Land Surface Data Assimilation

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DARC-UoR: Data Assimilation Training

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09/06/2025

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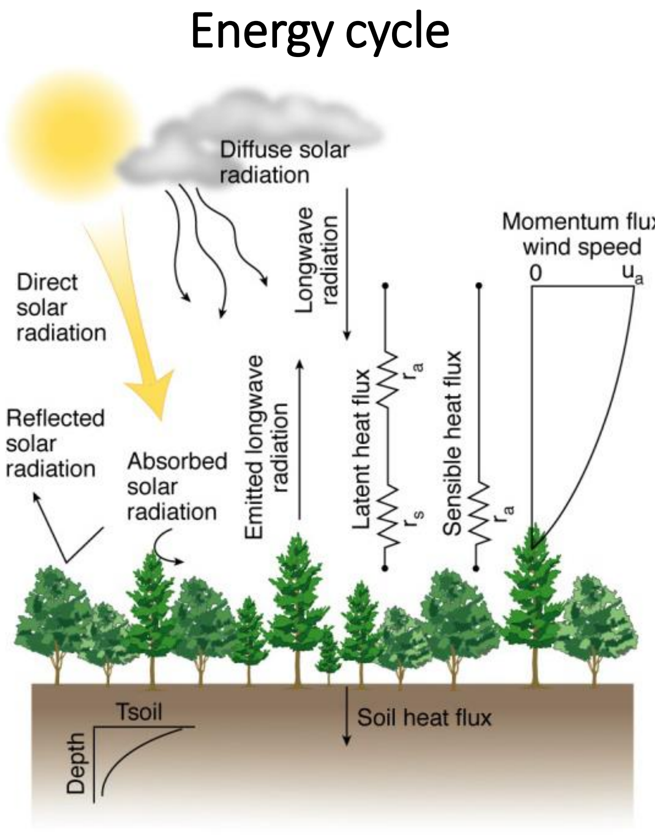
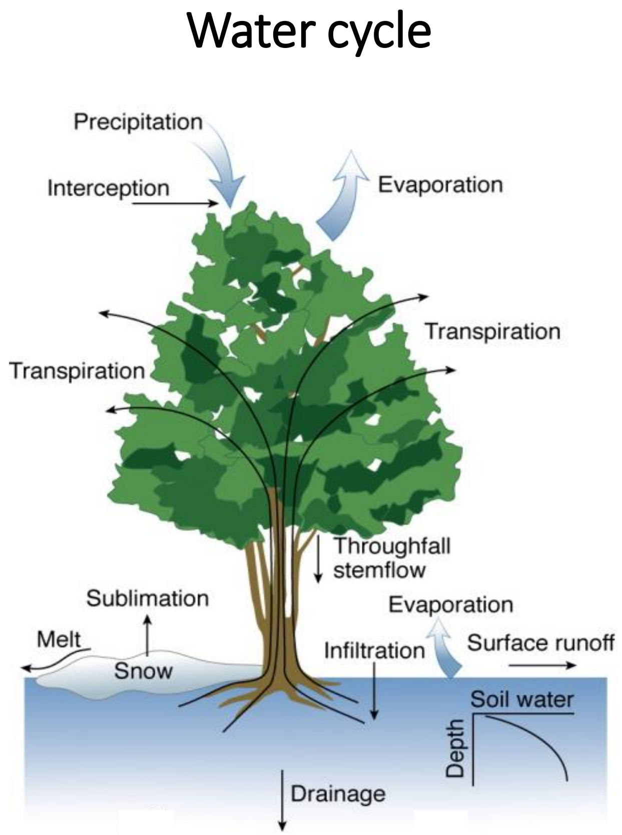
Land Surface Processes





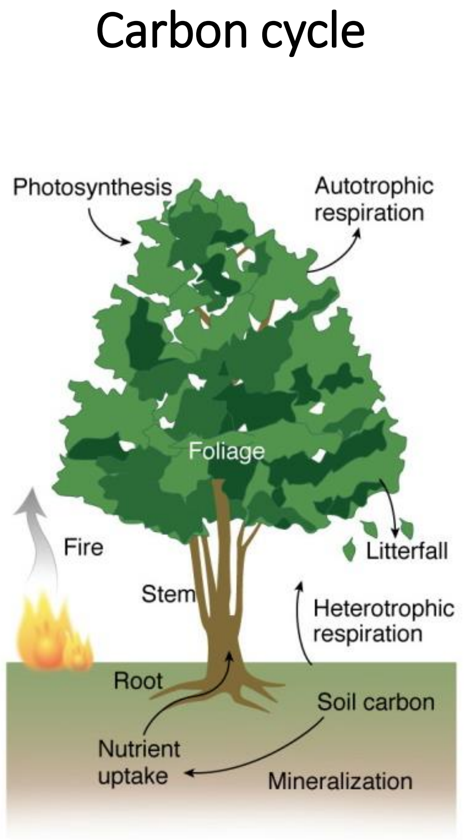
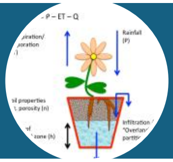
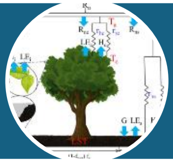


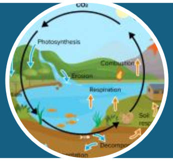
Figure: Different components of land surface processes. Bonan (2008)

Land surface processes describe the exchange of energy, water, and carbon between the land and the atmosphere.

Evolution of Land Surface Models (LSM)

1970s — 1st Gen 
Simple land hydrology and energy balance
Manabe's bucket model
Foundational Era

1980s — 2nd Gen 
Models included a veg. component (Veg–Atm interactions)
BATS (Dickinson 1986) and ISBA (Meteo-France scheme, 1989)
Era of "Big-leaf"

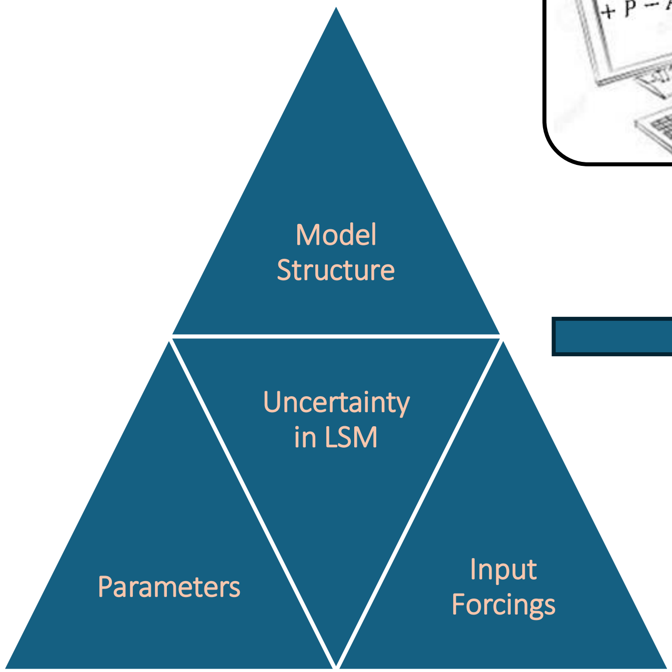
1990s — 3rd Gen 
LSMs began to incorporate terrestrial carbon cycle processes
NCAR LSM (Bonan 1996); UK's MOSES 2 (late 1990s)
Physiological Era

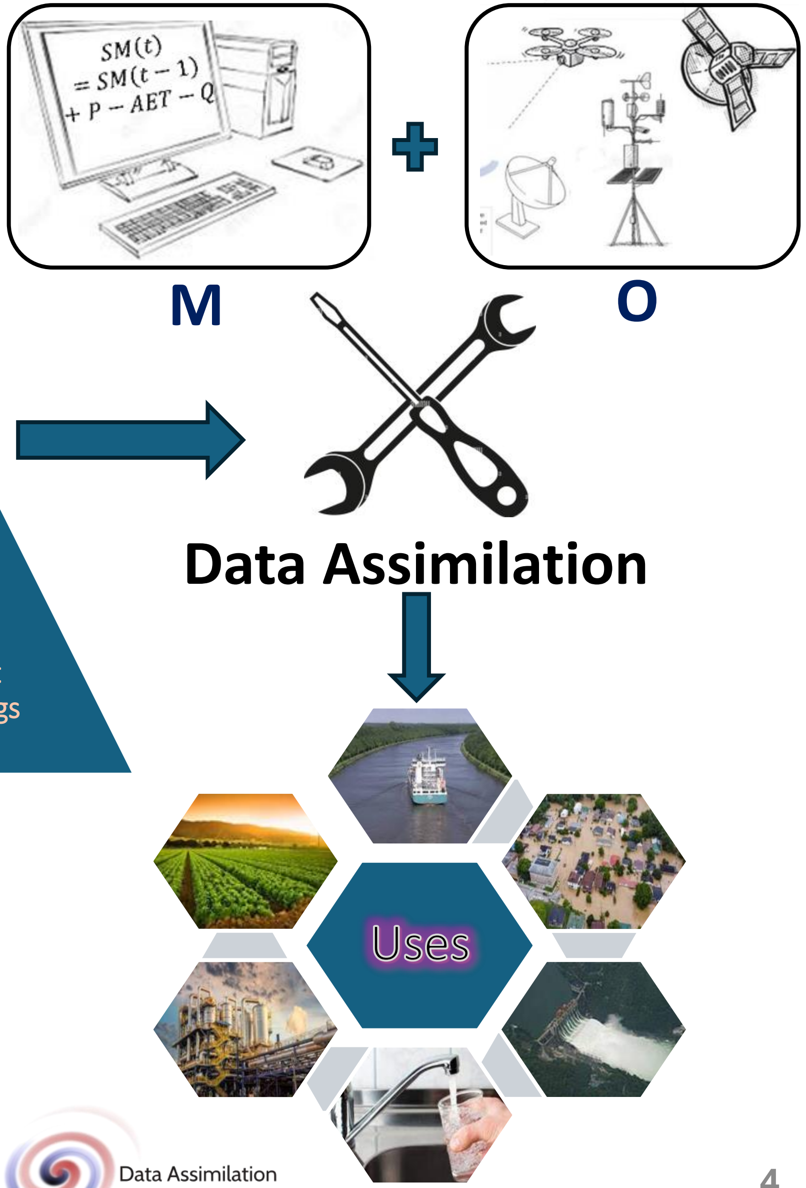
2010s — 4th Gen 
LSM now simulate human–environment interactions
Noah-MP; CLM; JULES; ORCHIDEE
Era of "DA"

2020s — 5th Gen 

A significant step toward operational "digital twin" models.
CLM5; JULES-ES; Physics-Informed Machine Learning (PIML)
Hyper-resolution Era

Land Surface Data Assimilation (LSDA)





