Vadose Zone Problem: Parameter Estimation Using Pedotransfer Functions and Inverse Modeling

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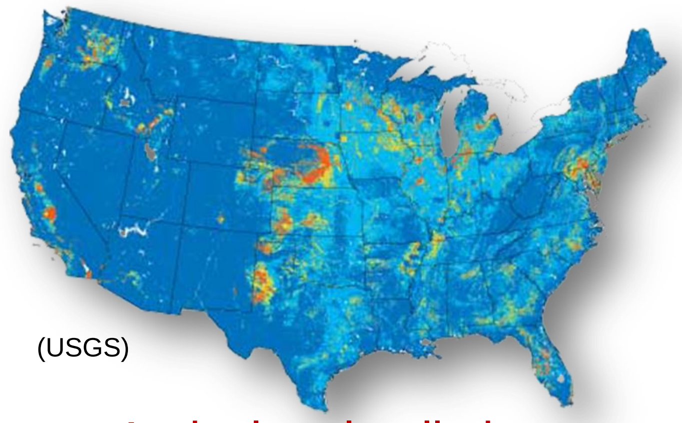
New Orleans, December 10, 2017

Unsaturated Zone (Vadose Zone) Problems

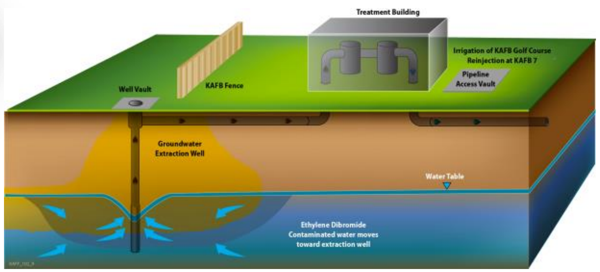
(Van Looy et al)

Crop yield



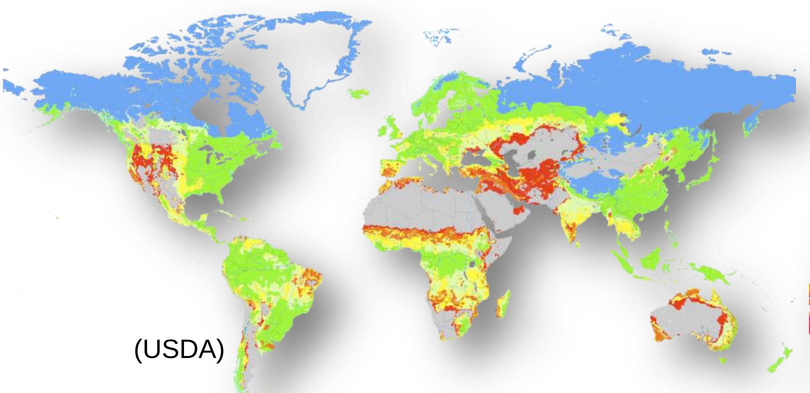
(USGS)

Agricultural pollution



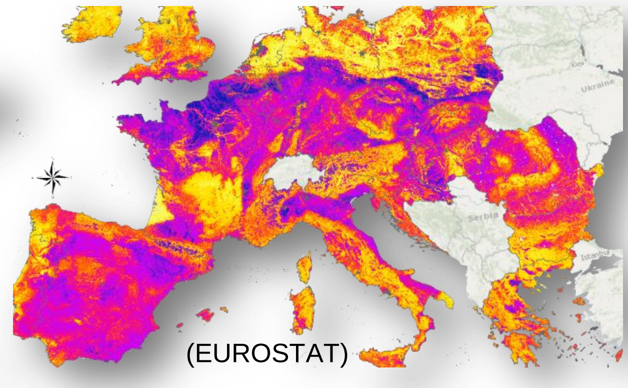
(www.env.nm.gov)

Soil remediation



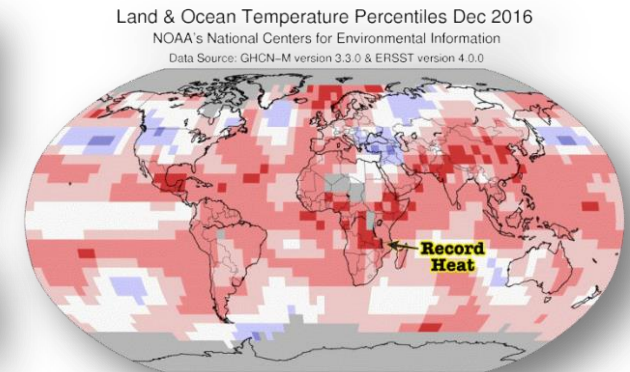
(USDA)

Flood & Drought



(EUROSTAT)

Water loss & soil erosion



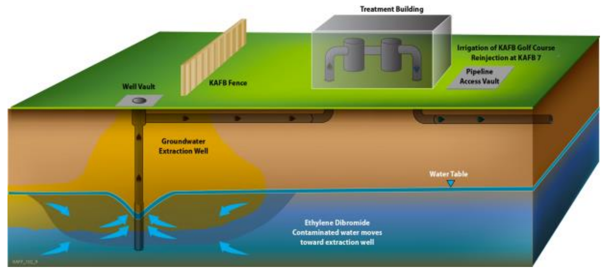
(NOAA)

Global warming

Motivation

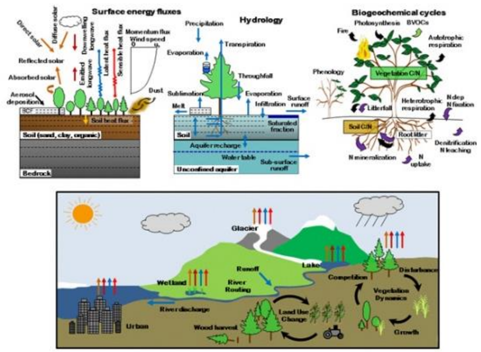
(From Van Looy et al)

water and solute transport



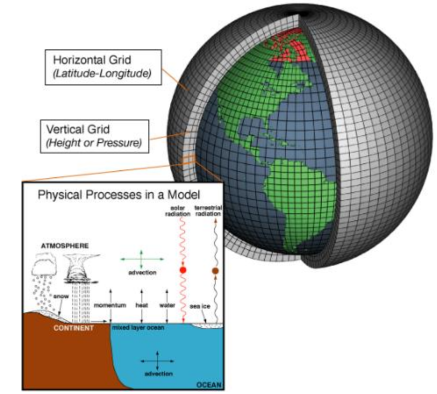
(www.env.nm.gov)

Soil remediation



(from NCAR)

Land Surface Model



(from NOAA)

Global Climate Model

- Modeling of unsaturated flow and transport processes requires the spatial distribution of the **soil hydraulic properties**.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta) \left(\frac{\partial h(\theta)}{\partial z} - 1 \right) \right] - S(\theta)$$ (1D Richards equation)

where θ is soil volumetric moisture content [L^3/L^3]; t is time [T]; h is soil water pressure head [L],

