Developing Machine-Learning Based Emulators for the JULES Land Surface Model

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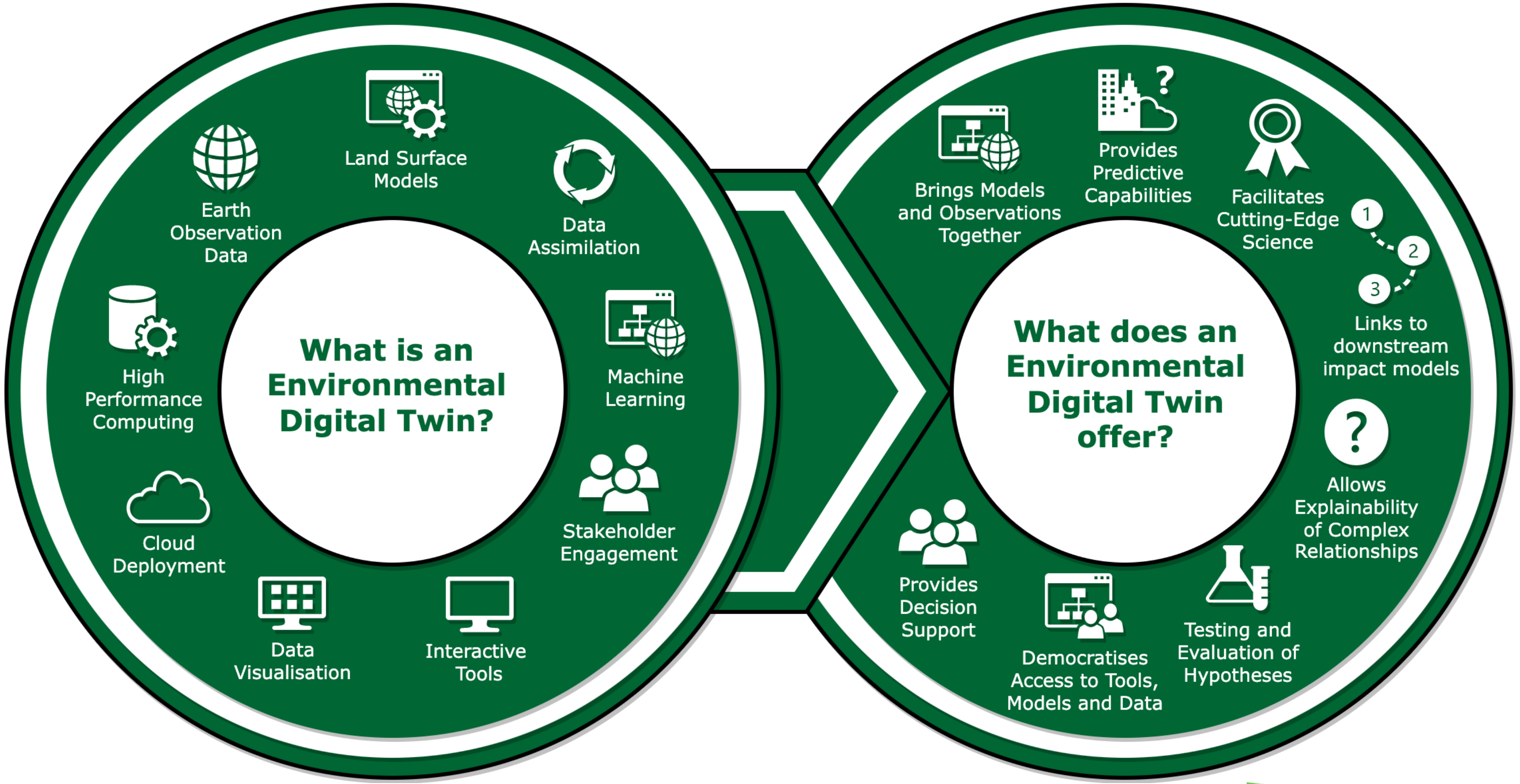
What is a Digital Twin?

- A digital representation of a physical system…
  - With some predictive capability (i.e. a model)…
  - That is data-driven (e.g. Earth Observation, in-situ, citizen data, etc)…
  - Capable of providing decision support to stakeholders
- Lots of different components and considerations that span a whole host of scientific, logistical, technical and IT areas
- Potentially hugely complex and ambitious
- Can extend beyond *just* environmental science (e.g. economics, social sciences, public health, etc)



Benefits of emulating the JULES land surface model

Emulator can accurately reproduce JULES simulations but also:

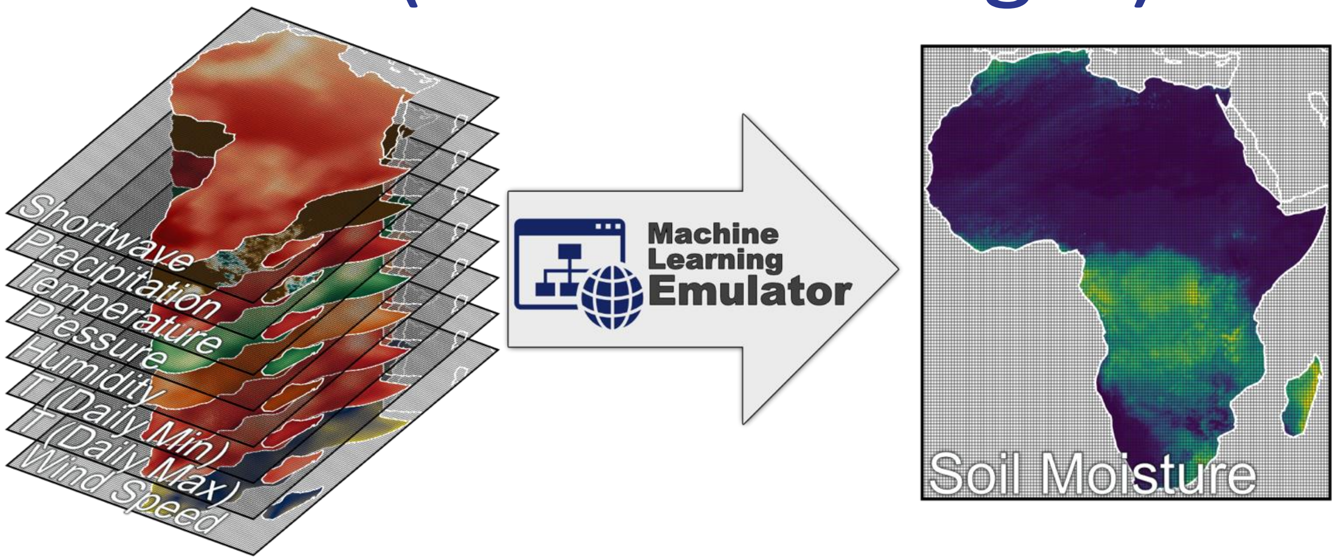
- is extremely fast (years per millisecond)
  - can run huge ensembles, sample uncertainties, etc
- is extremely simple/lightweight (deployed in cloud/notebook/etc)
  - makes JULES far more accessible to non-expert users
  - can be embedded into climate services
- allows explainability of model (Explainable AI methods)
- can be driven by other data (e.g. EO data)
  - constrained by the “physics” within JULES
  - but means we can potentially out-perform JULES by combining JULES and EO data
  - can run at whatever resolution we have available input data for

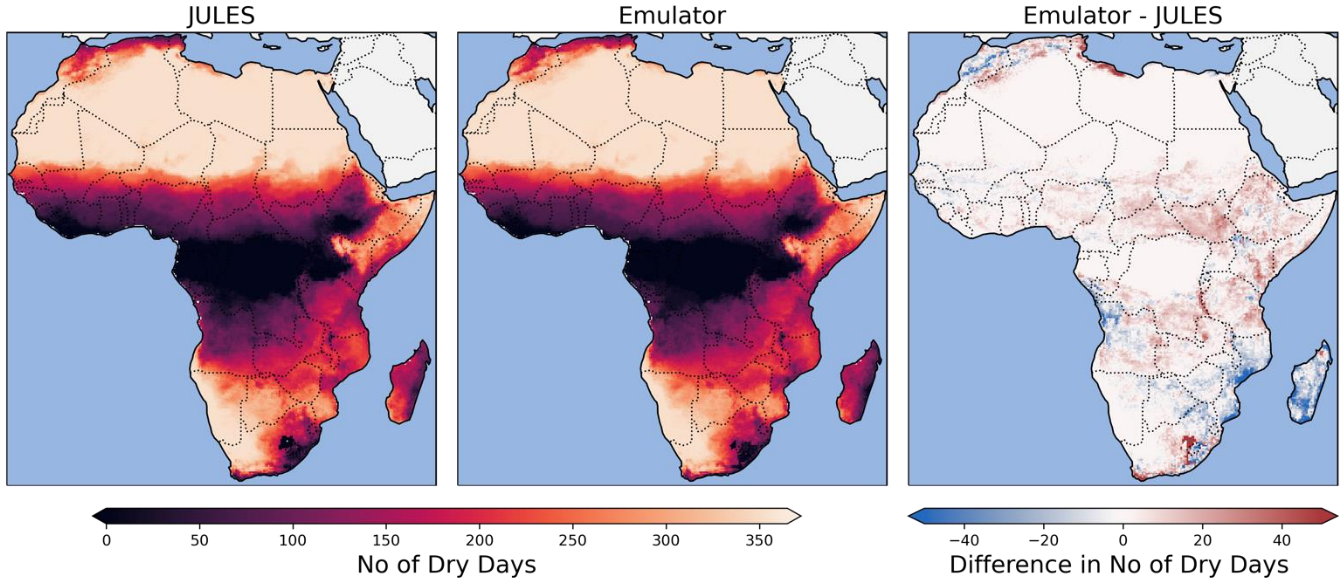
Two NCEO projects related to this work:

- ESA Digital Twin Earth - Drought - Soil moisture over Africa
- ESA IMITATE - Carbon Cycle - GPP over Europe

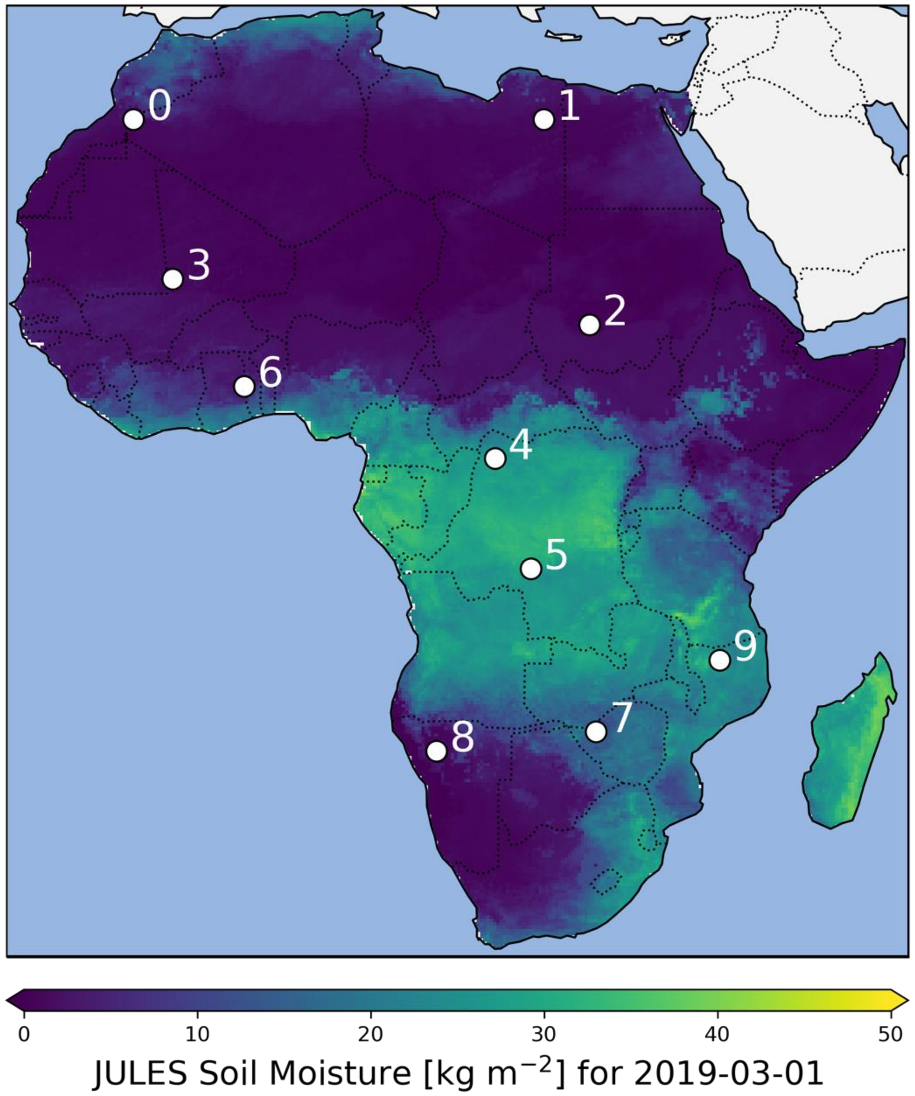
ESA Digital Twin Earth Precursor (African Drought)

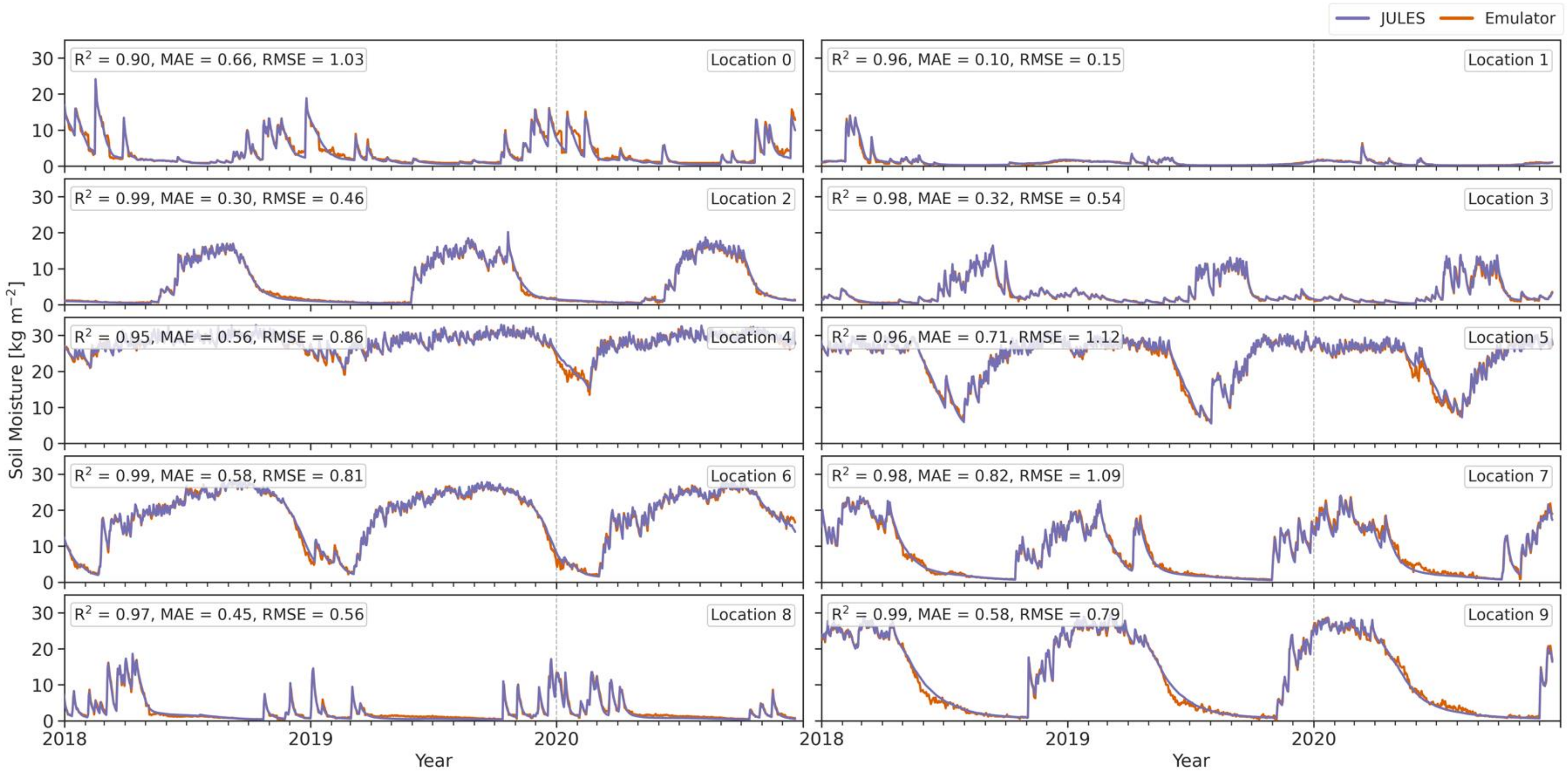
- We've used machine learning to emulate the complex, computationally expensive model in a very fast and light-weight way
- Produce drought metrics - currently **wet season length**, **start date of wet season** and **number of dry days**
- Widgets for these are deployed within our **Interactive Data Portal**
- Emulator is **extremely fast** and **runs in the web-browser**, allowing users to ask their own questions based around soil-moisture response to climate