Variable	Satellite Obs.	Spatial Res.	Temporal Res.
Soil Moisture	SMAP	9 km	1–3 days
	SMOS	35–50 km	1–3 days
	ASCAT	25 km (resampled to 12.5 km)	Daily
	ESA CCI	0.25° (~25 km)	Daily
Snow Water Equivalent	MODIS Snow Cover	500 m	Daily
	AMSR2	25 km	Daily
	Sentinel-1	1 km	6–12 days
	GlobSnow	25 km	Daily
Land Surface Temperature	MODIS LST	1 km	Daily
	Sentinel-3 SLSTR	1 km	Daily
	VIIRS	750 m	Daily
	GOES-R ABI	2 km	5–15 minutes
Leaf Area Index (LAI)	MODIS LAI	500 m	8 days
	Copernicus Global Land Service LAI	300 m	10 days
	PROBA-V	1 km	10 days
	Sentinel-2	10–20 m	5 days
Gross Primary Production (GPP)	MODIS GPP	500 m	8 days
	Copernicus Global Land Service GPP	300 m	10 days
	Sentinel-2	10–20 m	5 days
	VIIRS	500 m	Daily

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Optimizing Soil Moisture Assimilation Strategies for Improved Hydrological Predictions in JULES Model

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Part 1: JULES Land Surface Model

Joint UK Land Environment Simulator (JULES)

By Met Office Surface Exchange Scheme (MOSES)

Soil water content for each layer

$$\frac{d\boldsymbol{V}_k}{dt} = W'_{k-1} - W'_k - E'_k - \cancelto{0}{R_k}$$

$\boldsymbol{V}_k$ represent soil water content at layer k

W'_k represent diffusive fluxes determined through Darcy's law

E'_k is SM extraction which follows exponential distribution

~~R_k is subsurface lateral runoff~~ (i.e. 1D Jules)

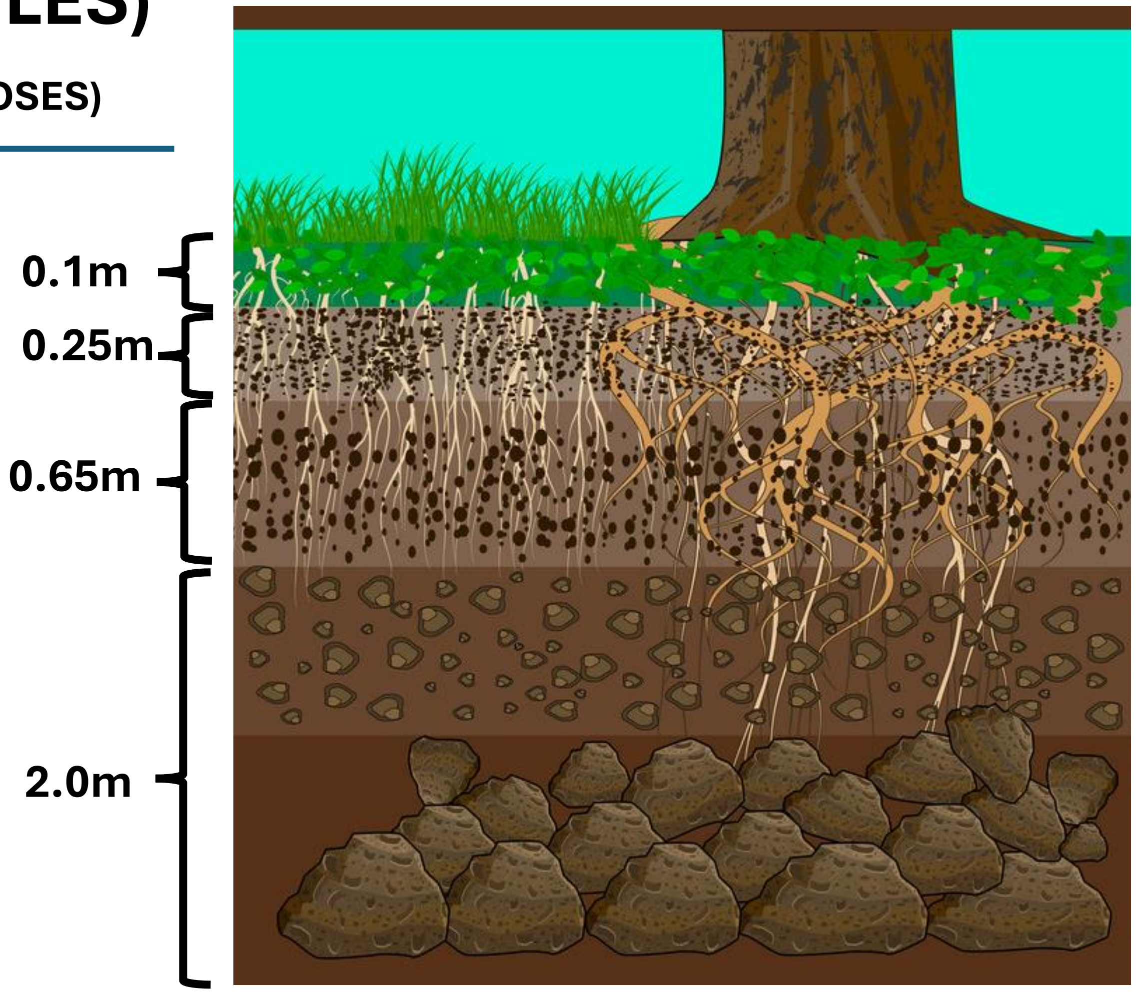


Figure: Soil layer configuration

Part 1: JULES - Soil Hydraulics Module

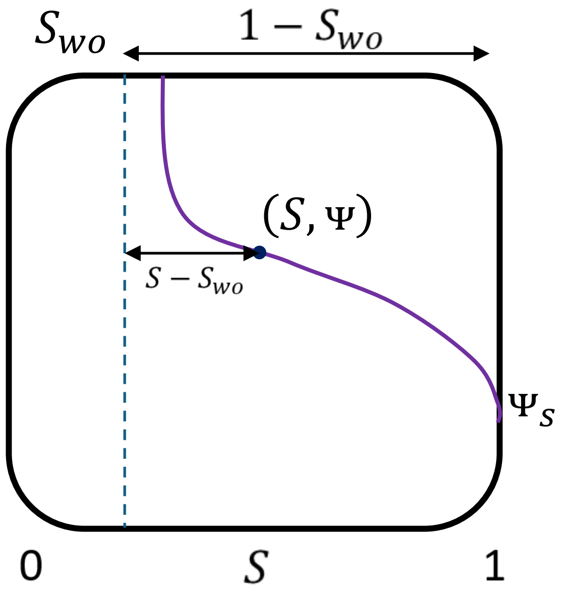
Flow in the unsaturated zone: Brooks and Corey

$$S_e = \left(\frac{S - S_{wo}}{1 - S_{wo}}\right) = \left(\frac{\Psi}{\Psi_s}\right)^{-1/b}$$

$$S = S_{wo} + (1 - S_{wo})\left(\frac{\Psi}{\Psi_s}\right)^{-1/b}$$

$$\boldsymbol{V} = V_{wo} + (V_{sat} - V_{wo})\left(\frac{\Psi}{\Psi_s}\right)^{-1/b}$$ and $$\frac{\boldsymbol{K}}{K_s} = \left(\frac{V}{V_{wo}}\right)^{2b+3}$$

Soil characteristic curve



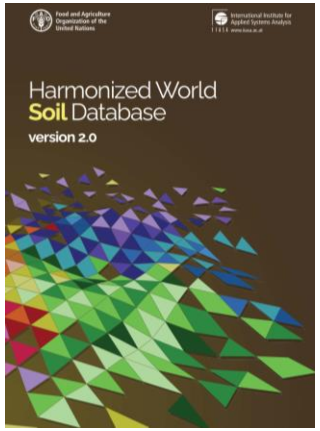
V_{wo}: Irreducible water content
Ψ: Capillary pressure
S_e: Effective saturation

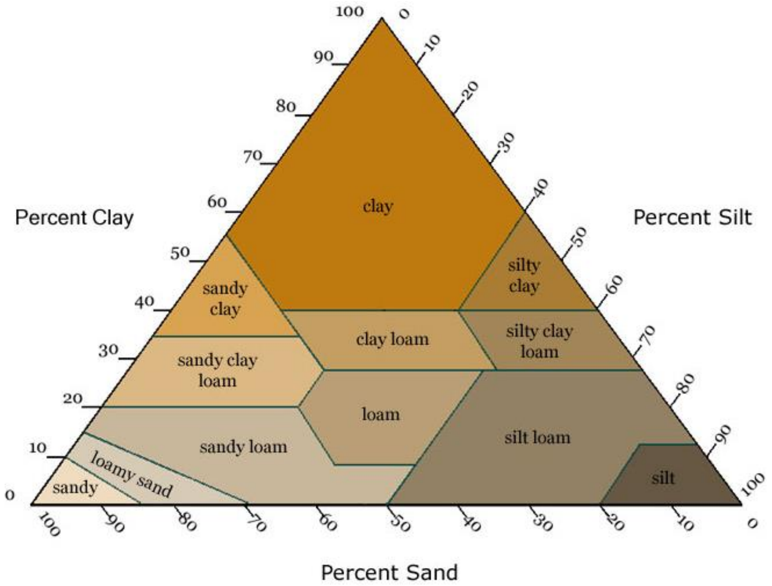
V_{sat}: Saturated water content
Ψ_s: Bubbling pressure (AEP)
b: Fitting coefficient

$\boldsymbol{K}$: **Hydraulic conductivity**
K_s: Hydraulic conductivity at saturation
$\boldsymbol{V}$: **Soil water content**

Part 1: PedoTransfer Function (PTF)

Easily Measurable Variables → **Pedotransfer function** → **Difficult-to-Measure Variables**





$$b = \boldsymbol{K_1} + \boldsymbol{K_2}\, f_{Clay} - \boldsymbol{K_3}\, f_{Sand}$$

$$V_{sat} = \boldsymbol{K_4} - \boldsymbol{K_5}\, f_{Clay} - \boldsymbol{K_6}\, f_{Sand}$$

$$\Psi_S = 0.01 * 10^{(\boldsymbol{K_7} - \boldsymbol{K_8}\, f_{Clay} - \boldsymbol{K_9}\, f_{Sand})}$$

$$K_S = 10^{(-\boldsymbol{K_{10}} - \boldsymbol{K_{11}}\, f_{Clay} + \boldsymbol{K_{12}}\, f_{Sand})}$$

$$V_{crit} = V_{sat}\left(\frac{\Psi_S}{3.364}\right)^{\frac{1}{b}}$$

$$V_{wilt} = V_{sat}\left(\frac{\Psi_S}{152.9}\right)^{\frac{1}{b}}$$

$$h_{cap} = (1 - V_{sat})\left(2.376 * 10^6 f_{Clay} + 2.133 * 10^6 f_{Silt}\right)$$

$$h_{con} = 0.025^{V_{sat}}\left(1.16^{f_{Clay}(1 - V_{sat})} * 1.57^{f_{Sand}(1 - V_{sat})} * 1.57^{f_{Silt}(1 - V_{sat})}\right)$$