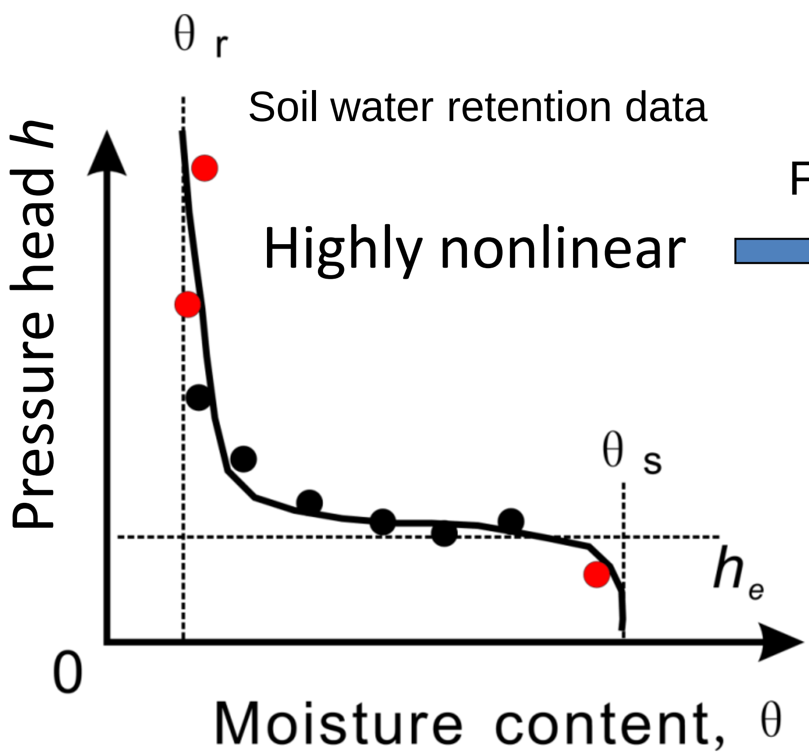
$K_{unsat}(h)$ is unsaturated hydraulic conductivity [L/T];

x and y are the horizontal coordinate [L]; z is the vertical coordinate,

and S is the source-sink term [T^{-1}]

Motivation

- Direct measurement procedures:



Fit

Soil water retention functions:

van Genuchten model (1980）

$$\theta(h)=\theta_r+\frac{\theta_s-\theta_r}{\left[1+|\alpha h|^{n}\right]^{m}} \qquad m=1-1/n$$

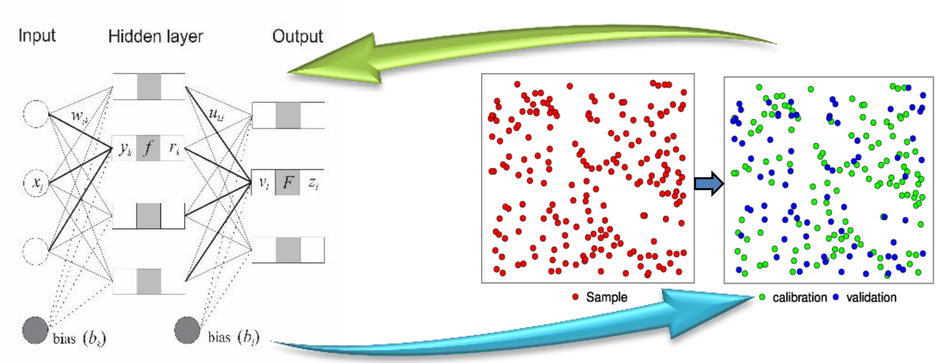
VG-*Mualem*（1976）to describe unsaturated hydraulic conductivities

$$K_{unsat}(\theta)=K_{sat}K_{rel}(\theta)=K_{sat}\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{0.5}\left\{1-\left[1-\left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right)^{1/m}\right]^{m}\right\}^{2}$$

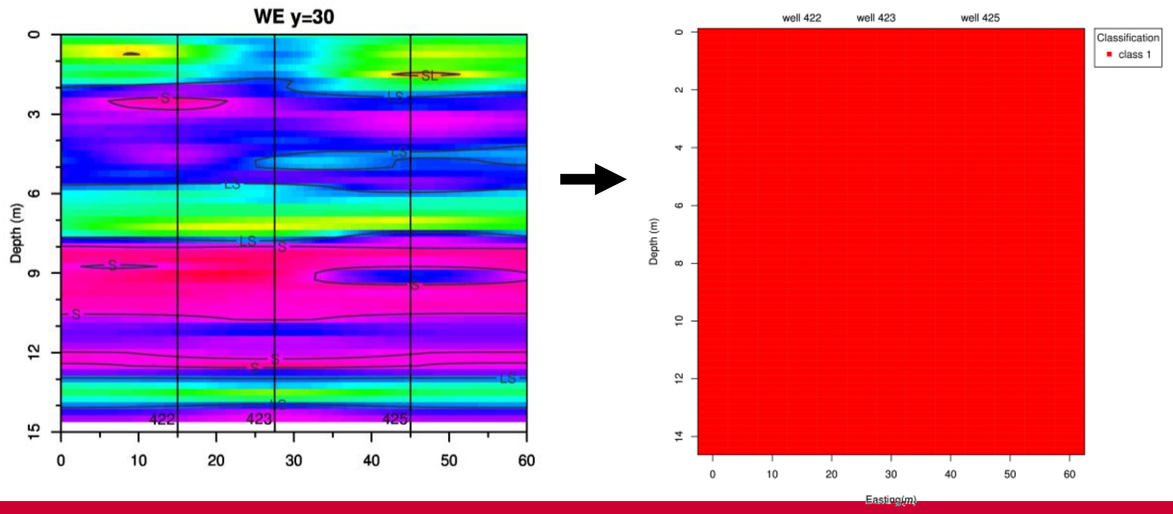
- Direct measurement is expensive, difficult, and time consuming, especially for deep vadose zones.
- Pedotransfer functions and/or inverse modeling are attractive.

New Rosetta and Inverse Modeling

- ❑ Part I: An Improved Rosetta Pedotransfer Function



- ❑ Part II: Inverse Modeling Using PTFs and Clustering



Part I: Pedotransfer Functions and Improved Rosetta

Easy to obtain

‚Standard' soil properties

Texture

Porosity

Soil minerals

(% sand, clay)

Organic matter

Bulk density

PedoTransfer Function

~

Difficult to obtain

- **Hydraulic parameters**
Moisture retention
Hydraulic conductivity

- **Solute transport parameters**
Strength preferential transport
Solute transport velocity

- **Thermal parameters**
Heat capacity
Thermal conductivity

- **Biogeochemical parameters**
Soil carbon parameterization
Soil mineralization and decomposition parameterization

Methods to establish PTFs: lookup tables, linear/nonlinear regression, neural networks, support vector regression, nearest neighbor methods, regression trees, et al.