Evaluation of Emulator





- ❑ Emulator performs exceptionally well and reproduces results of JULES model

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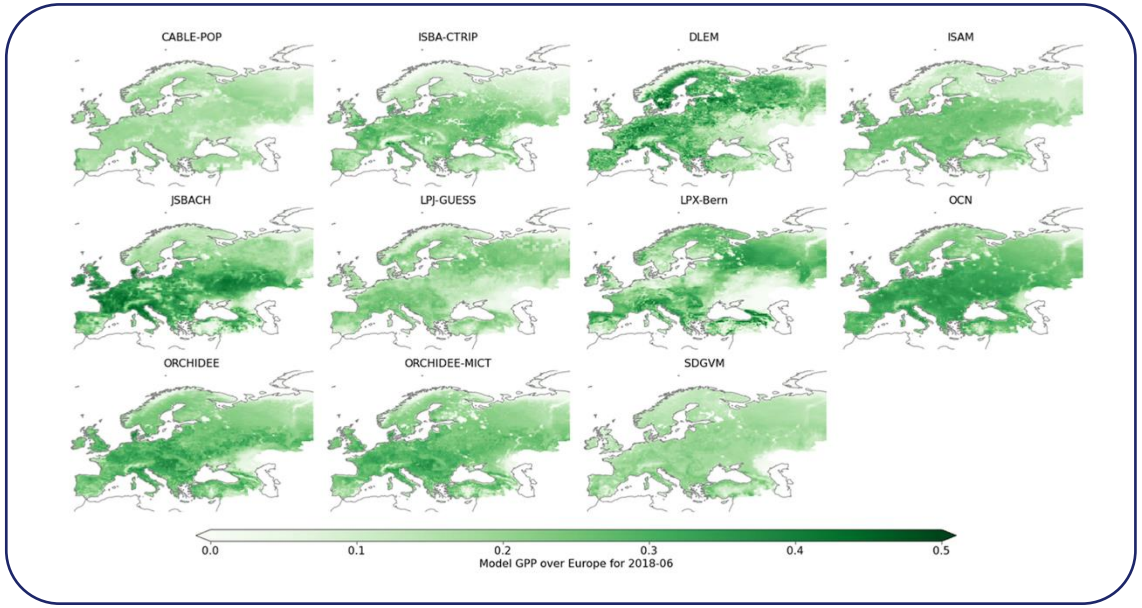
ESA IMITATE (Carbon Cycle)

IMITATE – Introducing Machine-learning Into Targeted Analysis for Terrestrial Ecosystems

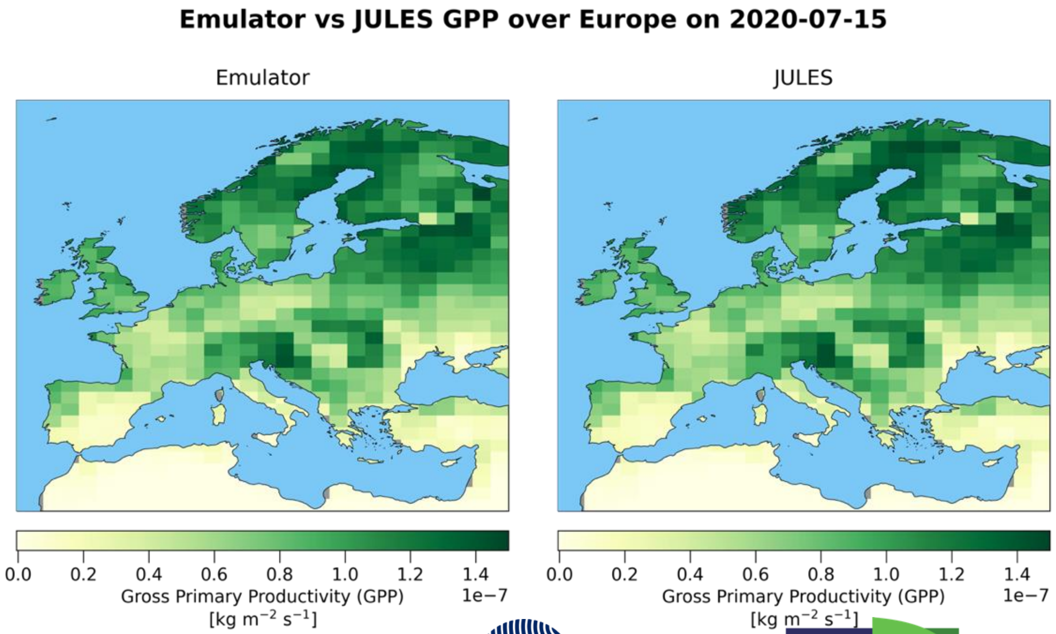
The carbon cycle over Europe is still **highly** uncertain and neither observations nor models alone are capable of addressing these issues.



We are developing machine-learning model **emulators** to replicate simulations from complex land surface model.

Emulators allow greater **understanding** of the model behaviour and let us explore the different relationships between the drivers and carbon fluxes.

We can then use emulator **with** Earth Observation data to derive **new** datasets that are explicitly tied to observations and can make use of their uncertainties.



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JULES Data

All GPP-related inputs

Gridbox emulator | Per-PFT emulator

- Minimum Temperature
- Maximum Temperature
- Soil moisture (**all layers**)
- Soil Moisture Availability Factor
- FAPAR
- SW Downwelling Radiation

Observable inputs

Per-PFT emulator

- Minimum Temperature
- Maximum Temperature
- Soil moisture (**top layer**)
- Diffuse VIS albedo
- Diffuse NIR albedo

EO Data

EO inputs

Per-PFT emulator

- Minimum LST
- Maximum LST
- Soil moisture (surface)
- White-sky VIS albedo
- White-sky NIR albedo

Features used in emulator training

1) Can we emulate JULES GPP using all available (relevant) JULES variables?

2) Can we emulate JULES GPP using only JULES variables that have an EO equivalent?

3) Can we use the EO data directly to produce an EO-based GPP data product constrained by JULES process representation?

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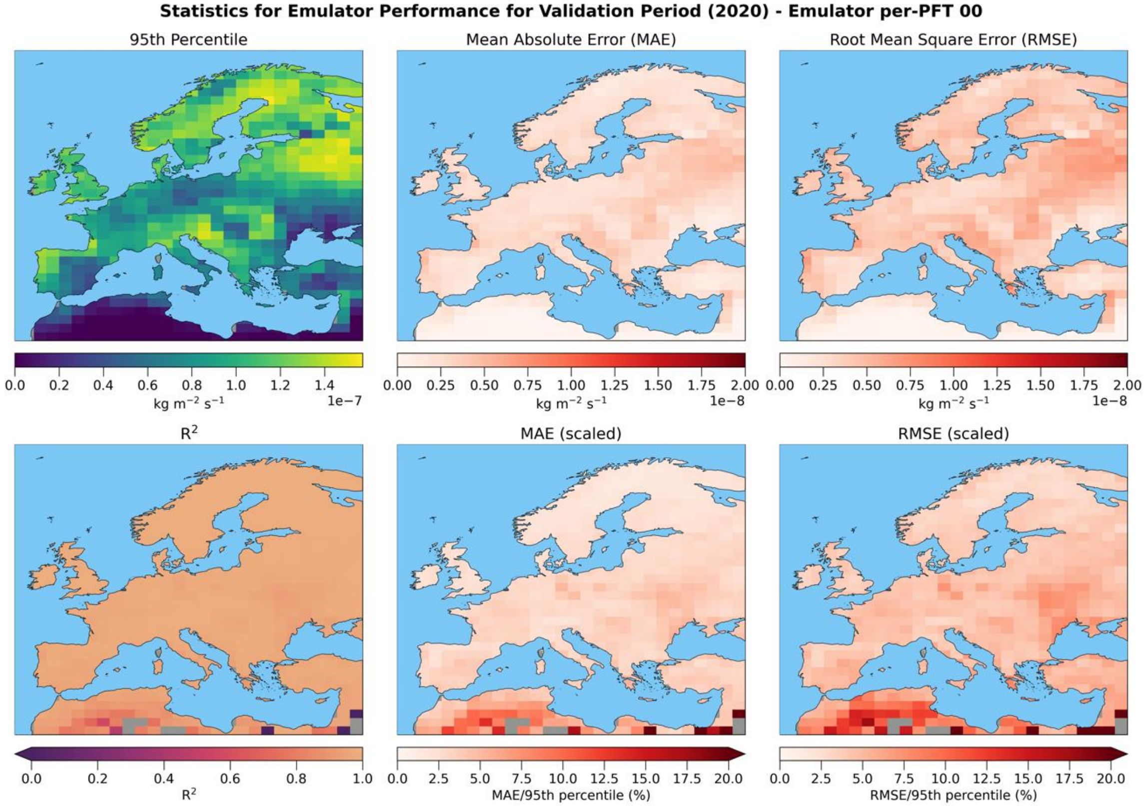
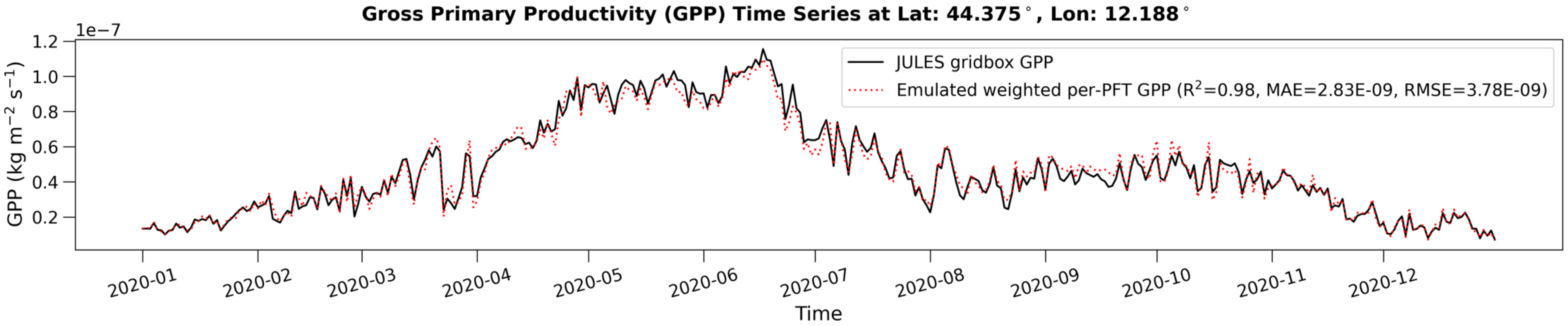
1) Can we emulate JULES GPP using all available (relevant) JULES variables?

