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A clustering approach to reduce computational expense in land surface models: a case study using JULES vn5.9

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Abstract. Land surface models such as JULES (the Joint UK Land Environment Simulator) are usually run on a regular, rectilinear grid, resulting in gridded outputs for variables such as soil moisture and water fluxes. Here we investigate a method of clustering grid cells with similar characteristics together in JULES. Clustering grid cells has the potential to reduce computational expense as well as providing an alternative to tiling approaches for capturing sub-grid heterogeneity. In this study, we cluster grid cells exclusively in the land surface part of modelling, i.e., separate from river routing. We compare gridded and clustered soil moisture outputs from JULES with measurements from the UK Centre for Ecology and Hydrology (UKCEH) COSMOS-UK network and show that the clustering approach can model soil moisture well while reducing computational expense. However, soil moisture results are dependent on the characteristics used to create the clusters. We investigate the effect of using clusters on predicted river flows, and compare routed JULES outputs with NRFA gauge data in the catchment. We show that less expensive JULES clustered outputs give similar river flow results to standard gridded outputs when routed at the grid resolution, and are able to match observed river flow better than gridded outputs when routed at higher resolution.

1 Introduction

Land surface models such as JULES (Joint UK Land Environment Simulator) were originally designed to enable weather and climate forecasting by capturing the feedbacks between the land and the atmosphere (e.g., Blyth et al., 2021); they were therefore typically run on regular grids at various scales which match those used by atmospheric models. More recently, land surface models have been extended to model other parts of the earth system (e.g., Fisher and Koven, 2020; Blyth et al., 2021, and references therein), and while often run as part of an atmospheric model, they can also be run independently ('standalone'). Land surface models are increasingly used for hydrological predictions (e.g., Lewis and Dadson, 2021; Lewis et al., 2018; Martínez-de la Torre et al., 2019), and JULES has a number of in-built options for routing surface and subsurface runoff outputs into river flow predictions, including RFM (Bell et al., 2007; Dadson et al., 2011) and TRIP (Oki et al., 1999).

Dedicated hydrological models generally have a simpler representation of land surface processes than LSMs. Such models may be designed to run in a gridded configuration (e.g., Bell et al., 2007; Grogan et al., 2022; Samaniego et al., 2010), or with catchments or hydrological response units (HRUs) as the smallest spatial modelling unit, as in, e.g. (Coxon et al., 2019; Arnold et al., 1998). In Coxon et al. (2019), the authors introduce DECIPHeR (Dynamic fluxEs and ConnectIvity for

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Predictions of HydRology), a highly flexible HRU model framework simulating river and hydrological flows using a rainfall-runoff model. DECIPHeR uses rainfall and potential evapotranspiration (PET) as meteorological inputs, and allows users to cluster underlying grid cells into HRUs in a similar way to this study. The difference with this work is that we target soil moisture as a key simulated variable rather than river flow, and while we neglect flows between response units, we use a more sophisticated land surface model able to simulate land-surface processes.

It is also possible to apply clustering methods to models which explicitly include both land surface and hydrological processes. This approach is taken in a number of recent studies in which an HRU or hillslope approach has been applied to a land surface model. In Chaney et al. (2016) the authors introduce HydroBlocks, which couples the Noah-MP land surface model (Ek et al., 2003) and the Dynamic TOPMODEL hydrological model (Beven and Freer, 2001). Clusters, or HRUs are defined based on high-resolution characteristics related to both land and hydrological processes. This concept is extended in Chaney et al. (2018), in which the authors use a hierarchical multivariate clustering (HMC) approach and more explicitly take catchment structure into account in the clustering process. The HydroBlocks approach is further extended in Chaney et al. (2021) to include two-way coupling between river networks and the land surface. In Swenson et al. (2019) a related approach is used with the CLM (Lawrence et al., 2019) land surface model; here the domain is divided into representative hillslopes rather than grid cells.