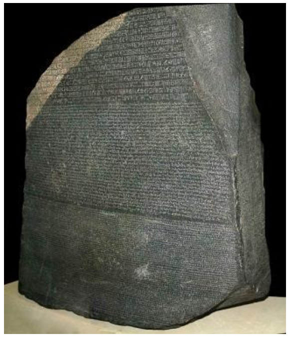
Van Looy et al, Reviews of Geophysics (Accepted)

PTFs to estimate soil hydraulic parameters

PTF	Source	Region	Model	No. of samples	Input				
					Sand	Silt	Clay	BD	OM
1	Clapp & Hornberger, 1978	USA	BC	1446	(+)	(+)	(+)	-	
2	Pachepsky et al., 1982	Hungary	BC	230	+	+	+	+	-
3	Rawls et al., 1982	USA	BC	5320	(+)	(+)	(+)	-	(+)
4	Cosby et al., 1984	USA	BC	1448	+	+	+	-	-
5	Rawls and Brakensiek, 1985	USA	BC	5320	+	-	+	+	-
6	Carsel and Parrish, 1988	USA	MvG	5097-5693	(+)	(+)	(+)	-	-
7	Vereecken et al., 1989	Belgium	MvG	182	+	-	+	+	+
8	Wösten et al 1999	Europe	MvG	1136-2894	+	+	+	+	+
9	Schaap et al., 2001	USA, Europe	MvG	2134/1306	+	+	+	+	-
10	Weynants et al., 2015	Belgium	MvG	136 (HCC), 166 (MRC)	+	-	+	+	+
11	Zhang and Schaap, 2017	USA, Europe	MvG	2134/1306	+	+	+	+	-

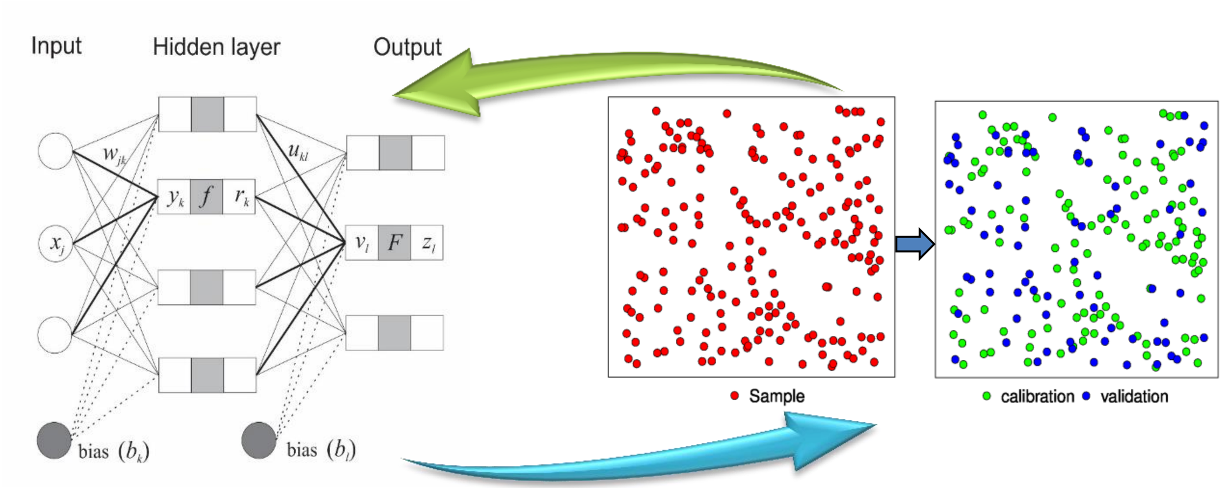
Van Looy et al, Reviews of Geophysics (Accepted)

Model parameters from PTF development: Rosetta



Rosetta stone
(196 BC)

- Rosetta (Schaap et al., 2001, JH) is based on Artificial Neural Network and bootstrap sampling (2134 samples from North America and Europe).



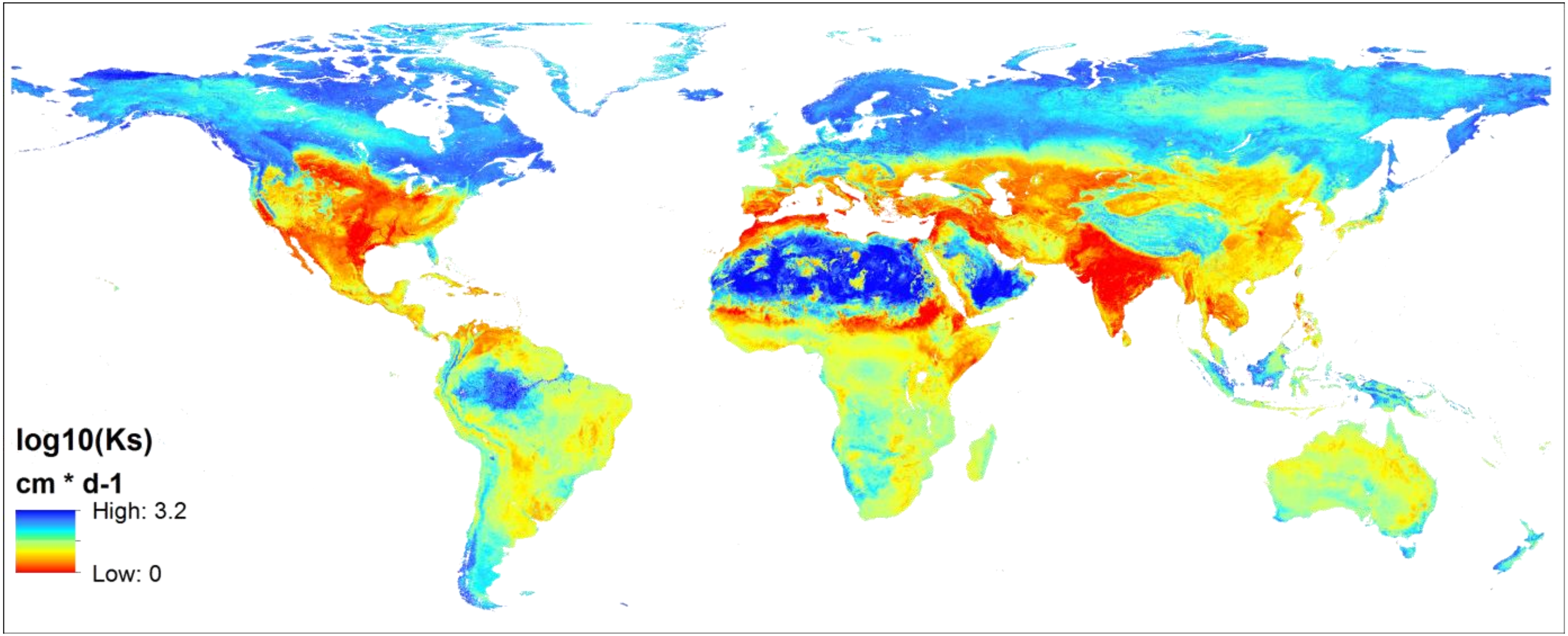
Artificial Neural Network Bootstrap sampling

Model	Input
H1	Textural class
H2	SSC
H3	SSCBD
H4	SSCBD θ_{33}
H5	SSCBD $\theta_{33}\theta_{15\ 000}$
Direct fit to data	

(5 hierarchical models)

- Rosetta is cited more than 1450 times in Google scholar, 900 in Web of Science, implemented in Hydrus1D, 2D, and 3D applications (Šimůnek et al., 2012; 2008) .