Cosby PTF

Cosby, B. J. et, al., (1984). *Water Resources Research*, https://doi.org/10.1029/WR020i006p00682,1984

Part 2: Ensemble Variational (En-Var) Hybrid Assimilation

4D Var: Cost function

\+

Ensemble model run

En-Var DA

$$J(x_0) = \underbrace{\frac{1}{2}(x_0 - x_b)^T \boldsymbol{B}^{-1}(x_0 - x_b)}_{\textbf{Prior}} + \underbrace{\frac{1}{2}\sum_{t=0}^{N}\left(h_t\left(m_{0\to t}(x_0)\right) - y_t\right)^T \boldsymbol{R}_t{}^{-1}\left(h_t\left(m_{0\to t}(x_0)\right) - y_t\right)}_{\textbf{Observations}}$$

Gradient

$$\nabla J(x_0) = \boldsymbol{B}^{-1}(x_0 - x_b) + \frac{1}{2}\sum_{t=0}^{N} \boldsymbol{M}_{t,0}^T \boldsymbol{H}_t^T \boldsymbol{R}_t{}^{-1}\left(h_t\left(m_{0\to t}(x_0)\right) - y_t\right)$$

To avoid computing the AM and reduce the computational time of estimating B^{-1}, a preconditioned matrix is used using **control variable transform**

$B \approx X_b' \, X_b'^T$ and $x_0 = \overline{x_b} + X_b' w$

$$J(\boldsymbol{w}) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \sum_{t=0}^{N}\left(h_t\left(m_t(\overline{x_b})\right) + \boldsymbol{H}_t\boldsymbol{M}_t X_b'\boldsymbol{w} - y_t\right)^T \boldsymbol{R}_t{}^{-1}\left(h_t\left(m_t(\overline{x_b})\right) + \boldsymbol{H}_t\boldsymbol{M}_t X_b'\boldsymbol{w} - y_t\right)$$

$$\nabla J(\boldsymbol{w}) = \boldsymbol{w} + \sum_{t=0}^{N}(\boldsymbol{H}_t\boldsymbol{M}_t X_b')^T \boldsymbol{R}_t{}^{-1}\left(h_t\left(m_t(\overline{x_b})\right) + \boldsymbol{H}_t\boldsymbol{M}_t X_b'\boldsymbol{w} - y_t\right)$$

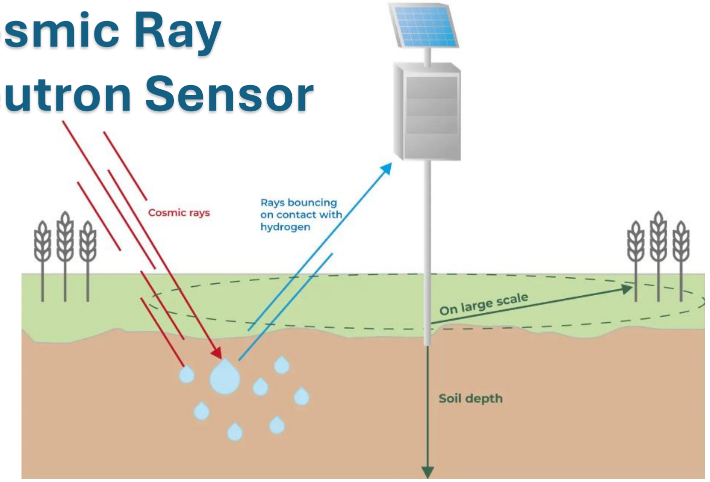
<u>Perturbation matrix in Observation space</u>

$$\boldsymbol{H}_t\boldsymbol{M}_t X_b' \approx Y_b' = \frac{1}{\sqrt{m-1}}\begin{pmatrix} h_t\left(m_t(X_b^1)\right) - h_t\left(m_t(\overline{x_b})\right),\ h_t\left(m_t(X_b^2)\right) - h_t\left(m_t(\overline{x_b})\right), \ldots, \\ \ldots, h_t\left(m_t(X_b^m)\right) - h_t\left(m_t(\overline{x_b})\right) \end{pmatrix}$$

Part 3: COSMOS-UK Observations

Variables	Purpose
Meteorological data	JULES Model Forcing
Soil Moisture	Assimilation and validation

Cosmic Ray Neutron Sensor



Temporal resolution: Daily
Spatial resolution: Field scale across UK
Duration: Three years
2016 (Warm-up period)
2017 (DA run) and 2018 (Forecast period)

Figure: Typical COSMOS-UK observation site (https://cosmos.ceh.ac.uk/)

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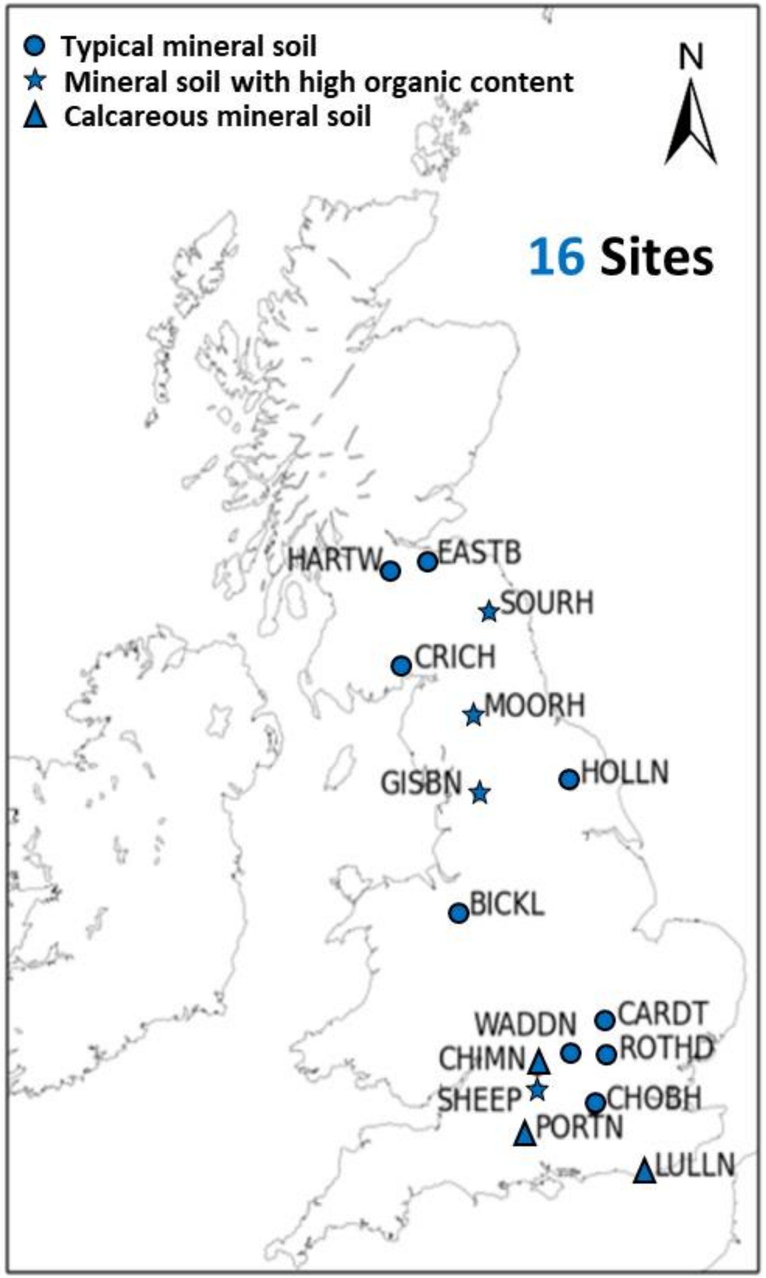
Site Locations



Site name and abbreviation	Land cover	Soil description
Cardington (CARDT)	Grassland	Typical mineral soil
Bickley Hall (BICKL)	Grassland	Typical mineral soil
Crichton (CRICH)	Grassland	Typical mineral soil
Waddesdon (WADDN)	Grassland	Typical mineral soil
Hollin Hill (HOLLN)	Grassland	Typical mineral soil
Easter Bush (EASTB)	Grassland	Typical mineral soil
Rothamstead (ROTHD)	Grassland	Typical mineral soil
Chimney Meadows (CHIMN)	Grassland	Calcereous mineral soil
Sheepdrove (SHEEP)	Grassland	Mineral soil, fairly high organic carbon content
Porton Down (PORTN)	Grassland	Highly calcareous mineral soil
Hartwood Home (HARTW)	Grassland/woodland	Typical mineral soil
Gisburn Forest (GISBN)	Coniferous forest	Mineral soil, high organic carbon content
Chobham Common (CHOBH)	Heath	Highly variable soil
Lullington Heath (LULLN)	Grassland/heath	Highly calcareous mineral soil
Moorhouse (MOORH)	Grassland/heath	Mineral soil with very high organic content
Sourhope (SOURH)	Grassland	Mineral soil with very high organic content

Assimilation Scenarios

Three Scenarios

1) State estimation of initial soil moisture condition

2) Parameter estimation of PTF constants

3) Dual state-parameter estimation

SC 1

(4 Layers/site)

$$
\left.\begin{bmatrix} \left.\begin{matrix} SM_1 \\ SM_2 \\ SM_3 \\ SM_4 \end{matrix}\right\} \text{Site 1} \\ . \\ . \\ \left.\begin{matrix} SM_1 \\ SM_2 \\ SM_3 \\ SM_4 \end{matrix}\right\} \text{Site 16} \end{bmatrix}\right\} X_b^i = \text{Augmented Initial SM condition}
$$