In this study we test the effect of a clustering approach on outputs from JULES. In contrast to Chaney et al. (2016, 2021) and Swenson et al. (2019) we apply clustering only to the land surface process part of JULES, and in this way we focus on the effect of clustering exclusively on the land surface component of modelling, rather than the hydrological component. We therefore prioritise land surface processes over hydrology when clustering, and refer to our clusters as Land surface Response Units (LRUs) rather than HRUs. We aim to take advantage of reduction in computational expense by running JULES simulations with fewer LRU clusters than grid cells. However, we note that we are not taking advantage of the full approach of Chaney et al. (2016, 2021); Swenson et al. (2019) in this first set of experiments - i.e. we do not include the functionality in which water can be moved through the soil from one cluster to another.

We have taken the hierarchical multivariate clustering technique from the HydroBlocks approach (Chaney et al., 2021; Chaney and Vergopolan) and applied it to the land surface part of JULES only, in part of the Thames catchment in the UK. We investigate the effect of the LRU approach on JULES soil moisture, and compare LRU and gridded JULES soil moisture predictions with measurements from the UKCEH COSMOS-UK soil moisture observation network (Stanley et al., 2023; Cooper et al., 2021b). We find that use of LRUs leads to good soil moisture prediction while reducing computational expense compared to a gridded approach, but that spatial soil moisture patterns can be strongly dependent on the characteristics used to create the LRUs.

JULES models surface and subsurface water fluxes as well as soil moisture, and these fluxes can be used as inputs to a river routing model to predict river flows either internally in JULES or using an independent flow routing model. We consider how the LRU approach impacts predicted river flows, comparing routed JULES outputs with observed river flow from a number of NRFA gauges in the catchment. We show that less computationally expensive LRU JULES outputs give similar river flow

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results to standard 1km gridded JULES outputs when routed at 1km resolution, and that the LRU approach can outperform gridded river flow predictions when routed at higher resolution.

The rest of this paper is organised as follows: in section 2 we describe the study domain and the simulations that we carried out in this study. In section 3 we present soil moisture and river flow results, showing that a clustering approach can provide a similar level of accuracy to a gridded approach for smaller computation cost. In section 4 we conclude that our results suggest that this is a promising method, and outline future developments for JULES.

2 Methods

2.1 Study domain

The area we chose for our proof-of-concept testing is a 10,450km^2 rectangle, covering part of the Thames catchment in the UK, and with the following OSGB 1936 / British National Grid corner co-ordinates: lower left corner (390000, 165000) and upper right corner (500000,260000). The 50m resolution digital elevation map of the domain, extracted from UK Centre for Ecology and Hydrology's Integrated Hydrological Digital Terrain Model dataset (see IHDTM) is shown in figure 1.

UKCEH runs the COSMOS-UK network of instruments, which measure soil moisture over a radius of approximately 200m using innovative cosmos ray neutron sensor technology. For more details about COSMOS-UK see Cooper et al. (2021b); Stanley et al. (2023). Three COSMOS-UK instruments are situated within our study domain, at Chimney Meadows (chimn), Waddeson (waddn) and Sheepdrove (sheep); their locations are shown with red crosses in figure 1.

2.2 Clustering approach

We use the IHDTM 50m resolution grid as the underlying grid for our study here, and use the hierarchical multivariate clustering approach from Chaney et al. (2016); Chaney and Vergopolan to cluster these 50m grid cells in various ways. Before clustering, each 50m square cell in the underlying fine scale grid was assigned a co-located elevation from the 50m resolution IHDTM dataset (see IHDTM). Meteorological driving data needed to run JULES was assigned to each 50m cell from the CHESS dataset (Robinson, 2020), according the the 1km CHESS grid cell it is located in. We assigned JULES ancillary data such as soil parameters and topmodel parameters from the 1km dataset used in Martinez-de la Torre (2018); Blyth et al. (2019). The CHESS landcover dataset assumes a tiled vegetation approach which was not appropriate here; we therefore assigned each 50m cell to be the dominant landcover type of the 1km CHESS cell which it is located in.

The HMC algorithm used here allows the user to specify a chosen number of clusters or LRUs. The user can also specify which grid cell characteristics should be used to form the clusters, i.e., which of the assigned 50m grid cell characteristics should be taken into account when clustering cells into LRUs.