Global map of *Ks*

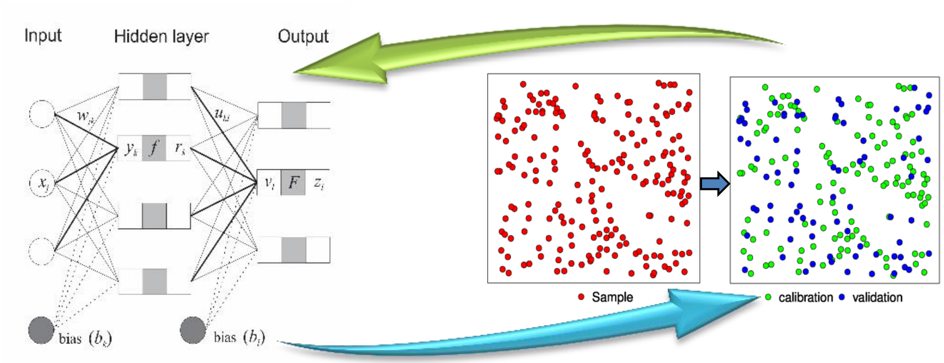


Global map of saturated hydraulic conductivity (log10(Ks) using Rosetta PTF. Calculations are based on the SoilGrids1km data set [Hengl et al., 2014].

Van Looy et al, Reviews of Geophysics (Accepted)

Several deficiencies of Rosetta1:

1. Pressure head-dependent **bias** in estimated water contents;
2. Uncertainty in the *fitted* VG parameters of was **ignored**; **noisy** data and **perfect** data are equally weighted;
3. Can provide only ***univariate*** uncertainties (**reason**); **covariance matrix** for VG & K_s is impossible;
4. Current published Rosetta1 software is nearly **unusable**.



Objective of Rosetta3:

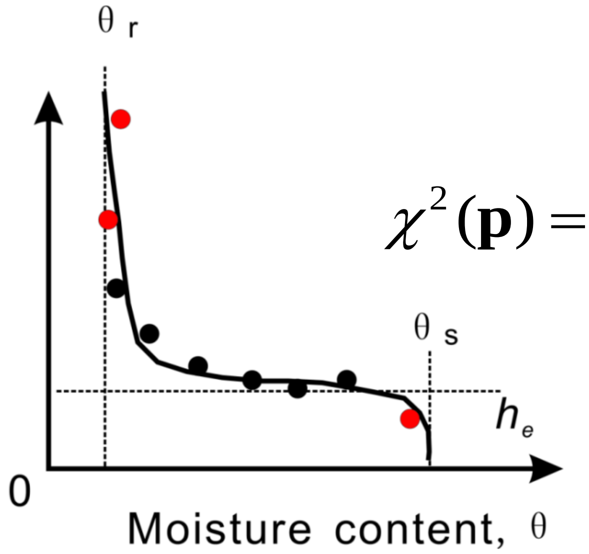
Recalibrate the Rosetta1 model and **solve** the above problems.

Rosetta3 procedure:

Obtaining weights → Adjusting weights → Coupling VG and K_s into one model → Rosetta3 obj function

$$O_{nn}(c_{nn}) = \sum_{i=1}^{N_s}\sum_{j=1}^{N_p} w''_{ij}\left(p_{ij} - p'_{ij}\right)^2$$

Obtaining weights:

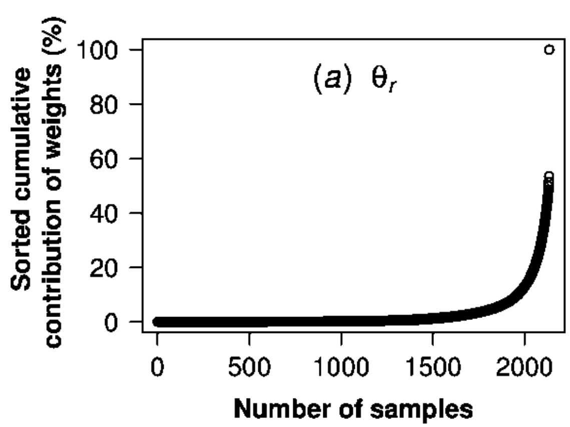


$$\chi^2(\mathbf{p}) = \sum_{i=1}^{N_w}\left[\theta_i - \theta'_i(h_i)\right]^2$$

$$\mathbf{Cov}_{\mathrm{VG}} = [\mathbf{J}^T\mathbf{J}]^{-1}$$

$$\mathbf{W}_{\mathrm{VG}} = \left[\mathrm{diag}(\mathbf{Cov}_{\mathrm{VG}})\right]^{-1}$$

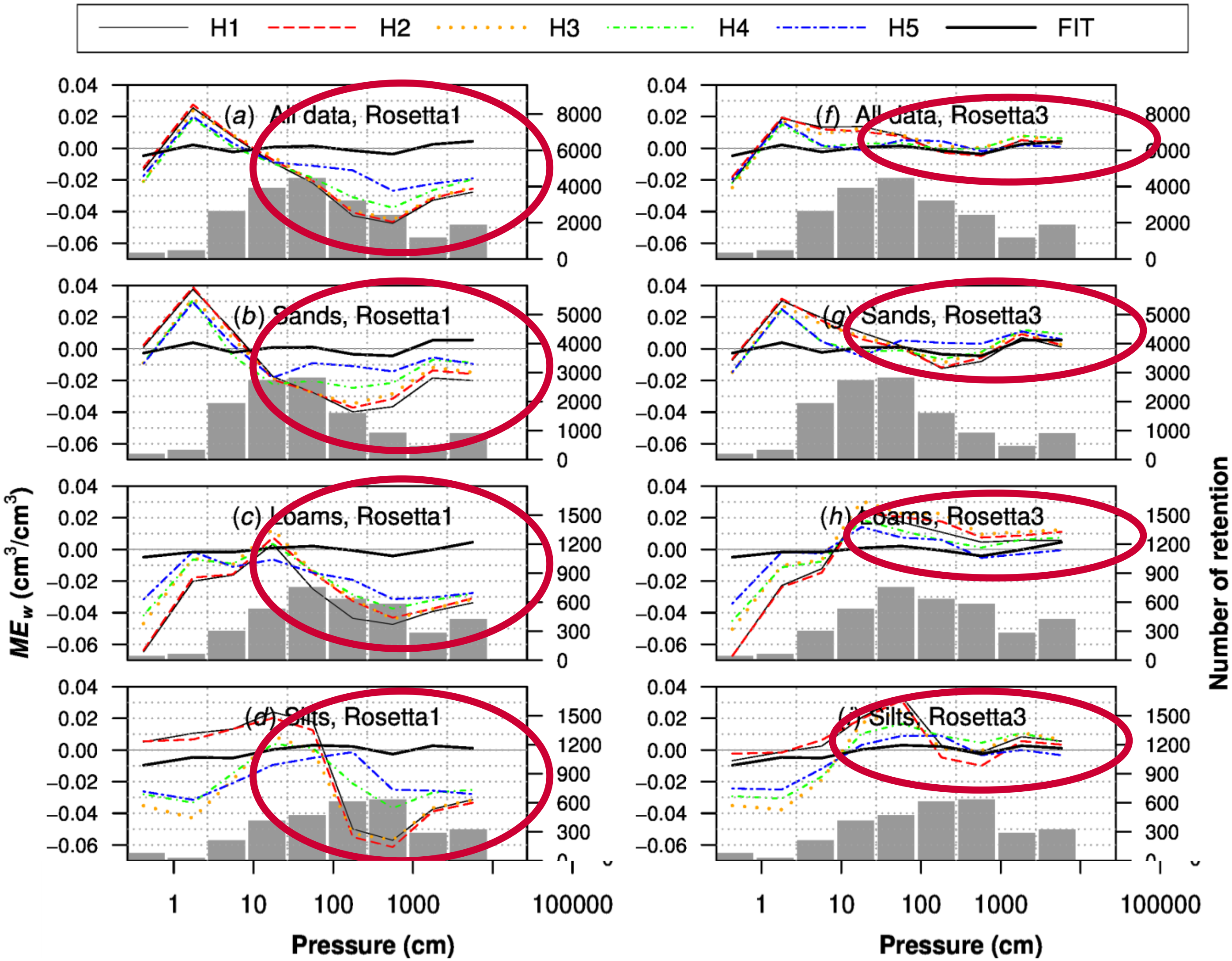
Adjusting weights:



VG: $$w'_{ij} = \begin{cases} w_{j,median} \times \Omega_U & \text{if } w_{ij} > w_{j,median} \times \Omega_U \\ w_{j,median} \times \Omega_L & \text{if } w_{ij} < w_{j,median} \times \Omega_L \end{cases}$$

$$w''_{ij} = \frac{w'_{ij}}{w_{j,median}}$$

ME (mean error) comparison of Rosetta1 and Rosetta3



Rosetta1 Rosetta3

- *ME* is reduced substantially by Rosetta3.
- Covariance matrix for VG & K_s can be obtained from Rosetta3

Rosetta3 Code: python (popular language)

Independent of Operating System, works in Linux, Windows 7+, and Mac OSX

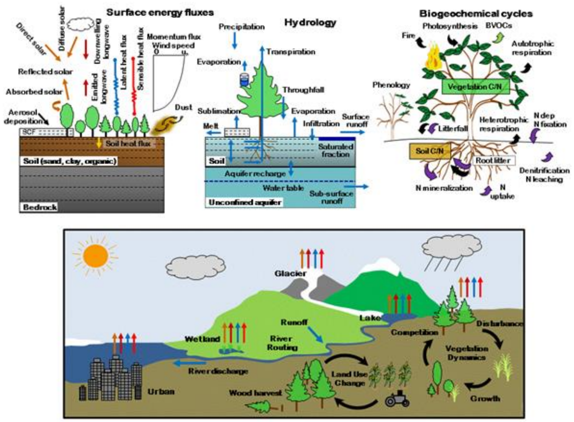
Can be downloaded from:
http://www.cals.arizona.edu/research/rosettav3.html
http://www.u.arizona.edu/~ygzhang/rosettav3

A web-based interface is under development.

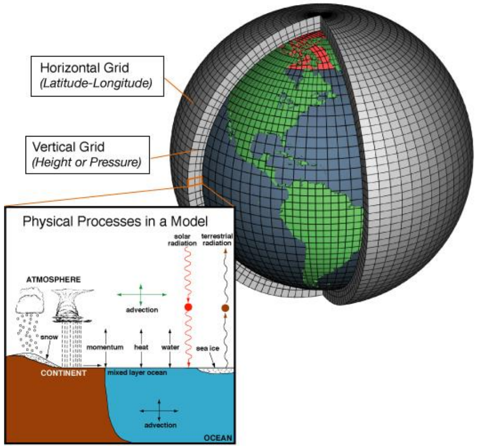
Zhang and Schaap (2017), JH

Different models need PTFs

(Van Looy et al)



(from NCAR)



(from NOAA)

Point Scale

Field Scale

Land Surface model

Global Climate model

(Agriculture, water and solute transport)

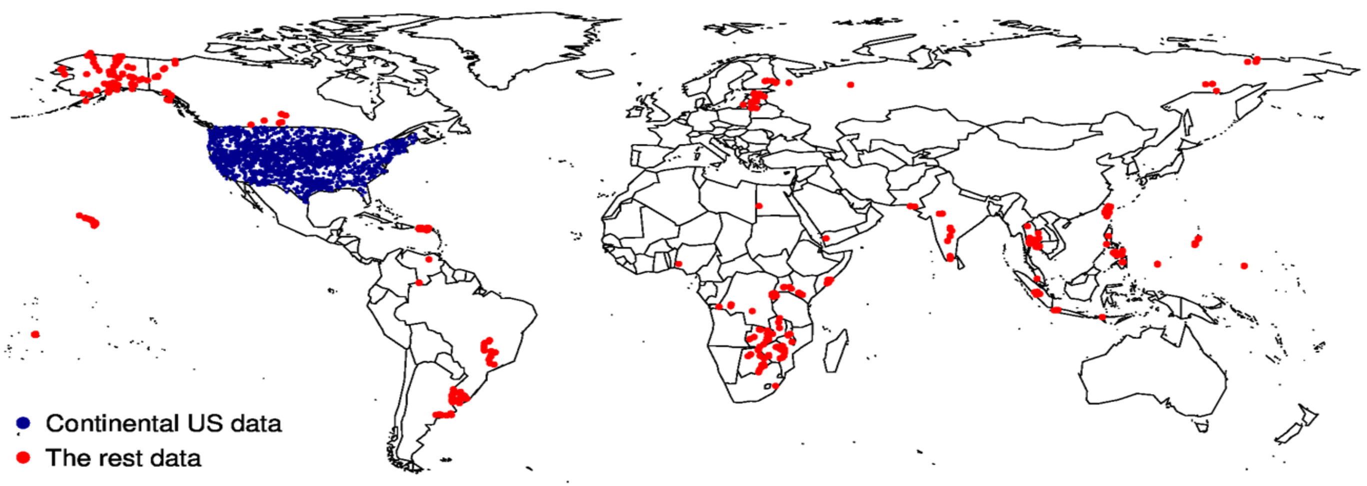
(Water, energy, carbon balance)

(Climate Change)