Ensemble size is 50
So, i = 1,2,..50

SC 2

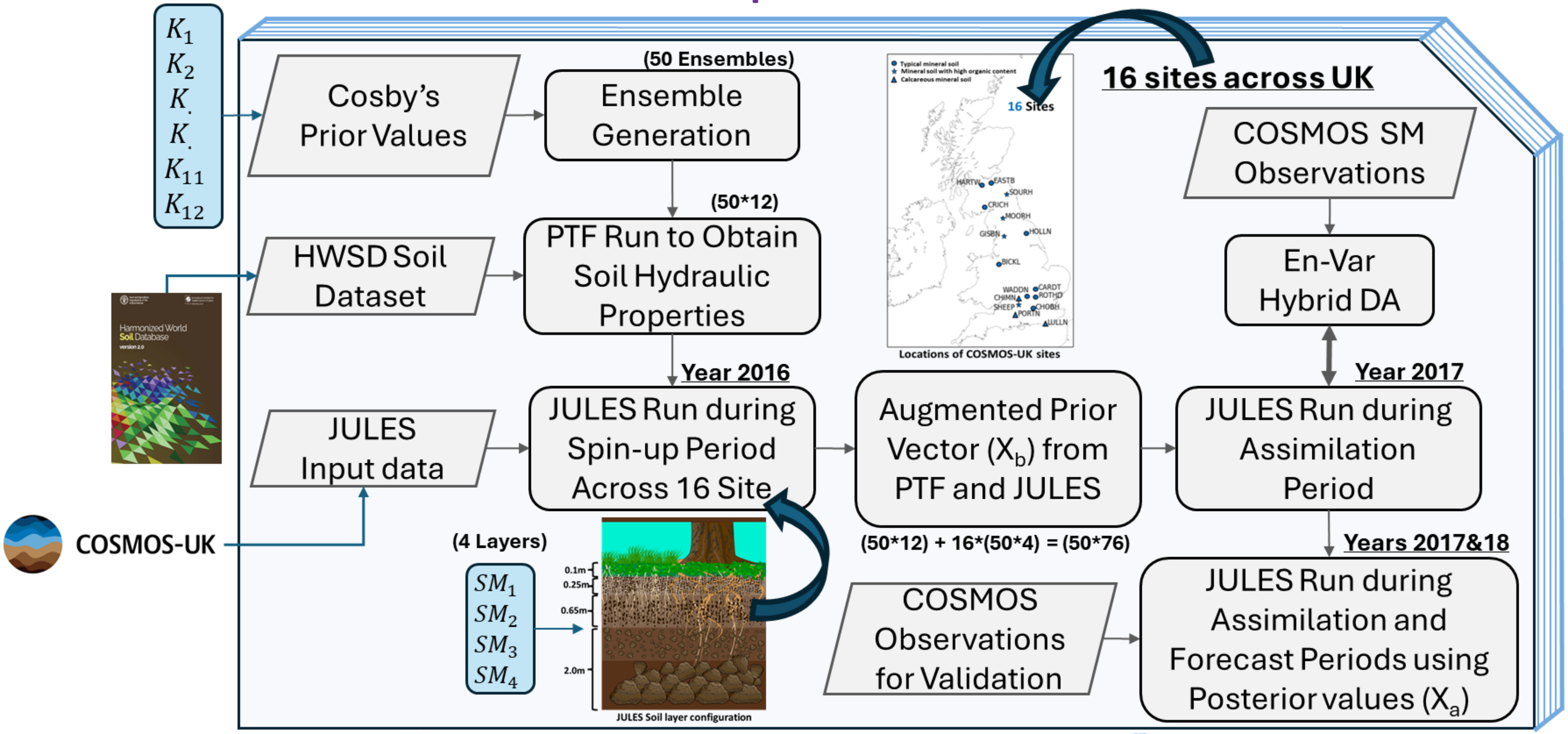
$$
\left.\begin{bmatrix} K_1 \\ K_2 \\ K_. \\ K_. \\ K_{11} \\ K_{12} \end{bmatrix}\right\} X_b^i = \text{Cosby's PTF values}
$$

SC 3

$$
\left.\begin{bmatrix} K_1 \\ K_. \\ K_. \\ K_{12} \\ SM_1 \\ SM_2 \\ SM_3 \\ SM_4 \\ . \\ . \\ SM_1 \\ SM_2 \\ SM_3 \\ SM_4 \end{bmatrix}\right\} X_b^i = \text{Augmented state-parameter vector}
$$

Methodology

Dual state-parameter estimation



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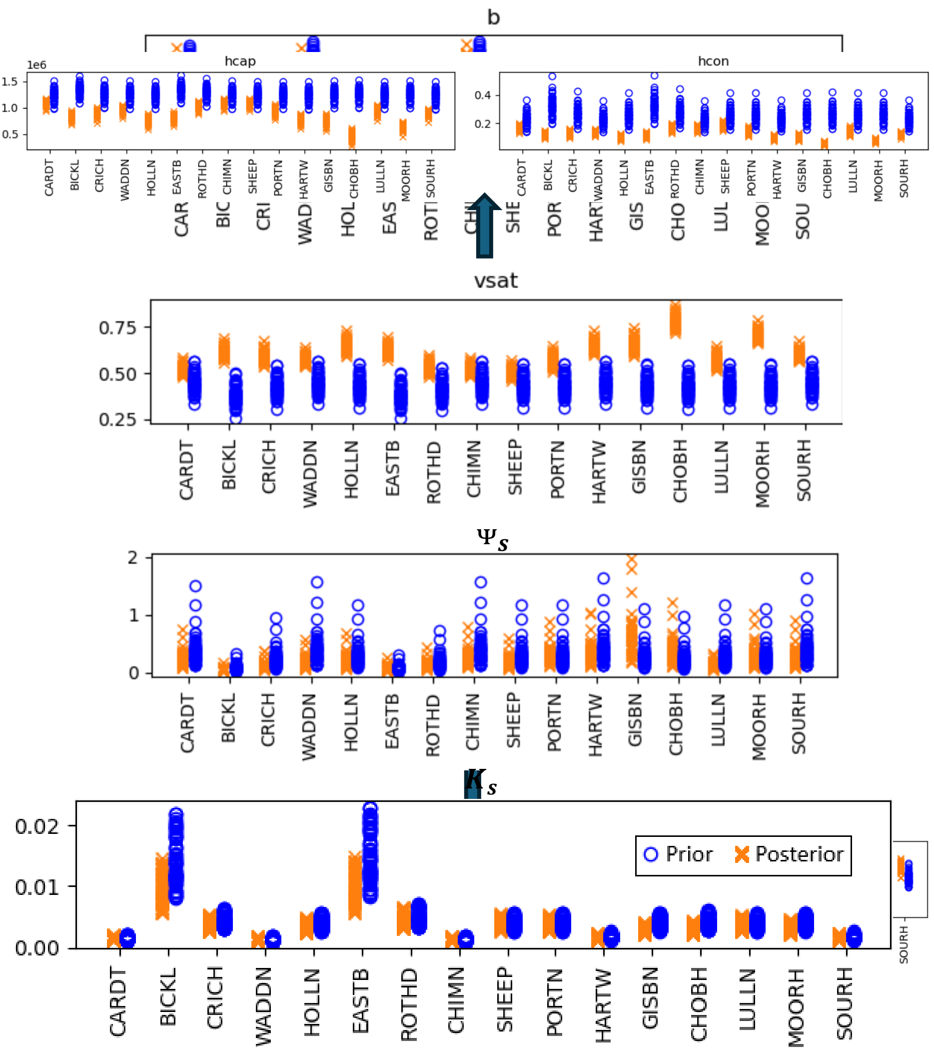
PTF parameter: Prior-Posterior Distributions