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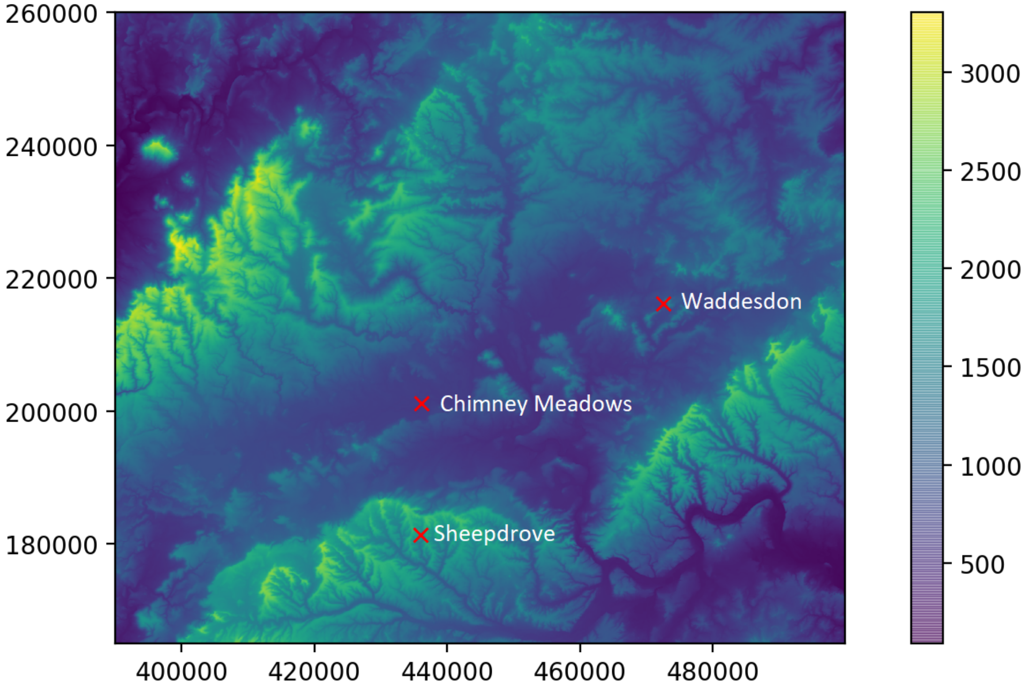

Figure 1. 50m digital terrain map (DTM) of study domain, comprising part of the Thames catchment in the UK. DTM data extracted from the IHDTM dataset. Red crosses show the locations of three COSMOS-UK soil moisture sensors in the domain.

2.3 Simulations

We ran various JULES simulations in our test domain for the period 2014 - 2017 inclusive. Daily meteorological drivers from Robinson (2020) were used to run JULES. Simulations were carried out in both a typical gridded 1km configuration (as in e.g. Martinez-de la Torre (2018)), and then for various clustering configurations in order to compare the results. For the clustering simulations we first ran a series of experiments with fixed clustering covariates and varying numbers of LRUs (number of clusters, N = 1,10,20,1000). The fixed clustering covariates for these simulations were: latitude, longitude, elevation, slope, land cover and soil type. Note that the slope covariate is calculated by the HydroBlocks clustering code, based on input elevation information. We then ran simulations over the same time period with a fixed number of N = 10 LRUs and different combinations of the aforementioned clustering covariates.

For a subset of the simulations we used surface and subsurface runoff outputs from JULES to give river flow predictions. We did this using the JULES runoff timeseries as an input to the river routing model RFM (Bell et al., 2007) as implemented in the UnifHy framework (Hallouin et al., 2022; Hallouin and Ellis, 2021).