Small scale

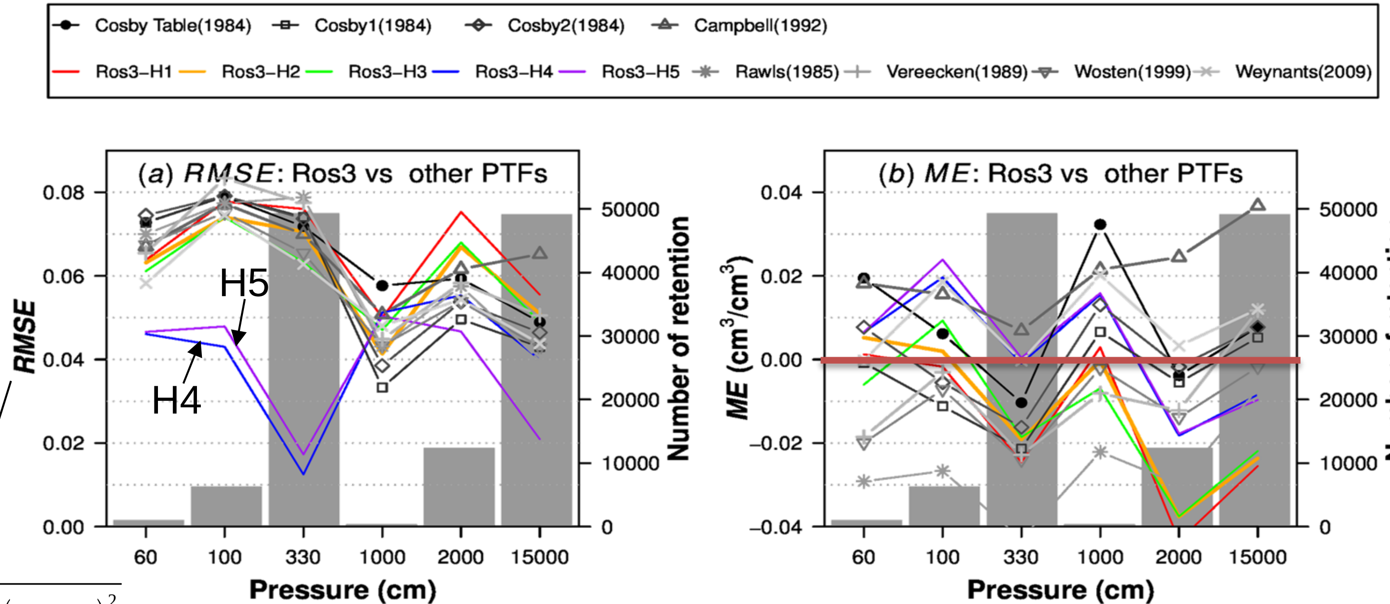
Large scale

Dataset



NCSS database contains 63565 soil pedons, 397212 soil layers across all of the world, but mainly focus on USA.
(WoSIS database [*Batjes et al.*, 2017] is also tried, but soil retention dataset of some samples is missing or different measurement of BD)

Different pedotransfer functions in different disciplines of the earth system models



$$\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\theta_i' - \theta_i\right)^2}$$

Clapp and Hornberger (1978)

$$\psi = \psi_s \left(\theta / \theta_s\right)^{-1/\lambda}$$

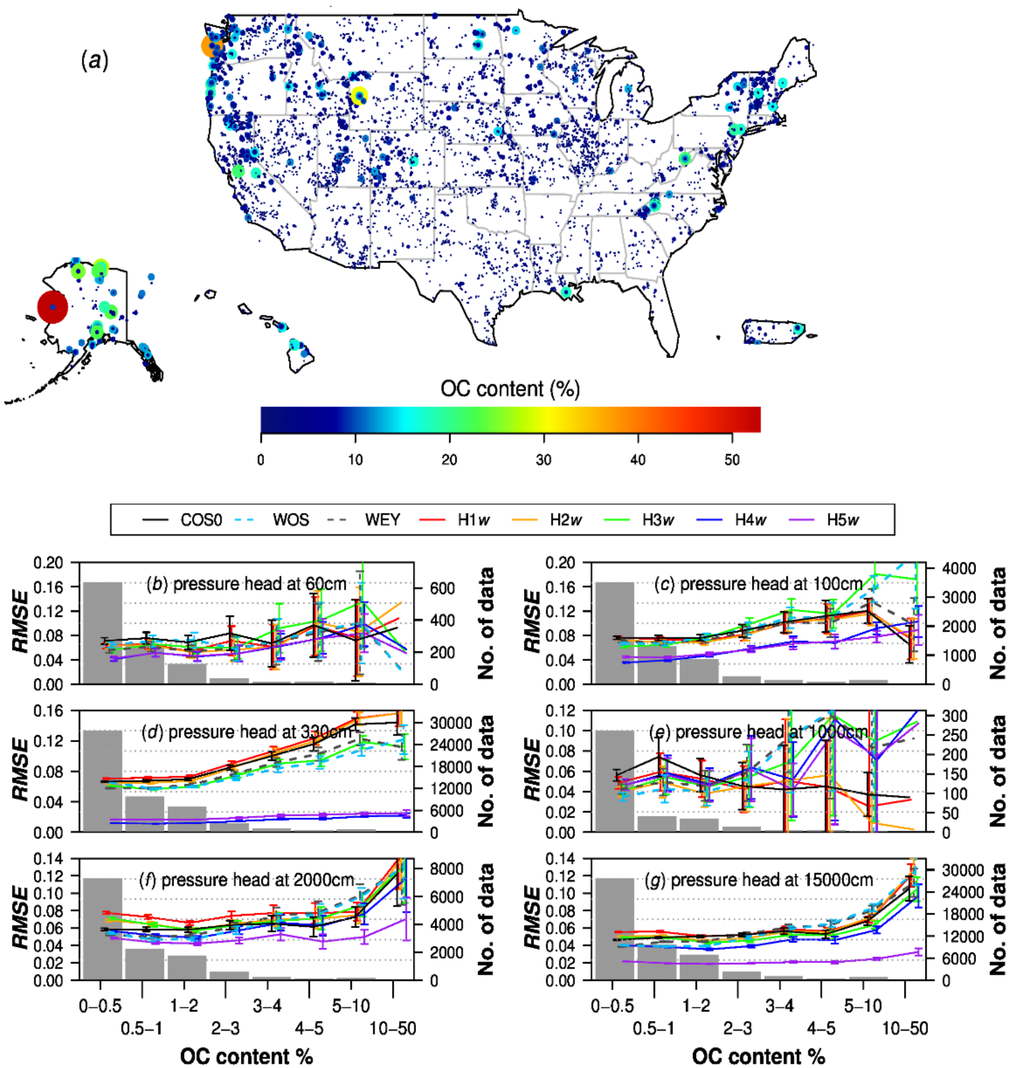
widely used in land surface models and global climate models.

