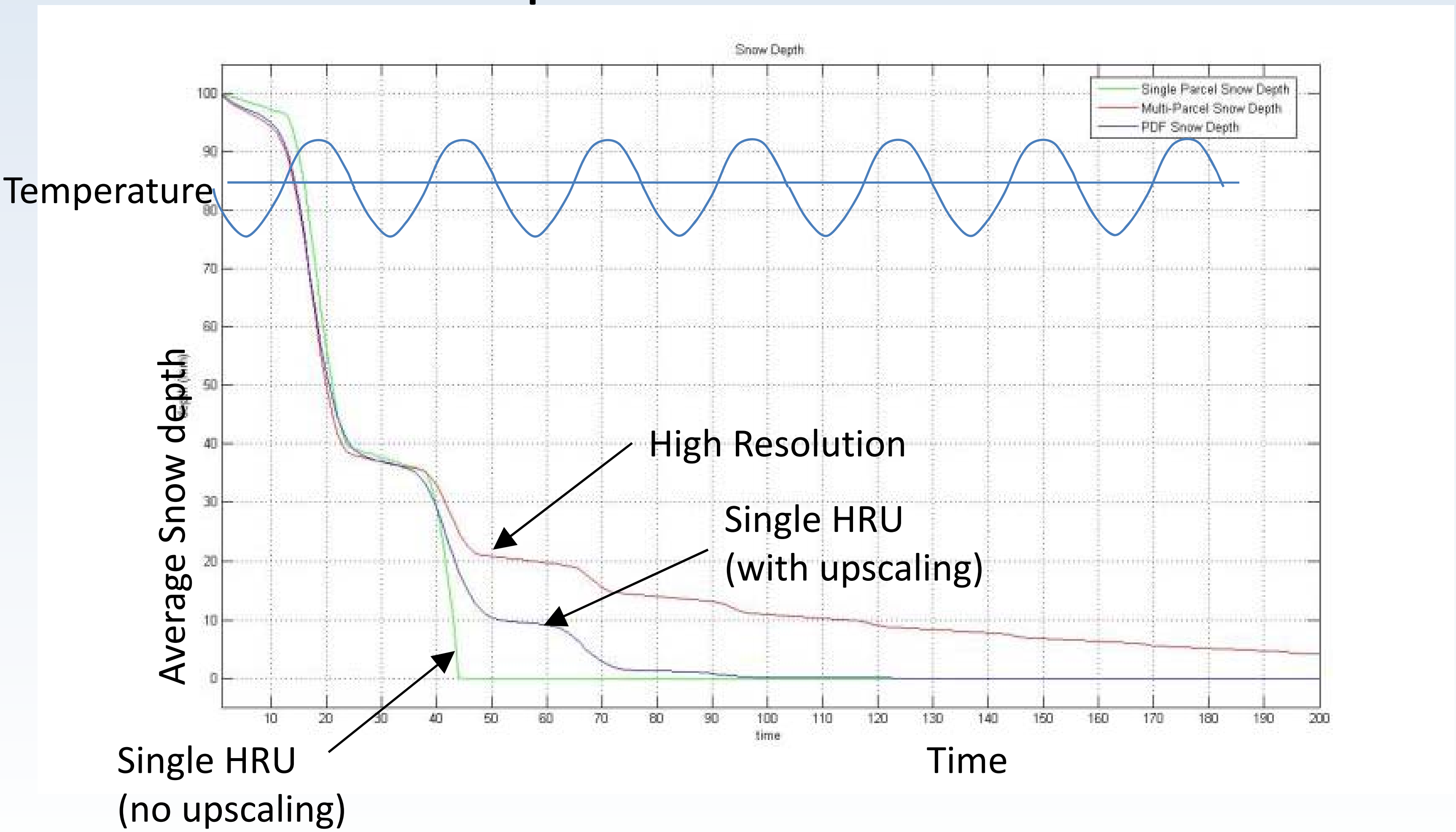
snowdepth.avi

Testing


Single Parcel Snow Depth
Multi-Parcel Snow Depth
PDF Snow Depth
High Resolution
Single HRU
(with upscaling)
Single HRU
(no upscaling)
Average Snow Depth [mm]
Time