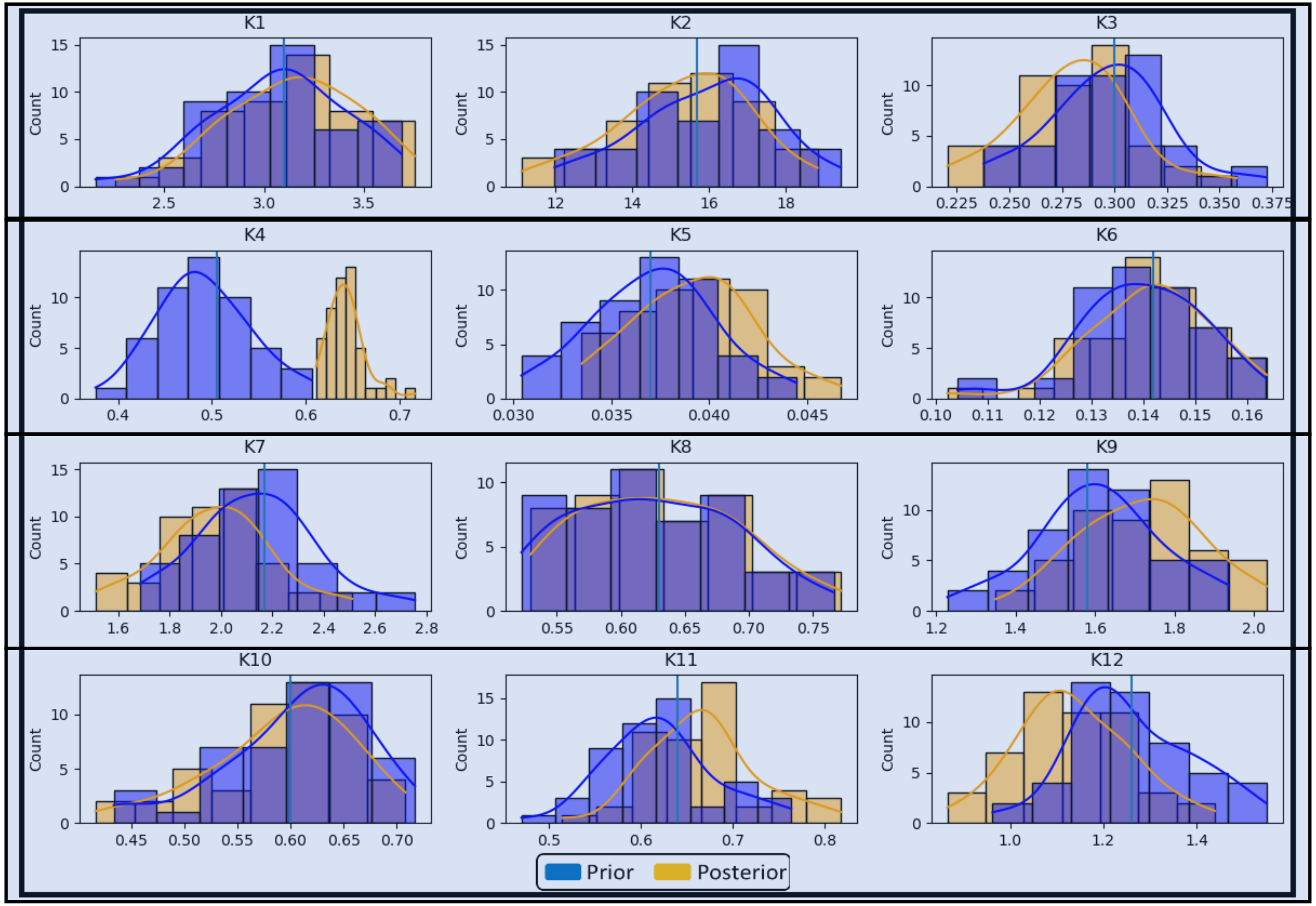


Fig: Prior and posterior PTF distribution for SC3

KGE Metrics

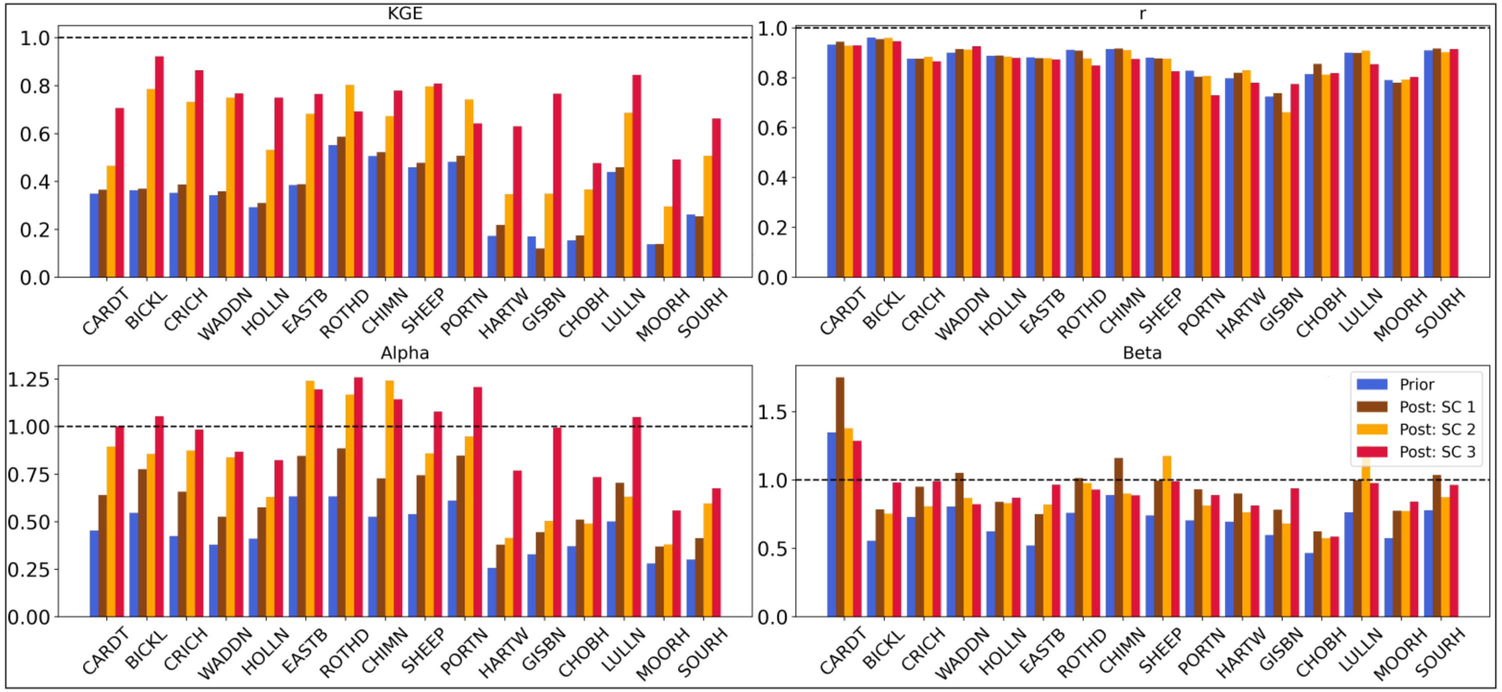


Figure: KGE metrics and its components showing the performance of JULES model across all the 16 sites in UK for three assimilation scenarios: state-only (SC 1), parameter-only (SC 2), and joint state-parameter (SC 3).

1. r (Correlation): JULES is already showing very good trend leaving less scope to improve them further after DA
2. α (Ratio of variability :– $\frac{\sigma_{model}}{\sigma_{obs}}$): This component influenced the KGE values maximum
3. β (Ratio of Bias :- $\frac{\mu_{model}}{\mu_{obs}}$): Increased V_sat and decreased K_s values after assimilation retained more water in the soil column reducing the bias difference.

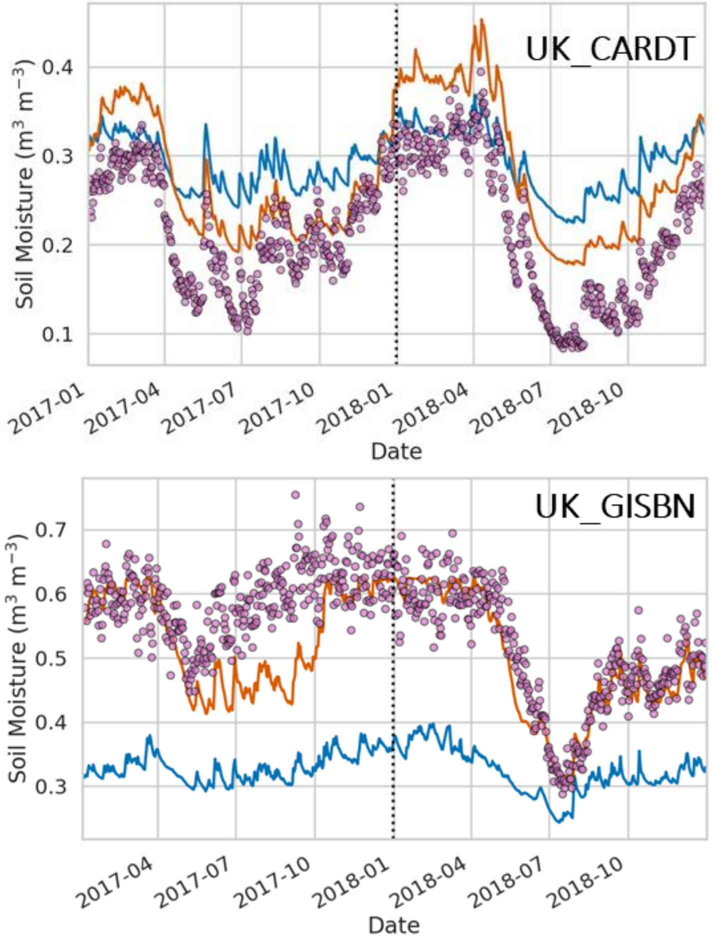


Figure: Modelled (ensemble mean) and observed soil moisture at GISBN and CARDT sites during assimilation (2017) and forecast periods (2018) for state-parameter assimilation scenario (SC 3)

Observation Prior Posterior

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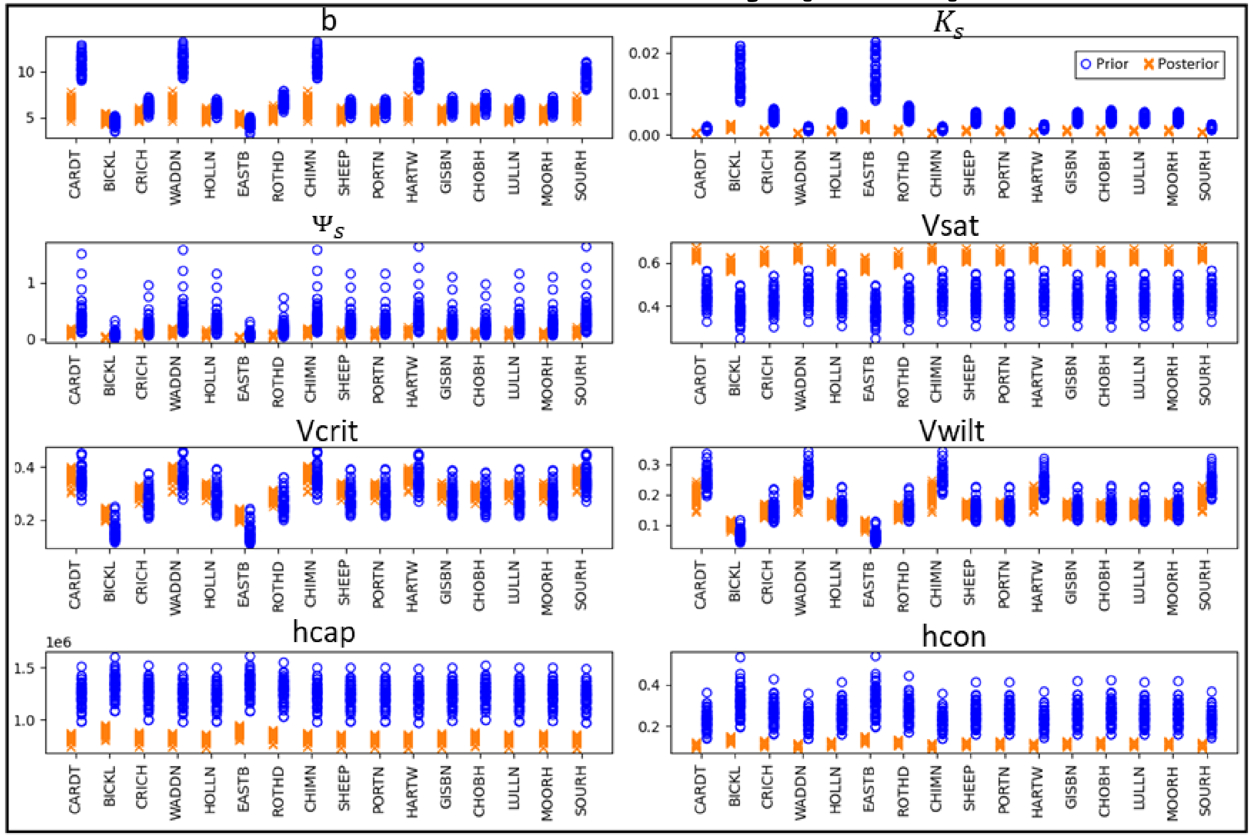
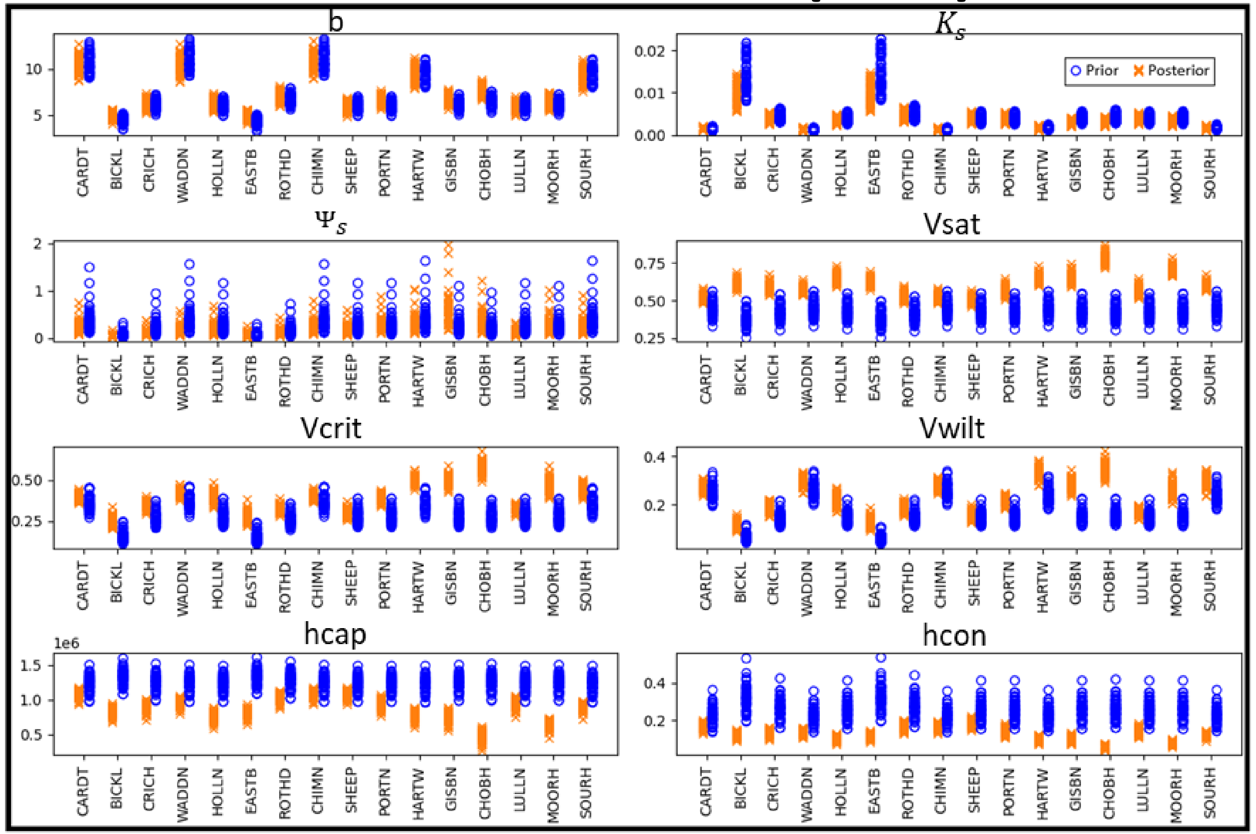
Scenario comparison