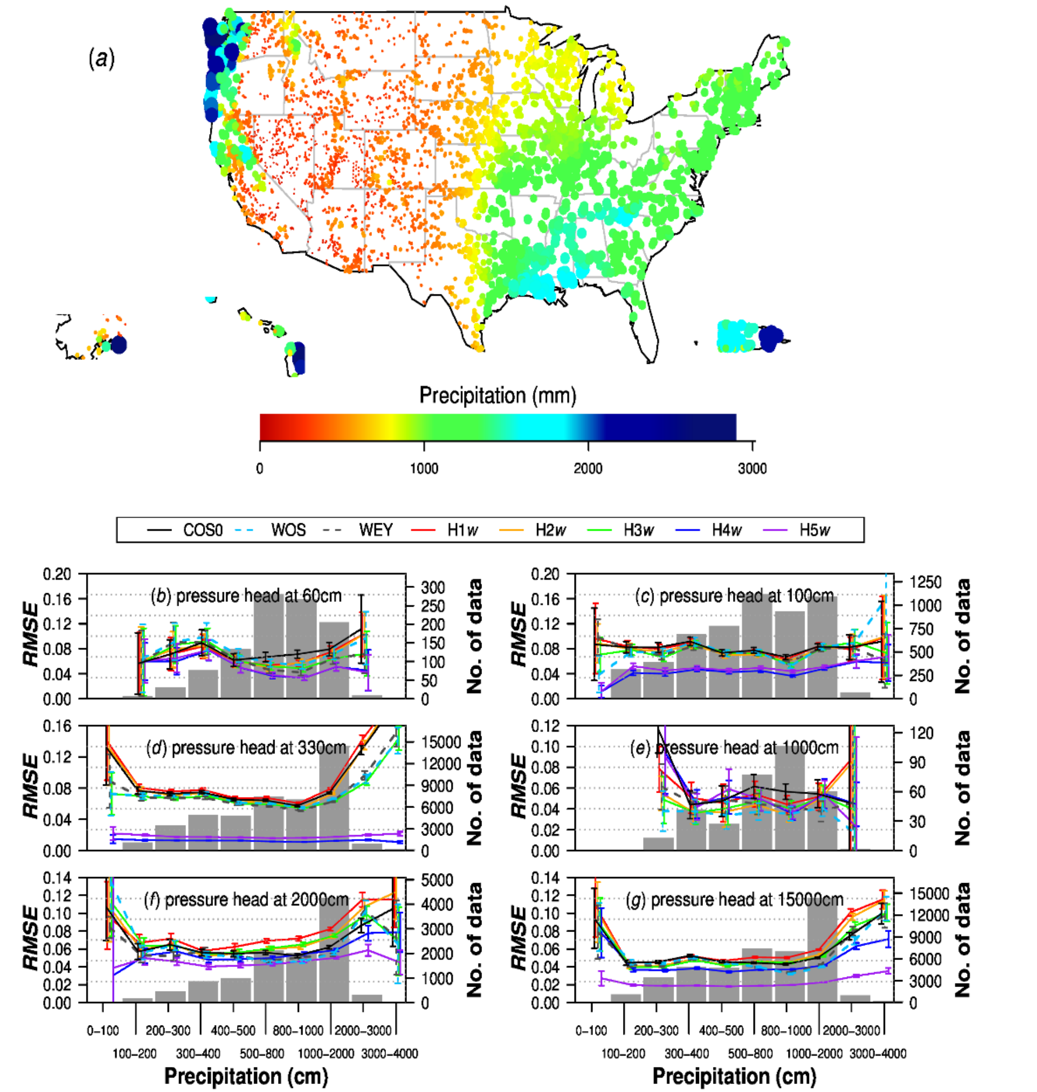
van Genuchten equation (1980)

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + |\alpha h|^n\right]^m}$$

more favored by soil scientists and hydrologists.

Part I: Improved Rosetta





RMSE is increasing as organic carbon content is increasing.

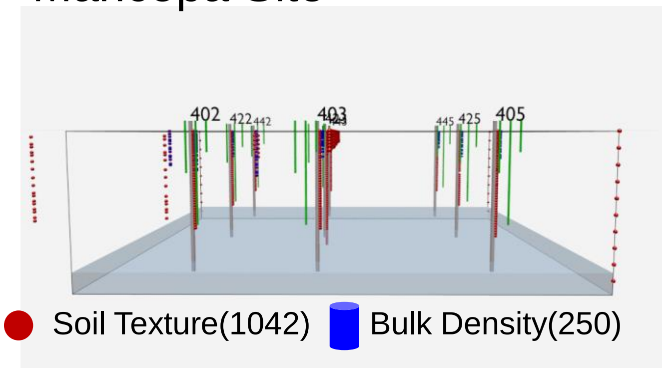
RMSE is increasing as precipitation is increasing.

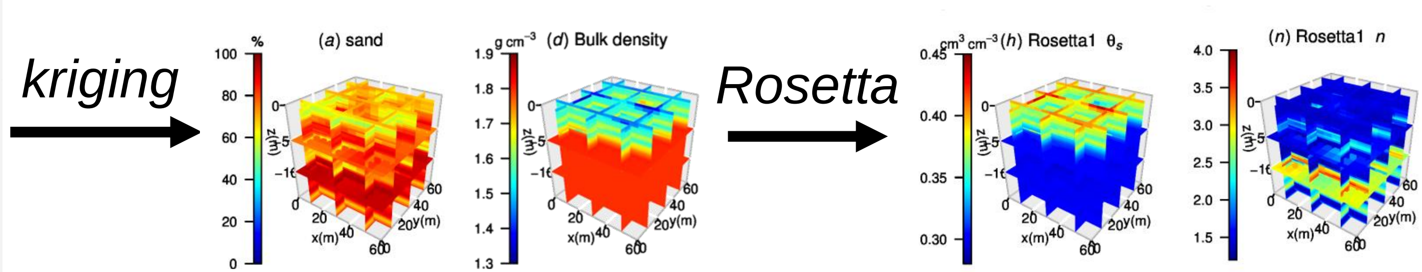
Zhang et al. (to be submitted)