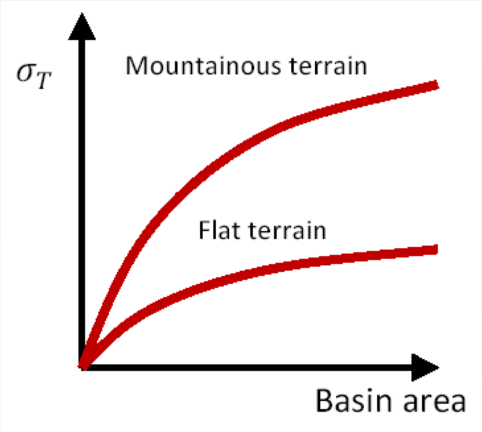
Testing

- Sinusoidal temperature variation:



Data needs

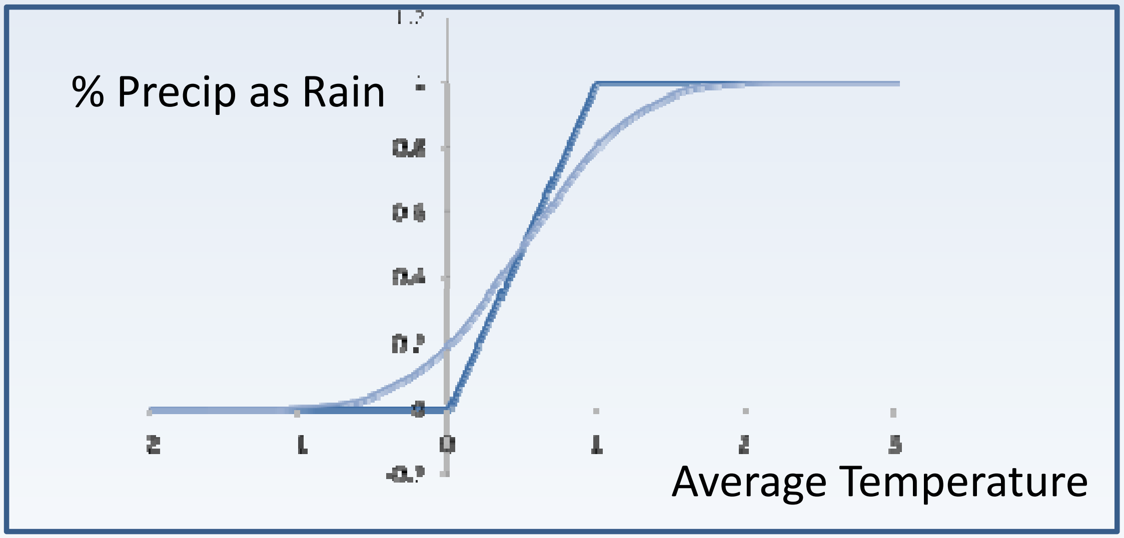
- In order to effectively use this approach, information regarding property and state variable distributions is needed
  - Empirical, generalizable relationships for distribution parameters as a function of scale



  - Understanding of evolution of distribution parameters over time

Extensions

- Similar upscaling methods can be applied to rates controlled by any forcing function or state variable with infinite limits



- Bounded variables require special attention (the math is a bit trickier)

Conclusions

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- A physically-based argument has been provided for threshold smoothing
  - Simple analytical upscaling approaches may improve calibration, stability, *and* accuracy of numerical models
  - Purely numerical smoothing parameters (Kavetski and Kuczera, 2007) replaced with measurable physical quantities
- Challenges arise from assumptions about correlation, distributions, etc. at the sub-computational scale
  - Despite imperfections, even naïve upscaling appears to be an improvement over the standard approach
  - Benefits of smoothing remain regardless of upscaling accuracy
- The next step is try to apply these methods to more sophisticated process models (e.g., a full energy balance model), address parameter correlation, etc.