Parameter-only (SC 2)



State-Parameter (SC 3)



Hydraulic parameter changes are more pronounced in SC2, leading to greater variability in JULES outputs.
Incorporating initial conditions moderated this effect, enabling JULES to align more closely with COSMOS observations.

Limitations

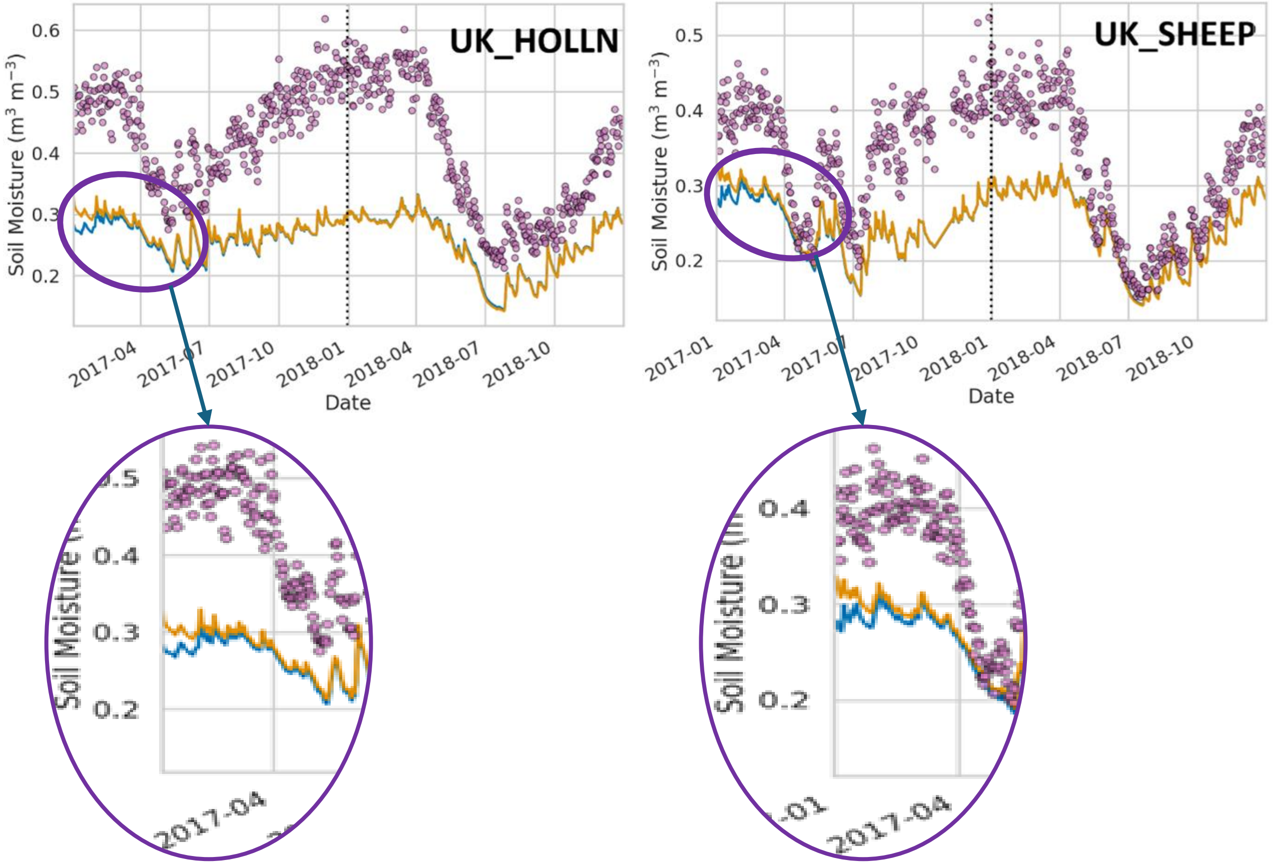


Figure: Modelled (ensemble mean) and COSMOS soil moisture time series at the HOLLN and SHEEP sites during the assimilation (2017) and forecast (2018) periods during state-only assimilation (SC 1)

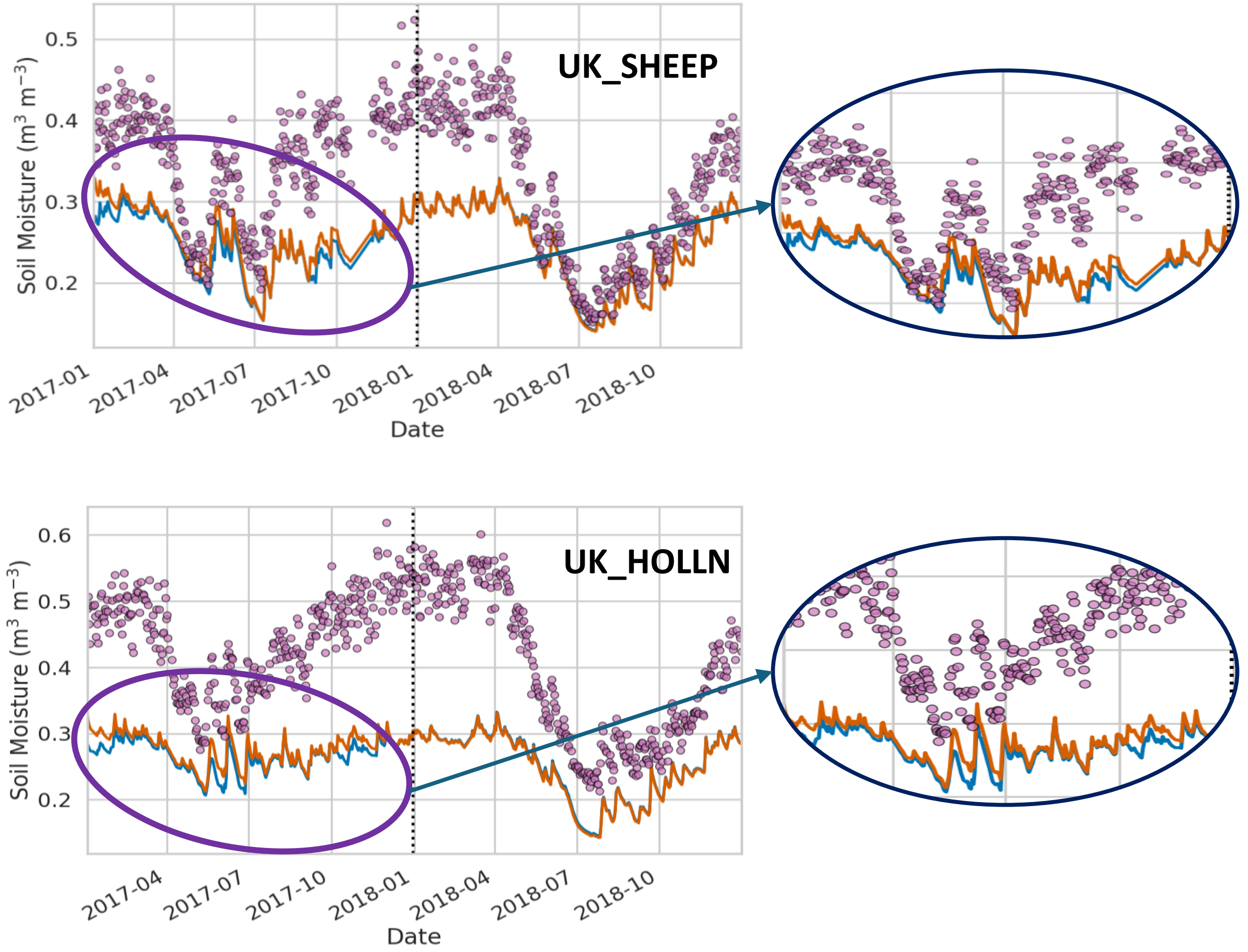


Figure: Modelled (ensemble mean) and COSMOS soil moisture time series at the HOLLN and SHEEP sites during the assimilation (2017) and forecast (2018) periods during dynamic state assimilation approach

Observation Prior Posterior

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Future directions

Ultimate Goal: Produce a KM scale soil moisture product for UK using JULES land surface model

- Potentially to be used by ***UKCEH*** and ***Met-office*** for their hydrological outlook portal