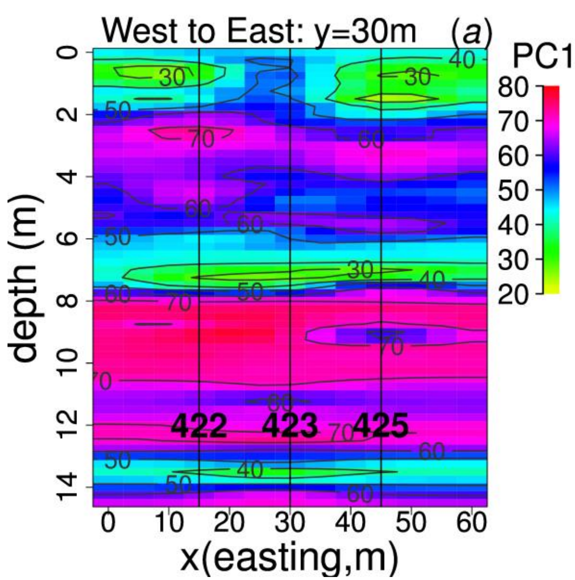
Part I: Improved Rosetta

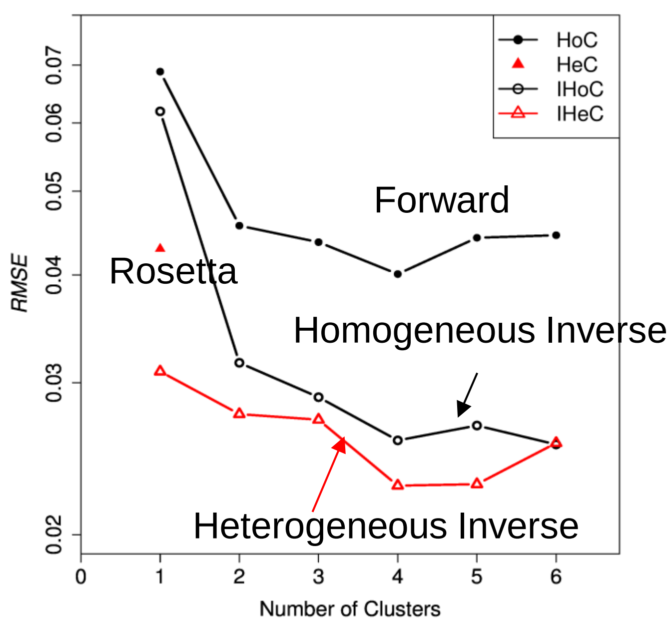
Part II: Inverse Modeling Using Clusters of Soil Texture

Maricopa Site









✓ Two inversions have the same number of parameters (5*N) to optimize.

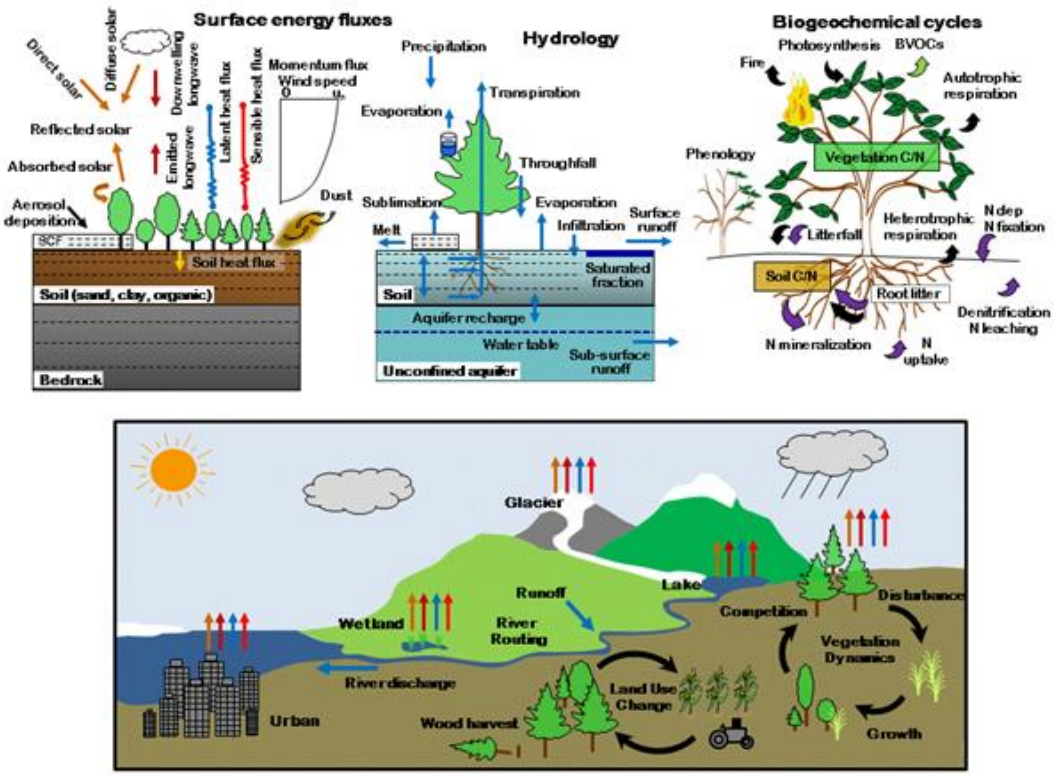
- Two inverse modeling are developed.
- Inversion can significantly improve soil moisture estimation with the aid of more information.

Zhang et al., (2016) WRR

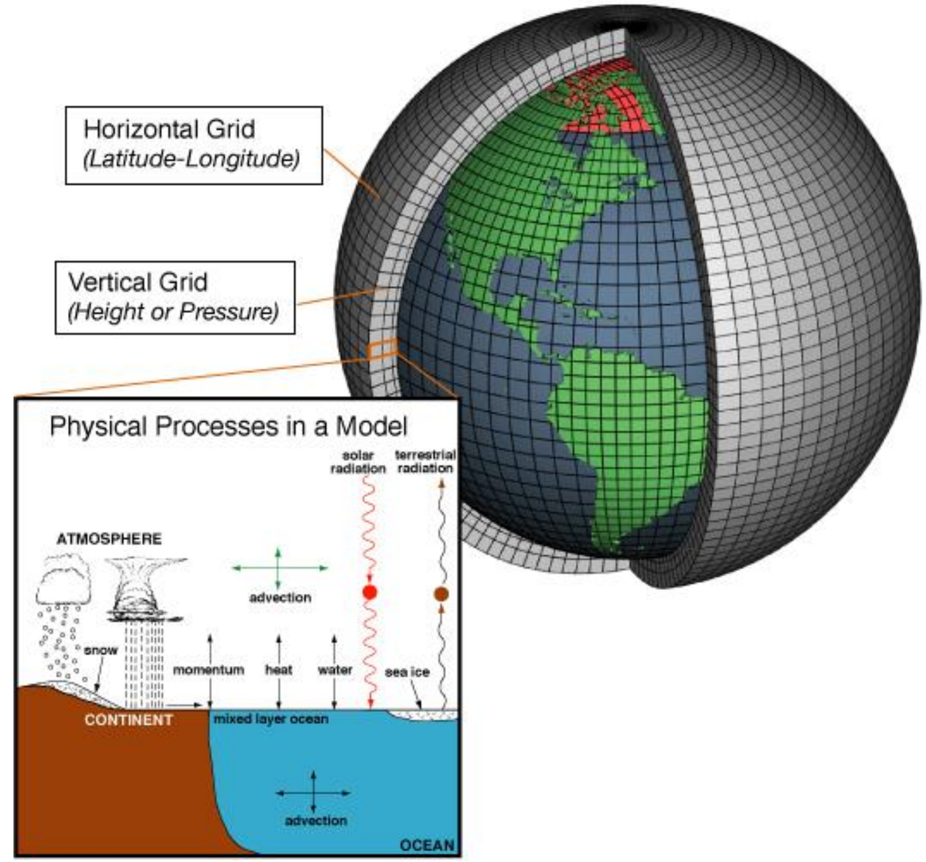
Summary

- An improved Rosetta model was developed: Rosetta-v3.
- Evaluation of current pedotransfer functions in different disciplines of the earth system models.
- Two inverse modeling of parameterizing vadose zone hydraulic properties are developed.

Application of Rosetta3 to Land Surface Model and General Circulation Model



Noah-MP, with Guo-yue Niu
(from NCAR)



General Circulation Model
(from NOAA)

Zhang et al. (in preparation)





Thanks