The methodology for creating soil moisture and runoff timeseries for LRU configurations is as shown in figure 2. To summarise:

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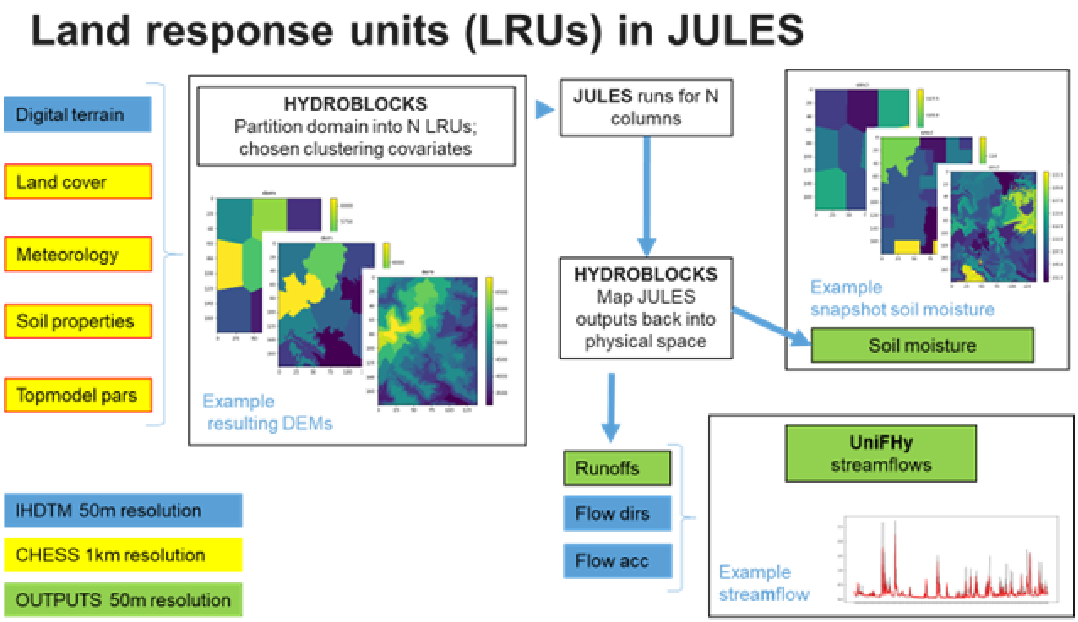

Figure 2. Method schematic

- each 50m cell is assigned characteristics from the 50m IHDTM or 1km CHESS dataset (as detailed in the previous paragraph)
- we choose a subset of cell characteristics as clustering covariates and the required number of LRUs, N.
- we apply the HMC algorithm from (Chaney and Vergopolan), which groups the 50m cells into a number, N, of LRUs such that cells with similar values of the chosen clustering covariates are grouped together
- this produces N sets of driving and ancillary data, i.e. one per LRU
- we run JULES for each LRU, resulting in N sets of JULES output time series, including soil moisture and runoff
- we map the JULES output values back into physical space using mapping files created by the clustering algorithm

3 Results and discussion

3.1 Soil moisture

3.1.1 Soil moisture results for various clustering configurations

In the first set of simulations we used fixed covariates for clustering and a variable number, N, of LRUs. Figure 3 shows resulting snapshots of the daily average soil moisture (kgm^{-1}) over the top JULES soil layer (10cm) in the domain on 15th

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December 2017. Panel (a) in figure 3 shows results for a 1km traditional gridded JULES run comprising 10,450 grid cells; panels b to e show results for 1, 10, 20 and 1000LRUs respectively. As expected, the results for 1, 10 and 20 LRUs provide less variation in the soil moisture values across the domain than the gridded run due to averaging out of input meteorology and grid cell characteristics. However, all the snapshots except for 1LRU show broadly similar spatial features in the soil moisture values. The differences between the gridded and 1000LRU soil moisture values are small; a direct comparison between values in the 1km and 50m grids is not straightforward, but the means and standard deviations of soil moisture values are similar (mean 31.9 kgm^{-1} (1000LRU) 32.1 kgm^{-1} (gridded), std 4.6 kgm^{-1}(100LRU) 4.4 kgm^{-1} (gridded)). This indicates that a ten fold reduction in JULES compute expense can yield comparable results to the 1km gridded approach.