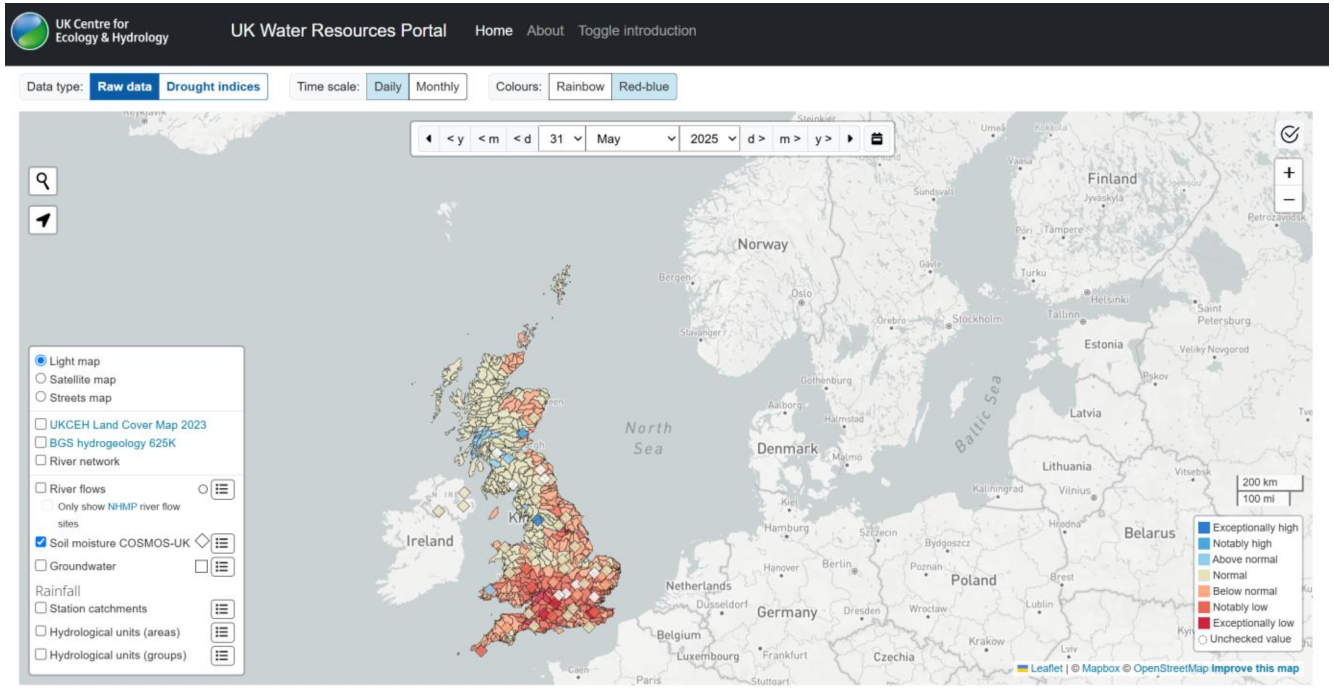

Fig: UKCEH's Hydrological Outlook Map

Step 1: Perform state-parameter assimilation on JULES for 16 COSMOS-UK sites across UK (https://doi.org/10.5194/egusphere-2024-3980)
Step 2: Identify optimal assimilation window length and perform cyclic update of JULES initial soil moisture condition (Ongoing)
Step 3: Multivariate assimilation of soil moisture and streamflow observations within state-parameter framework for gridded JULES model (Future)

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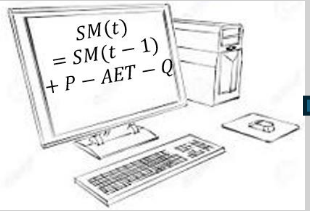
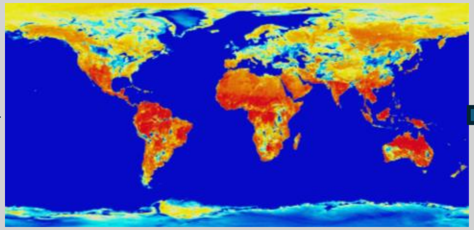
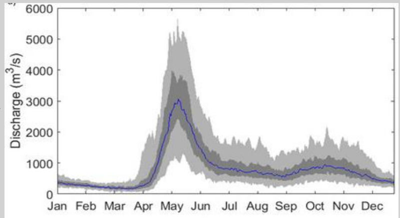
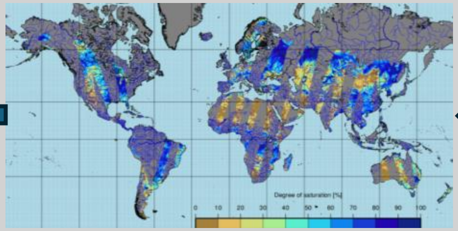
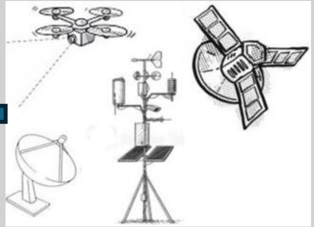

$SM(t)$
$= SM(t-1)$
$+ P - AET - Q$


Discharge (m^3/s)
6000
5000
4000
3000
2000
1000
0
Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec



Thank you

Part 1: JULES Parameter Estimation

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https://doi.org/10.5194/gmd-13-55-2020

Geoscientific Model Development
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The Land Variational Ensemble Data Assimilation Framework: LAVENDAR v1.0.0

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Abstract. The Land Variational Ensemble Data Assimilation Framework (LAVENDAR) implements the method of four-dimensional ensemble variational (4D-En-Var) data assimilation (DA) for land surface models. Four-dimensional ensemble variational data assimilation negates the often costly calculation of a model adjoint required by traditional variational techniques (such as 4D-Var) for optimizing parameters or state variables over a time window of observations. In this paper we present the first application of LAVENDAR, implementing the framework with the Joint UK Land Environment Simulator (JULES) land surface model. We show that the system can recover seven parameters controlling crop behaviour in a set of twin experiments. We run the same experiments at the Mead continuous maize FLUXNET site in Nebraska, USA, to show the technique working with real data. We find that the system accurately captures observations of leaf area index, canopy height and gross primary productivity after assimilation and improves posterior estimates of the amount of harvestable material from the maize crop by 74 %. LAVENDAR requires no modification to the model that it is being used with and is hence able to keep up to date with model releases more easily than other DA methods.

pacts on human life. Most land surface models will converge to a steady state; their state vector tends toward an equilibrium defined by forcing variables (i.e., the meteorology experienced by the model) and the model parameters. This is quite unlike fluid dynamics models used for the atmosphere and oceans, which exhibit chaotic behaviour; a small change in their initial state can lead to large deviations in the state vector evolution with time. Consequently, for some land surface applications parameter estimation can have greater utility than state estimation (Luo et al., 2015). This article deals primarily with the problem of parameter estimation in land surface models, although the technique we introduce could easily be used for state estimation problems too.

Data assimilation (DA) combines models and data such that resulting estimates are an optimal combination of both, taking into account all available information about respective uncertainties. DA techniques are typically derived from a Bayesian standpoint and have been largely developed to service the needs of atmospheric and ocean modelling, especially where there is a need to provide near-real-time forecasts. Typically the focus of such activities is on estimating the optimal model state as the fundamental laws underlying fluid dynamics are well understood and many of the model

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https://doi.org/10.5194/hess-25-1617-2021

Hydrology and Earth System Sciences
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Improving soil moisture prediction of a high-
land surface model by parameterising pedotr
functions through assimilation of SMAP sate

Ewan Pinnington[1], Javier Amezcua[1], Elizabeth Cooper[2], Simon Dadson[2,3], Ri
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Abstract. Pedotransfer functions are used to relate gridded databases of soil texture information to the soil hydraulic and thermal parameters of land surface models. The parameters within these pedotransfer functions are uncertain and calibrated through analyses of point soil samples. How these calibrations relate to the soil parameters at the spatial scale of modern land surface models is unclear because gridded databases of soil texture represent an area average. We present a novel approach for calibrating such pedotransfer functions to improve land surface model soil moisture prediction by using observations from the Soil Moisture Active Passive (SMAP) satellite mission within a data assimilation framework. Unlike traditional calibration procedures, data assimilation always takes into account the relative uncertainties given to both model and observed estimates to find a maximum likelihood estimate. After performing the calibration procedure, we find improved estimates of soil moisture and heat flux for the Joint UK Land Environment Simulator (JULES) land surface model (run at a 1 km resolution) when compared to estimates from a cosmic-ray soil moisture monitoring network (COSMOS-UK) and three flux tower sites. The spatial resolution of the COSMOS probes is much more representative of the 1 km model grid than traditional point-based soil moisture sensors. For 11 cosmic-ray neutron soil moisture probes l
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1 Introduction

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Using data assimilation to optimize pedotransfer functions using field-scale in situ soil moisture observations

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Abstract. Soil moisture predictions from land surface models are important in hydrological, ecological, and meteorological applications. In recent years, the availability of wide-area soil moisture measurements has increased, but few studies have combined model-based soil moisture predictions with in situ observations beyond the point scale. Here we show that we can markedly improve soil moisture estimates from the Joint UK Land Environment Simulator (JULES) land surface model using field-scale observations and data assimilation techniques. Rather than directly updating soil moisture estimates towards observed values, we optimize constants in the underlying pedotransfer functions, which relate soil texture to JULES soil physics parameters. In this way, we generate a single set of newly calibrated pedotransfer functions based on observations from a number of UK sites with different soil textures. We demonstrate that calibrating a pedotransfer function in this way improves the soil moisture predictions of a land surface model at 16 UK sites, leading to the potential for better flood, drought, and climate projections.

(PTFs) to relate readily available or easy-to-measure soil characteristics such as soil texture to the soil hydraulics parameters required by the model (e.g. Van Looy et al., 2017)

There are a number of different types of pedotransfer function, as noted in Van Looy et al. (2017) and Hodnett and Tomasella (2002), with different inputs and outputs depending partly on the representation of soil physics processes of the chosen land surface model. In "class" approaches, soil types are clustered into groups, and hydraulic model parameters are then obtained from a lookup table (Wösten et al., 1999); this results in discrete soil hydraulics parameter sets. Alternatively, continuous pedotransfer functions take soil characteristic information from each sample of interest and apply the function to produce continuous soil hydraulics parameter sets (e.g. Cosby et al., 1984; Hodnett and Tomasella, 2002; Schaap et al., 2001).