Features
- Minimum Temperature
- Maximum Temperature
- Soil moisture (**all layers**)
- Soil Moisture Availability Factor
- FAPAR
- SW Downwelling Radiation





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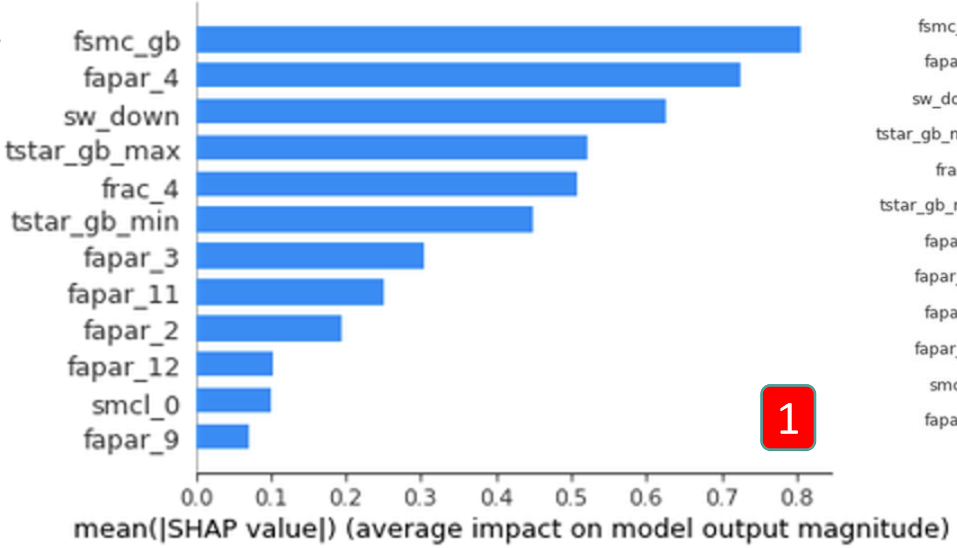
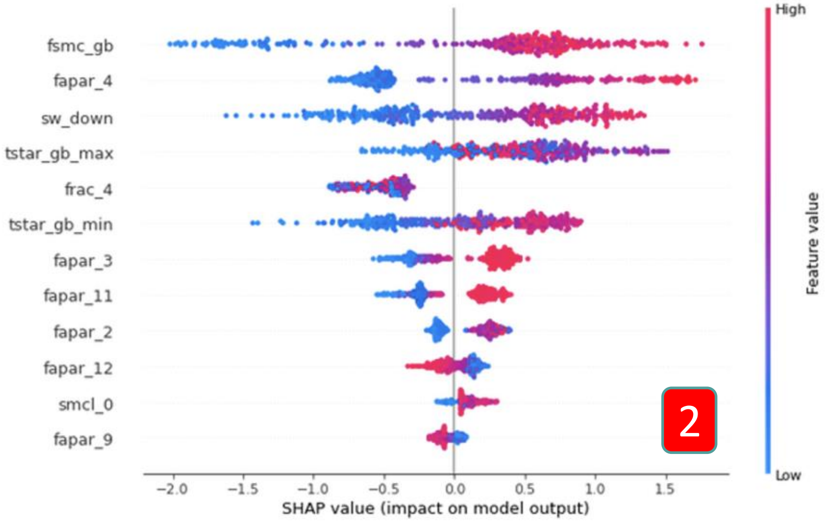
Explainability and Interpretability

work in progress

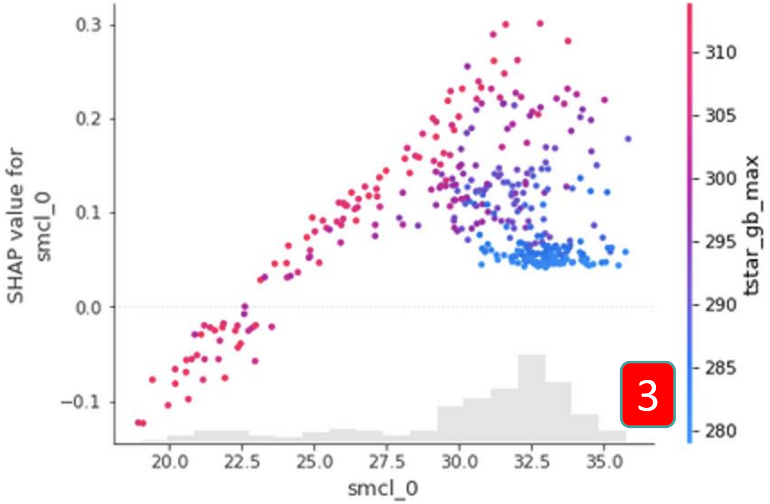
- ❑ SHAP values can be thought of as the influence a particular input feature has on the output
- ❑ It's referenced to the mean value of the output

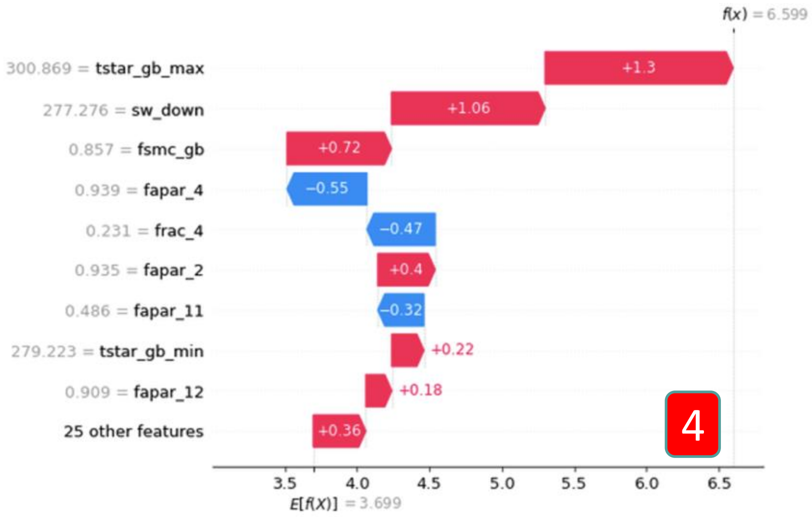




Plots show:

- ❑ (1) Overall feature importance
- ❑ (2) How each feature impacts on GPP over whole timeseries
- ❑ (3) Interactions between different features
- ❑ (4) What causes the GPP value for a single point





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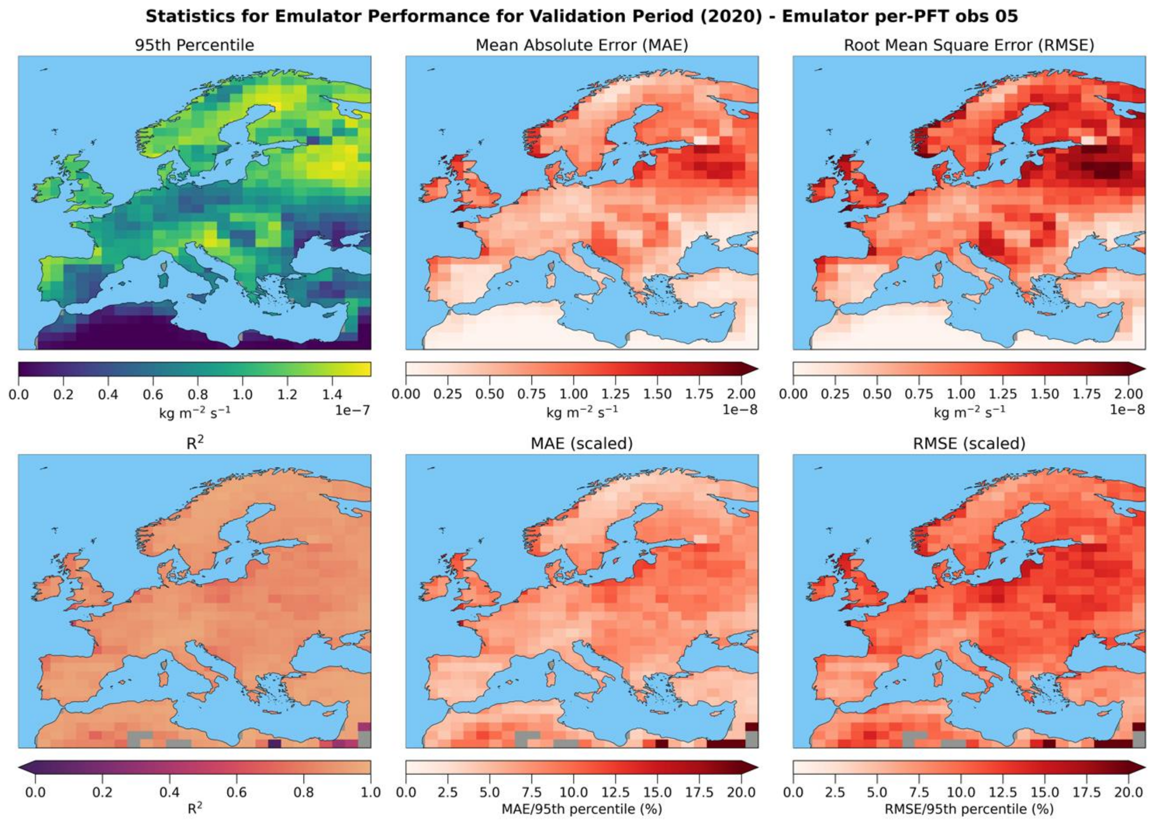
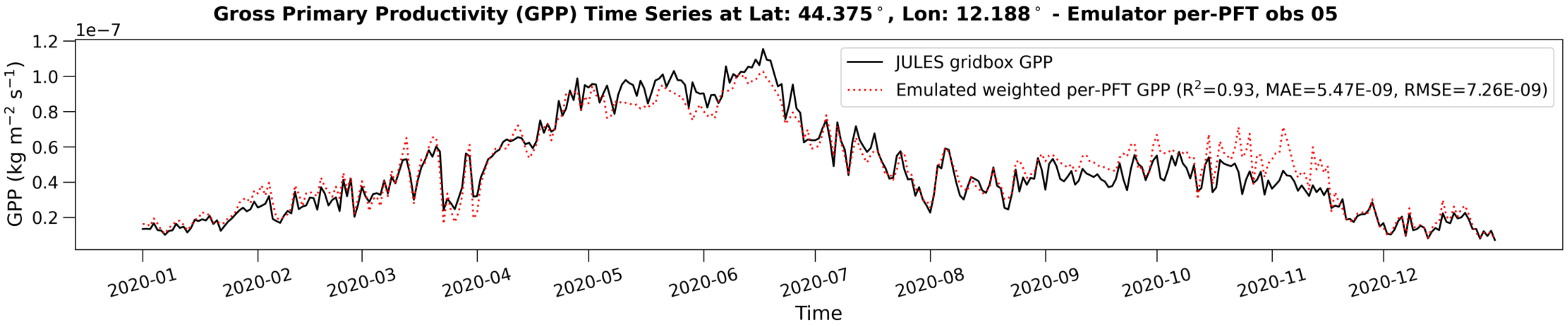
work in progress

2) Can we emulate JULES GPP using only JULES variables that have an EO equivalent?

Features

- Minimum Temperature
- Maximum Temperature
- Soil moisture (**top layer**)
- Diffuse VIS albedo
- Diffuse NIR albedo
- Soil Moisture Availability Factor



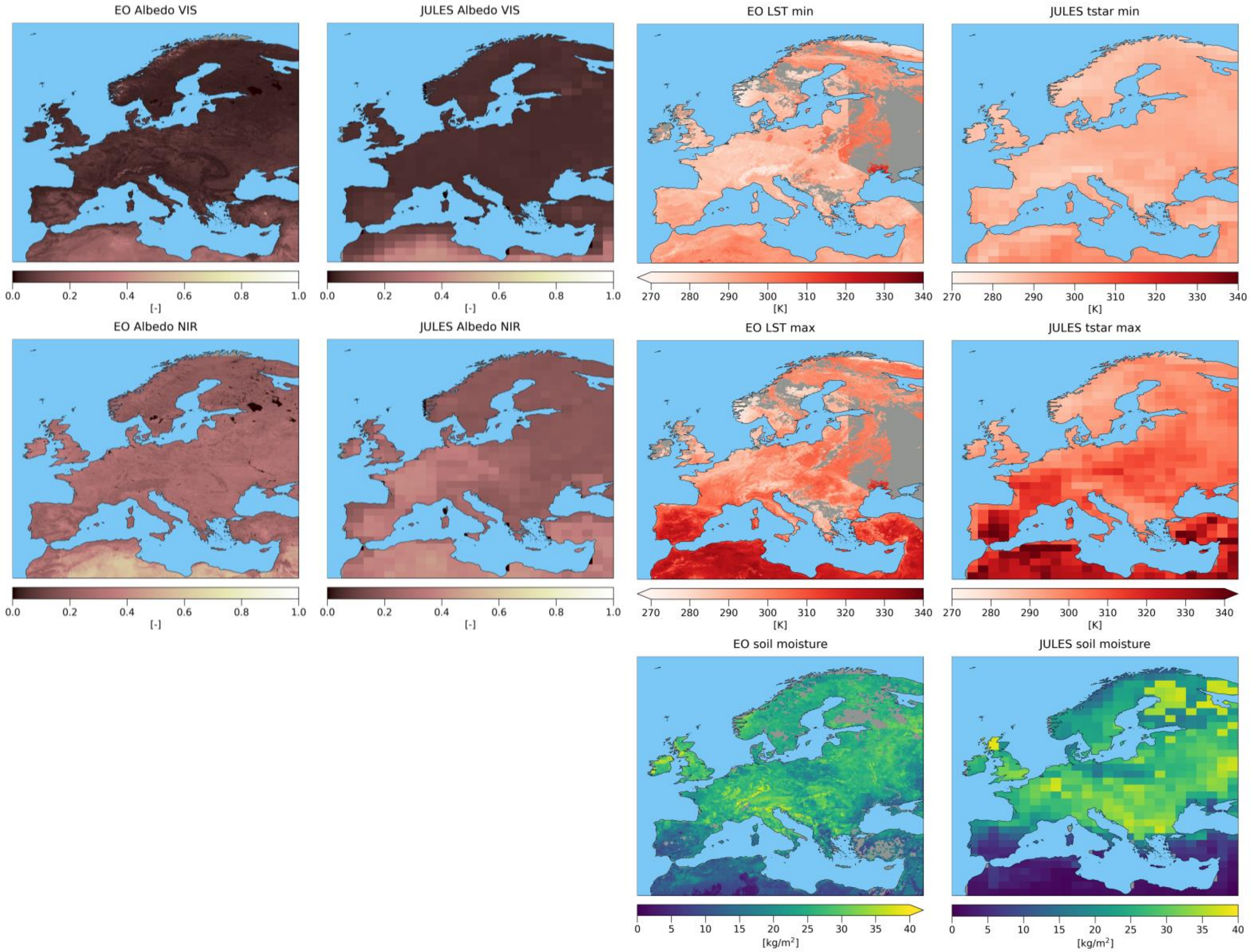


work in progress

3) Can we use the EO data directly to produce an EO-based GPP data product constrained by JULES process representation?