To date, pedotransfer functions have been derived by fitting to results from field or laboratory experiments on point- or small-scale soil samples (centimetre to metre), despite the fact that land surface models are generally applied at larger (field to kilometre) scales. The recent development of novel in situ techniques for measuring soil moisture over

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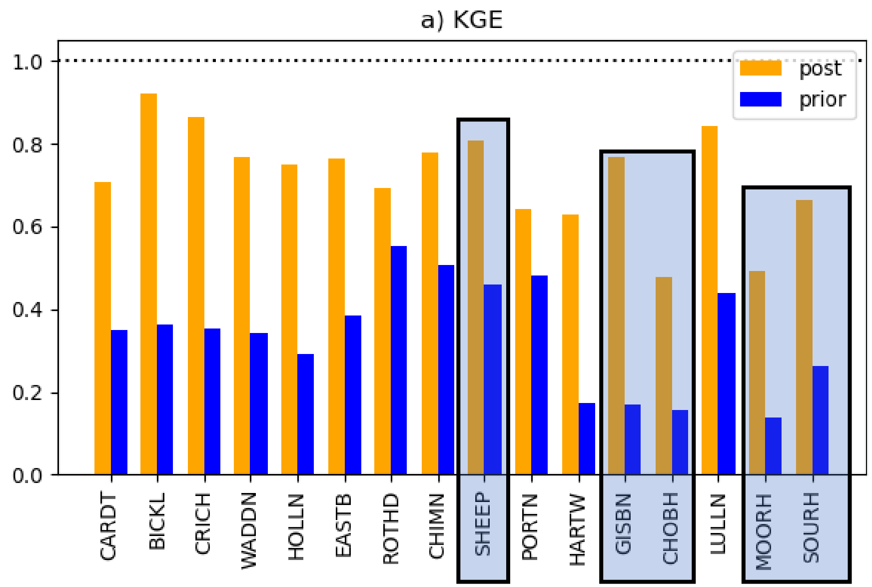
Effect of DA on Non-typical Soil Sites



Site name and abbreviation	Land cover	Soil description
Cardington (CARDT)	Grassland	Typical mineral soil
Bickley Hall (BICKL)	Grassland	Typical mineral soil
Crichton (CRICH)	Grassland	Typical mineral soil
Waddesdon (WADDN)	Grassland	Typical mineral soil
Hollin Hill (HOLLN)	Grassland	Typical mineral soil
Easter Bush (EASTB)	Grassland	Typical mineral soil
Rothamstead (ROTHD)	Grassland	Typical mineral soil
Chimney Meadows (CHIMN)	Grassland	Calcereous mineral soil
Sheepdrove (SHEEP)	Grassland	Mineral soil, fairly high organic carbon content
Porton Down (PORTN)	Grassland	Highly calcareous mineral soil
Hartwood Home (HARTW)	Grassland/woodland	Typical mineral soil
Gisburn Forest (GISBN)	Coniferous forest	Mineral soil, high organic carbon content
Chobham Common (CHOBH)	Heath	Highly variable soil
Lullington Heath (LULLN)	Grassland/heath	Highly calcareous mineral soil
Moorhouse (MOORH)	Grassland/heath	Mineral soil with very high organic content
Sourhope (SOURH)	Grassland	Mineral soil with very high organic content

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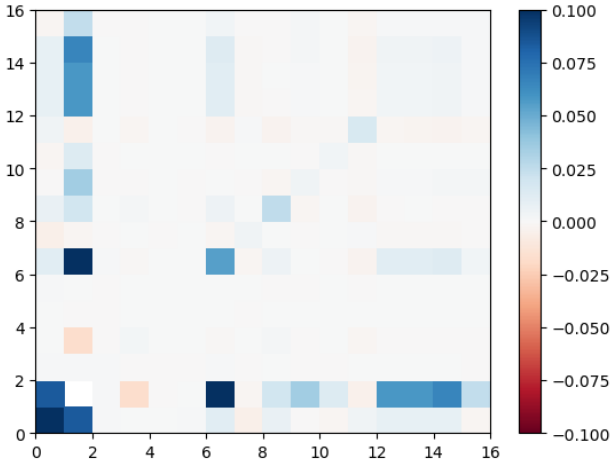
Place	KGE-Prior	KGE- Post.	% increase	Rank
CARDT	0.35	0.71	102.85	10
BICKL	0.36	0.92	155.55	6
CHRICH	0.35	0.86	145.71	8
WADDN	0.34	0.77	126.47	9
HOLLN	0.29	0.75	158.62	5
EASTB	0.38	0.76	100	11
ROTHD	0.55	0.69	25.45	16
CHIMN	0.51	0.78	52.94	14
SHEEP	0.46	0.81	76.08	13
PORTN	0.48	0.64	33.33	15
HARTW	0.17	0.63	270.58	2
GISBN	0.17	0.77	352.94	1
CHOBH	0.15	0.48	220	4
LULLN	0.44	0.84	90.90	12
MOORH	0.14	0.49	250	3
SOURH	0.26	0.66	153.84	7

Correlation and Error Co-variance plots



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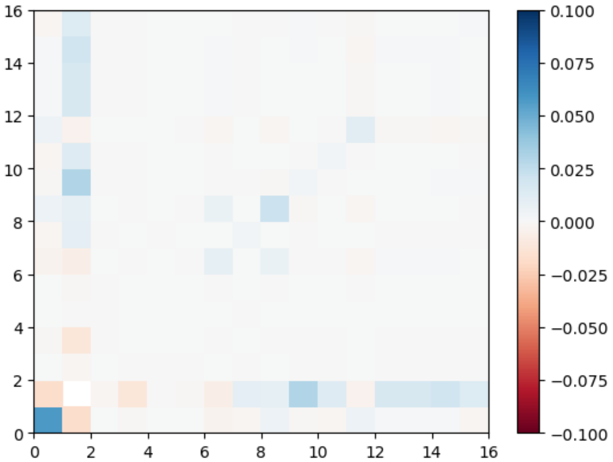

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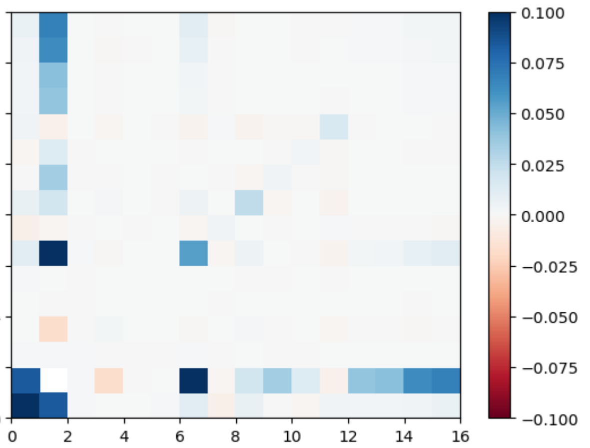

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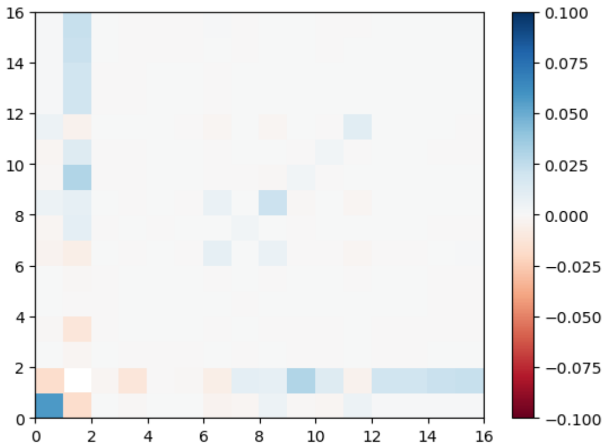

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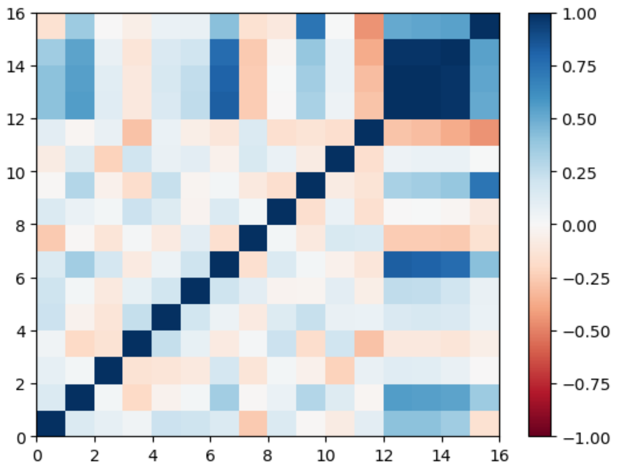

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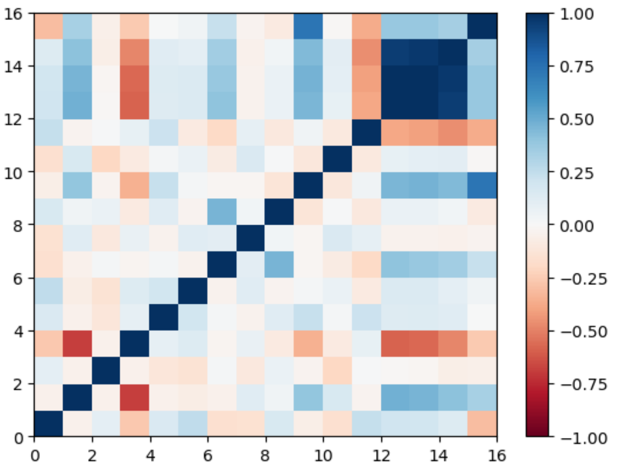

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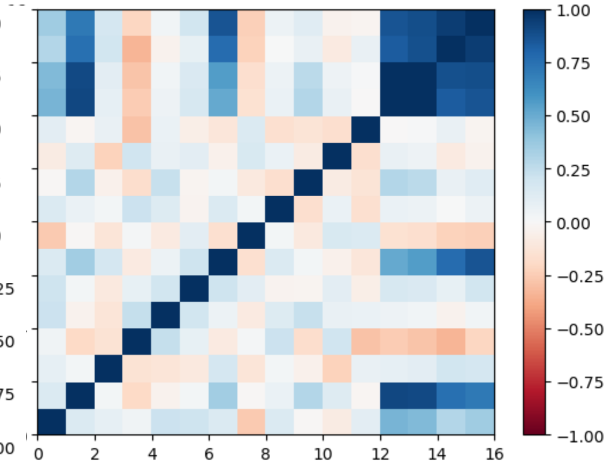

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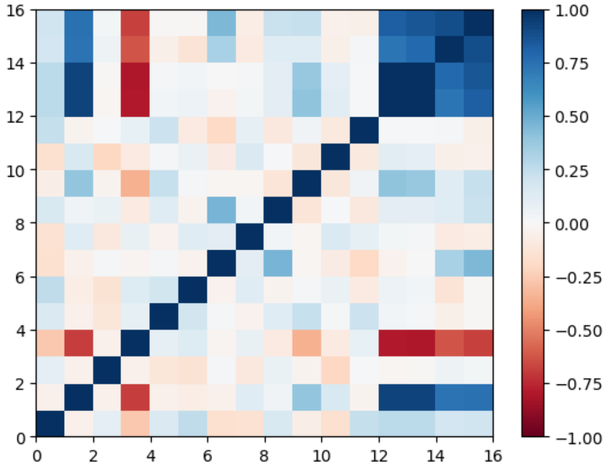

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