- Minimum LST
- Maximum LST
- Soil moisture (surface)
- White-sky VIS albedo
- White-sky NIR albedo
- Soil Moisture Availability Factor

Example of EO data vs JULES for a single day (July 2014)

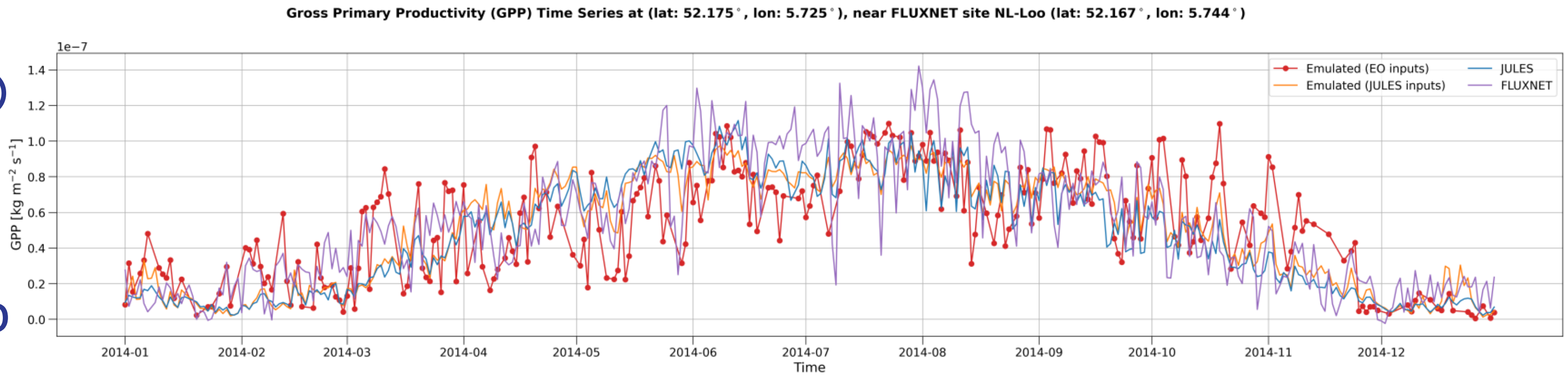


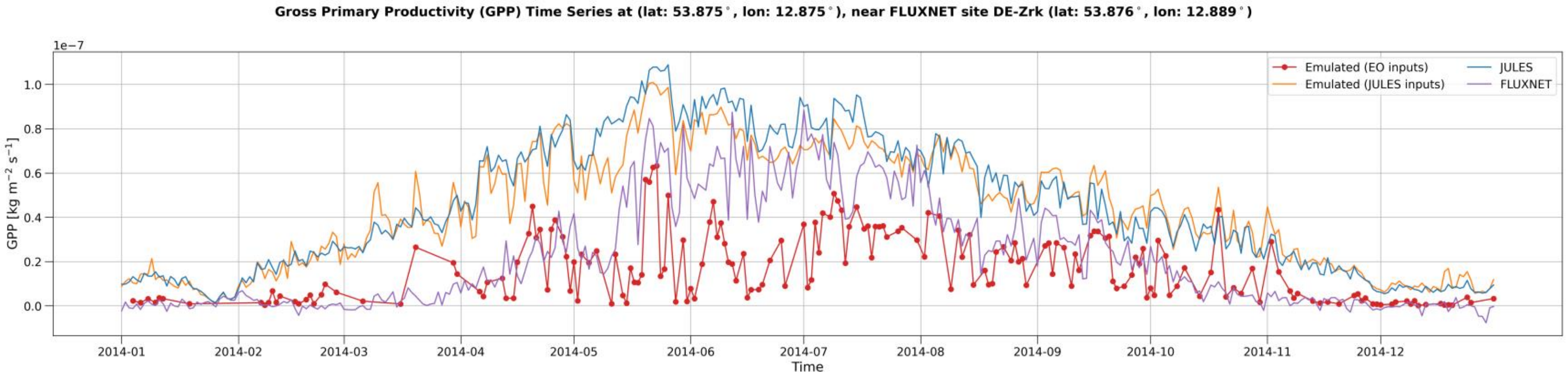
work in progress

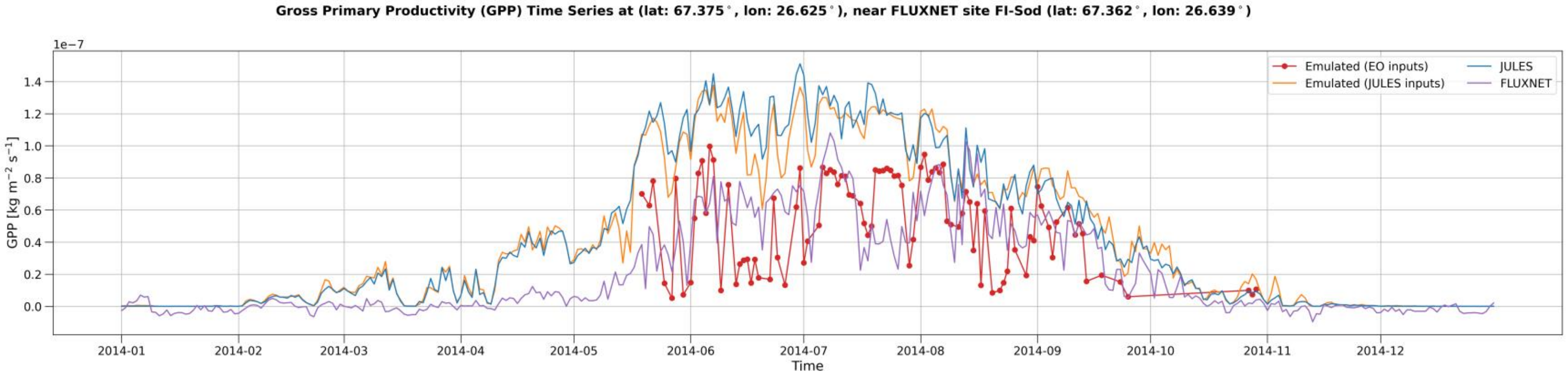
Some cherry-picked examples ☺

For some FLUXNET sites either:

- ❑ EO-based results are similar to JULES (and agree well with FLUXNET)
- ❑ Parts of the timeseries with EO-based emulator compares better to FLUXNET than JULES did (and parts don’t!)
- ❑ EO-based emulator does better than JULES at matching FLUXNET
- ❑ Some sites (not shown) are awful!







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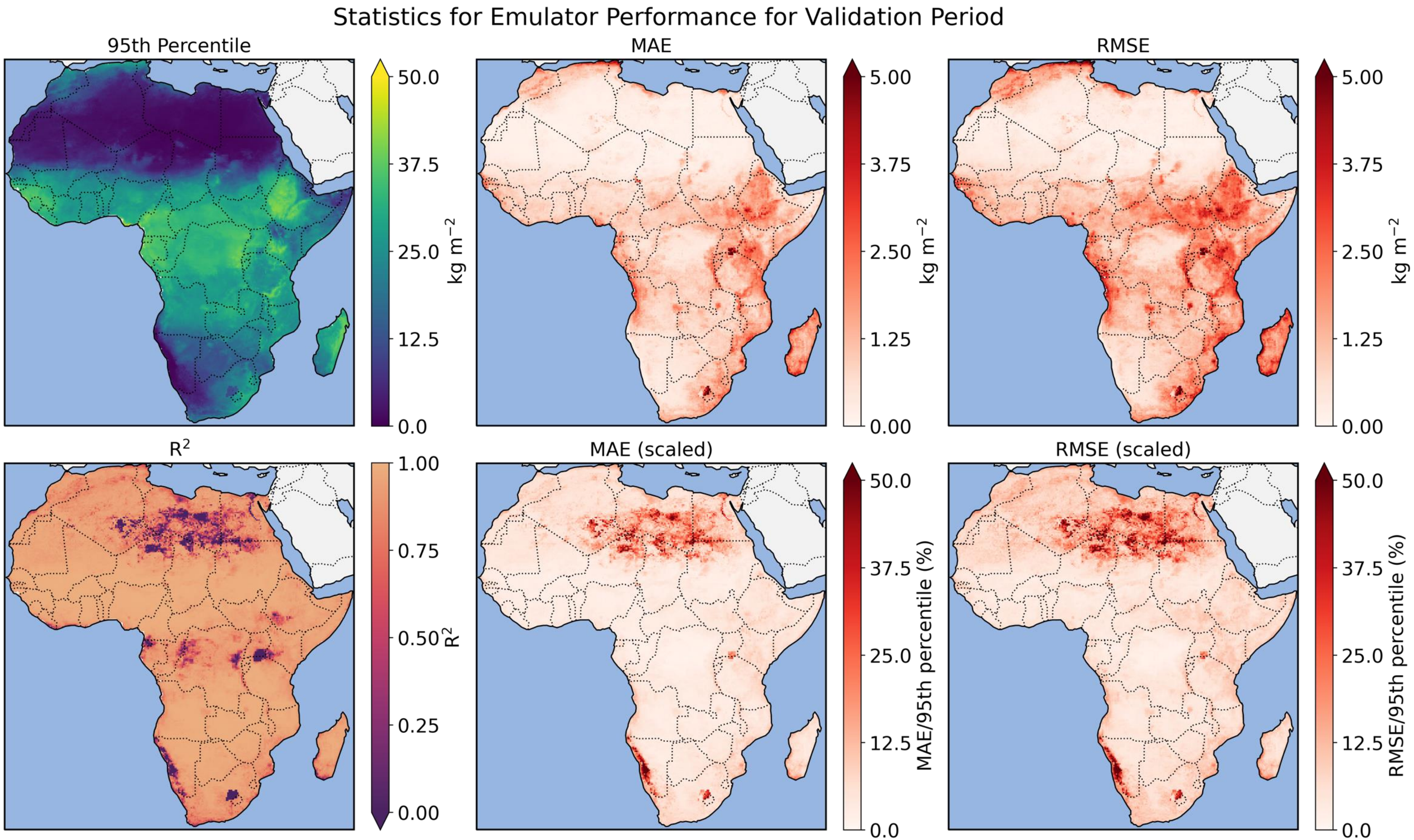
Summary and Conclusions

- We've successfully developed machine-learning based emulators for several different JULES applications (drought and GPP)
- These emulators are (very!) fast, easy to use, etc and open up a range of applications and potentially interesting science
- If we can successfully use EO data to drive emulator, we nicely bring together physics-based process models with power of satellite observations (and their uncertainties!)
- Explainability/Interpretability have the potential to help us really explain/understand model behaviour
- Lessons learned: If there are land surface model simulations where we can easily map the inputs to the output, we can probably build an emulator for it!
- Much more work to do in this area: deploying applications, Explainable AI, model-data fusion by driving with EO data, uncertainty propagation, extending beyond JULES to other land surface models, etc.
- Please do get in touch if this is interesting to you ☺

Extra Slides


Statistics for Emulator Performance for Validation Period
95th Percentile
50.0
37.5
25.0
12.5
0.0
kg m⁻²
MAE
5.00
3.75
2.50
1.25
0.00
kg m⁻²
RMSE
5.00
3.75
2.50
1.25
0.00
kg m⁻²
R²
1.00
0.75
0.50
0.25
0.00
R²
MAE (scaled)
50.0
37.5
25.0
12.5
0.0
MAE/95th percentile (%)
RMSE (scaled)
50.0
37.5
25.0
12.5
0.0
RMSE/95th percentile (%)

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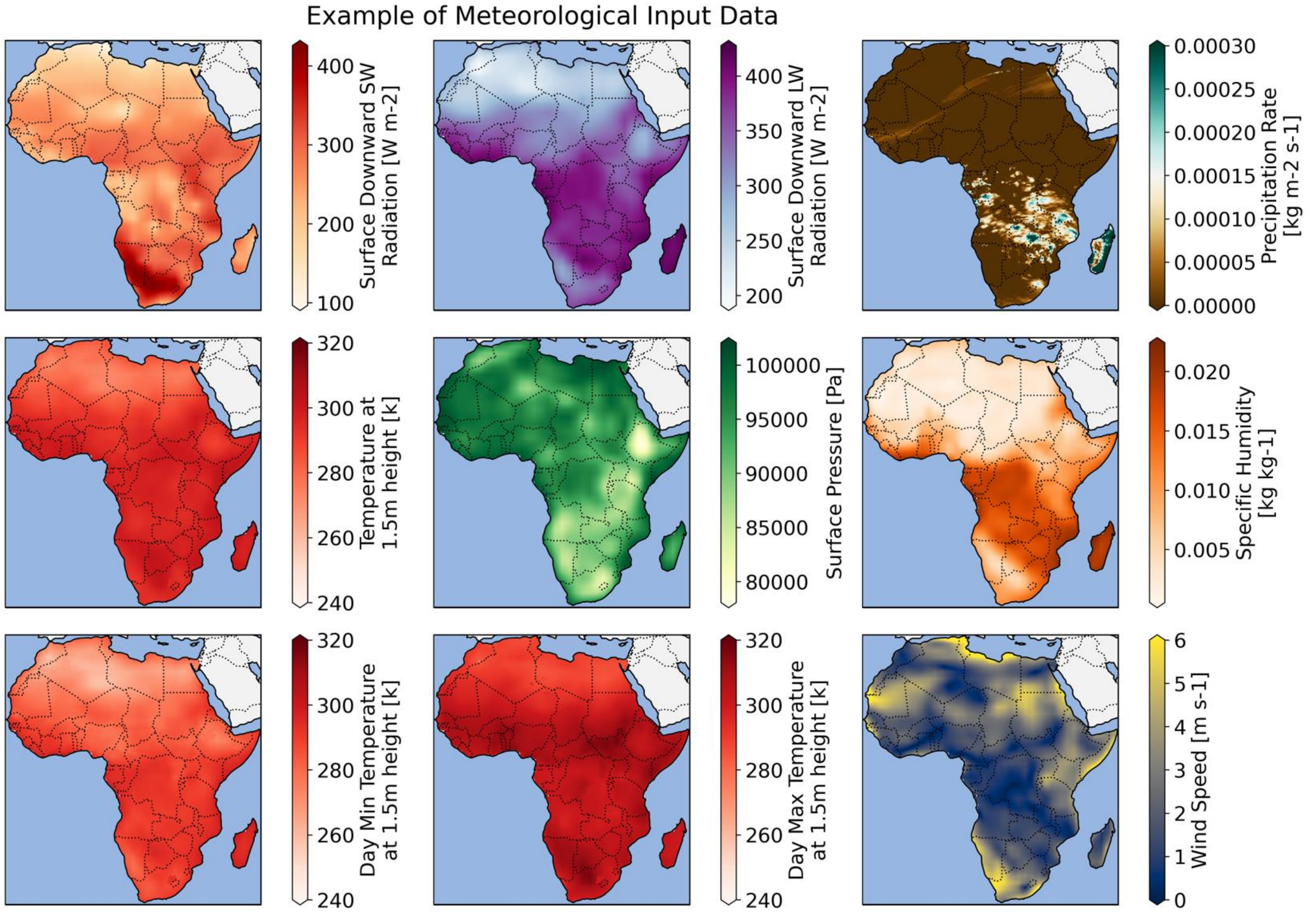
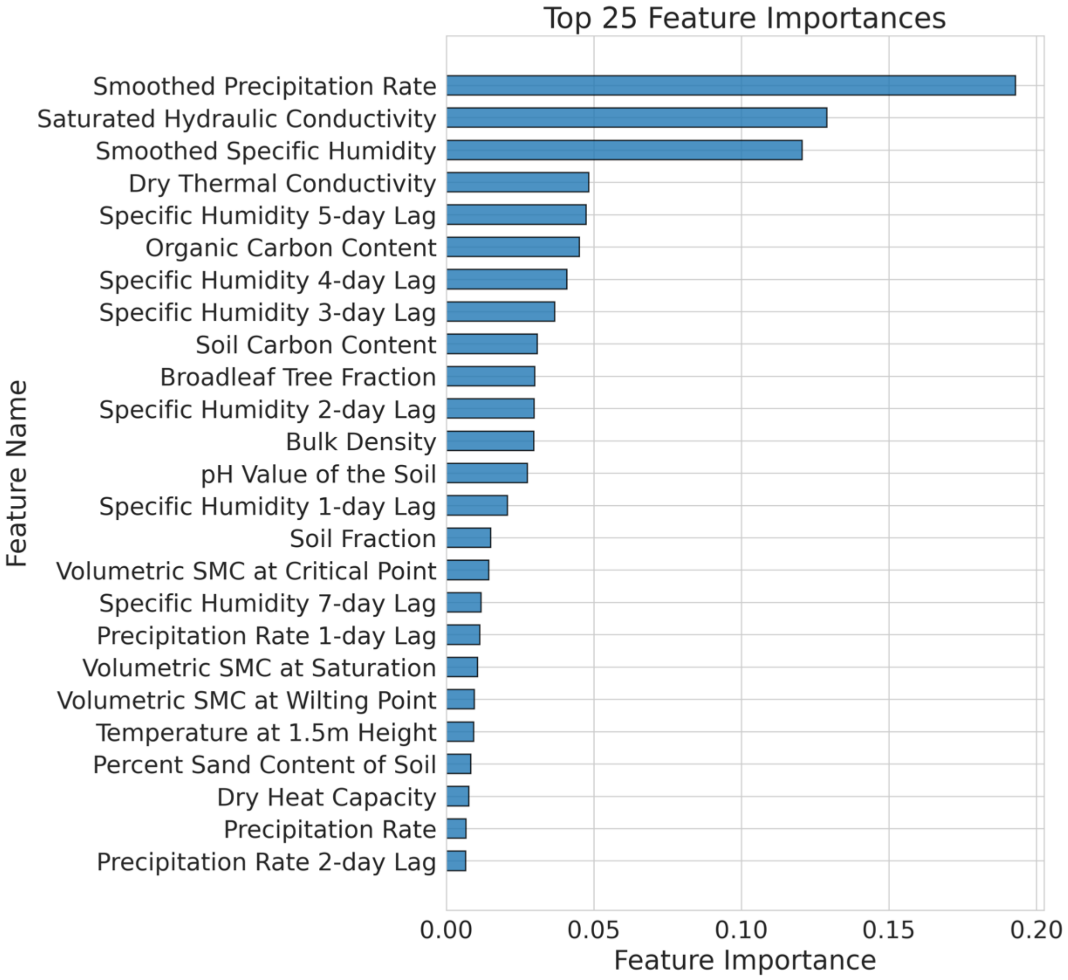
Explainability and Feature Importance





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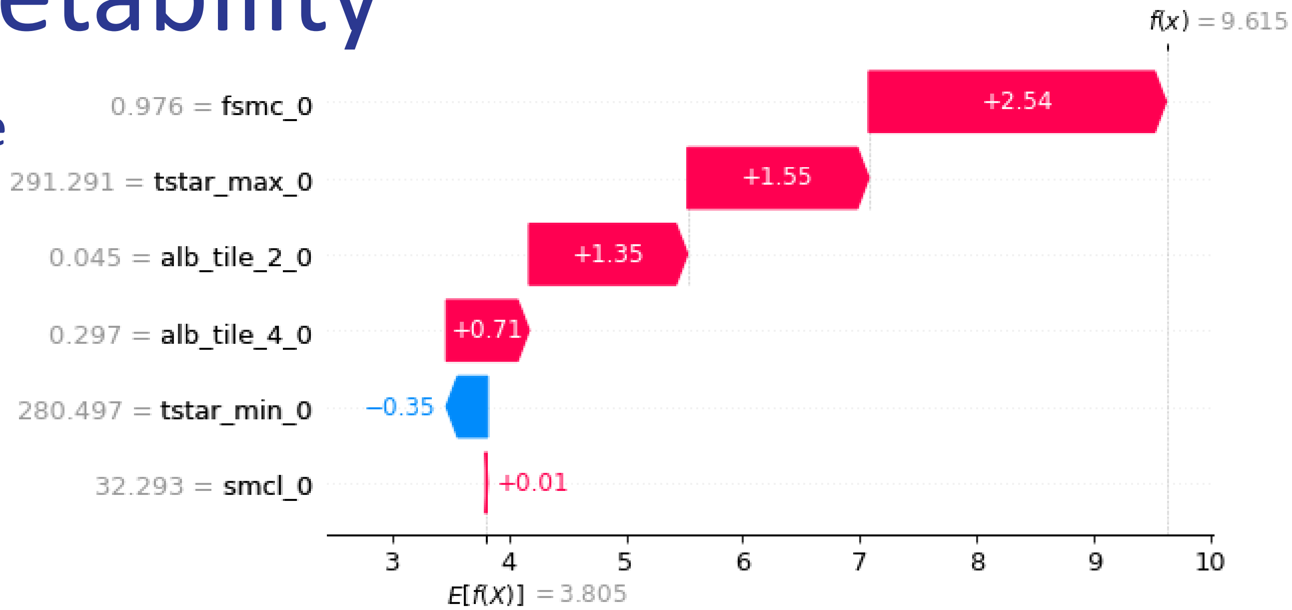
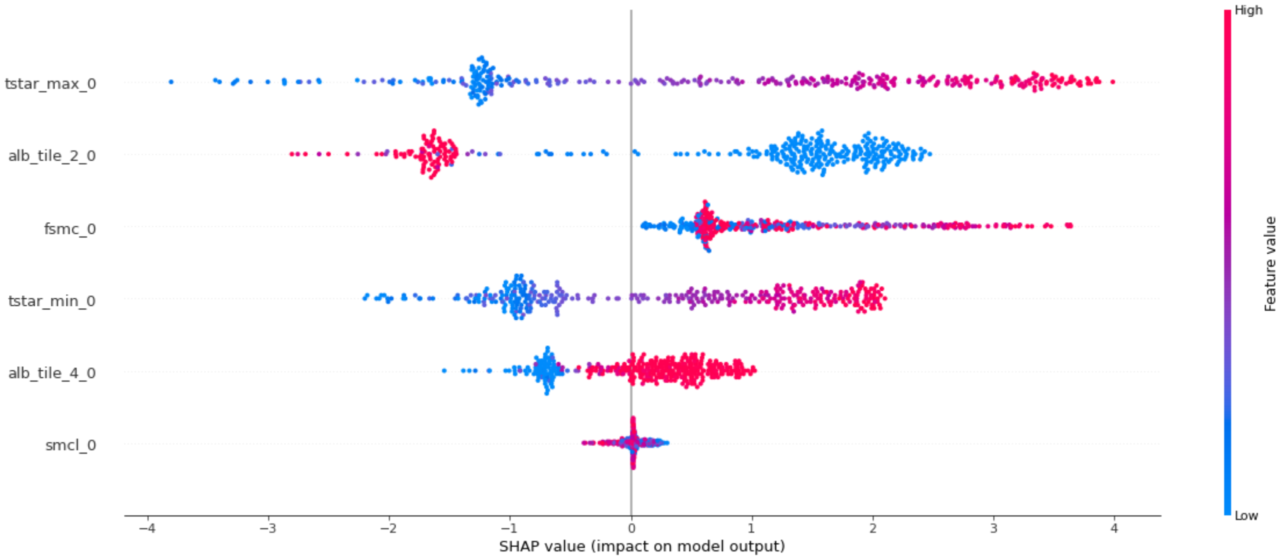
Explainability and Interpretability

- SHAP values can be thought of as the influence a particular input feature has on the output
- It's referenced to the mean value of the output
- Fig 1 shows the effect of the particular values of each input feature for **a particular data point** and how they moved the result from the mean expected value
- Fig 2 shows **for an entire timeseries** how each input feature has affected the result, i.e.
  - Low values of temperature reduce GPP
  - Low values of VIS albedo increase GPP
  - Low values of NIR albedo decrease GPP
- This sort of explainability can be very powerful!





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next steps

3) Can we use the EO data directly to produce an EO-based GPP data product constrained by JULES process representation?

	Soil Moisture	Land Surface Temperature	Albedo	Land Cover
Product	ESA CCI soil moisture v6.1 COMBINED	ESA CCI LST 3-hourly	MODIS MCD43C3 CMG Albedo	ESA CCI Global Land Cover Maps v2.0.7
JASMIN path	`/neodc/esacci/soil_moisture/data/daily_files/COMBINED/v06.1`	`/neodc/esacci/land_surface_temperature/data/MULTISENSOR_IRMGP/L3S/0.05/v1.00/daily`	N/A https://ladsweb.modaps.eosdis.nasa.gov/archive/allData/61/MCD43C3/	`/neodc/esacci/land_cover/data/land_cover_maps/v2.0.7`
Units	[m^3 m^{-3}]	[K]	[-]	[-]
Time range	1978-11-01 to 2020-12-31	2009-2020	2000-2022	1992 - 2015
Spatial resolution	0.25 degrees	0.05 degrees	0.05 degrees	300 metres

NERC Digital Twin Case Study

- In the ESA DTEP project we developed a ML-based emulator for JULES soil moisture over Africa
- This project builds on that and further develops interactive tools for stakeholder engagement
- NCEO (Leicester, Reading, CEDA) with Met Office and STFC-RAL as project partners