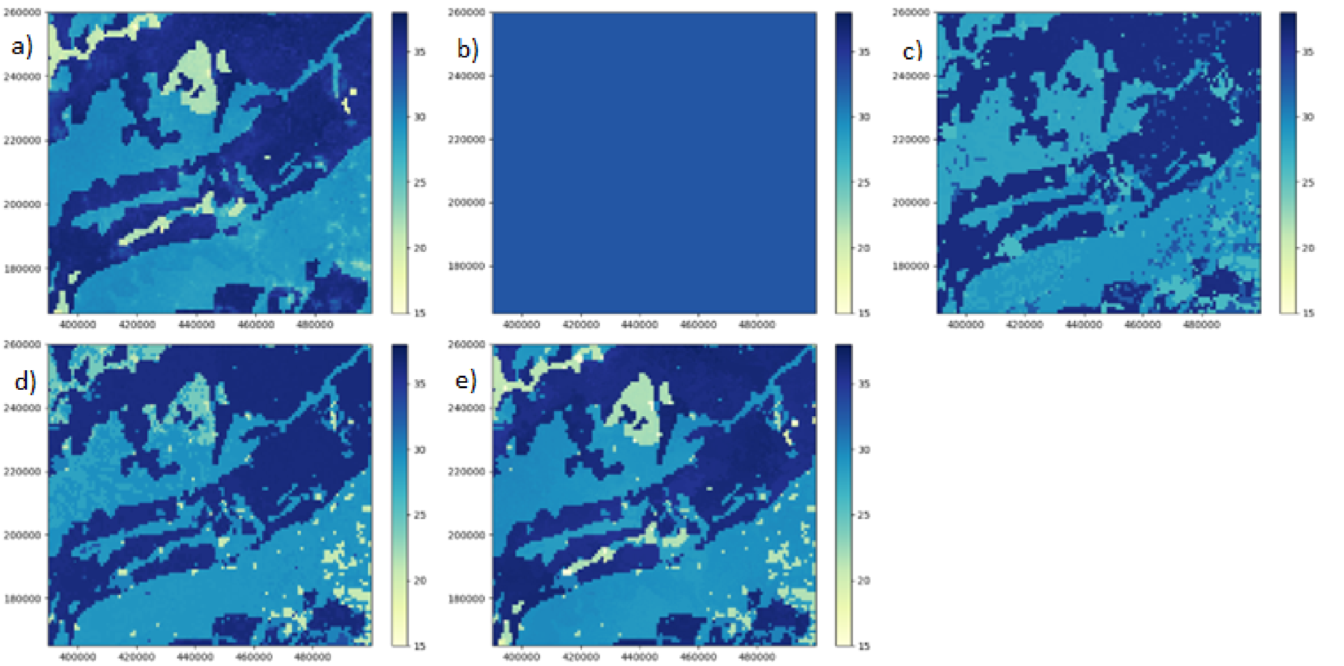

Figure 3. Snapshot average daily JULES top layer soil moisture in kgm^{-1} over the whole domain for different modelling approaches. Panel a shows is gridded soil moisture (10450 grid cells), other panels show JULES LRU with varying numbers of LRUs: b) 1LRU, c) 10 LRU, d) 20LRU and e) 1000LRU.

In the next set of simulations, we used a constant number of clusters (N=10) and varied our choice of clustering covariates. Figure 4 is similar to 3, showing snapshot daily top layer soil moisture kgm^{-1} in the domain on 15th December 2017. Panel (a) in figure 4 again shows results for a 1km traditional gridded JULES run comprising 10,450 grid cells; panels b to e show results for different covariate choices. Clustering covariates for the other panels are as follows. Panel (b): latitude, longitude, elevation, slope, soil type, land cover; (c) latitude, longitude, elevation; (d) latitude, longitude, soil type; (e) latitude, longitude, land cover and (f) land cover and soil type. Figure 4 demonstrates that the choice of clustering covariates can have a large impact on the spatial patterns observable in predicted soil moisture values, and that in some cases (b, d, f), 10 LRUs are able

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to capture most of the spatial features present in the gridded simulation. The similarities between panels a and f in figure 4 indicate that the gridded soil moisture outputs are closely related to the clustering convariates chosen here: elevation and soil properties. This implies that in this area, elevation and soil properties significantly influence soil moisture.

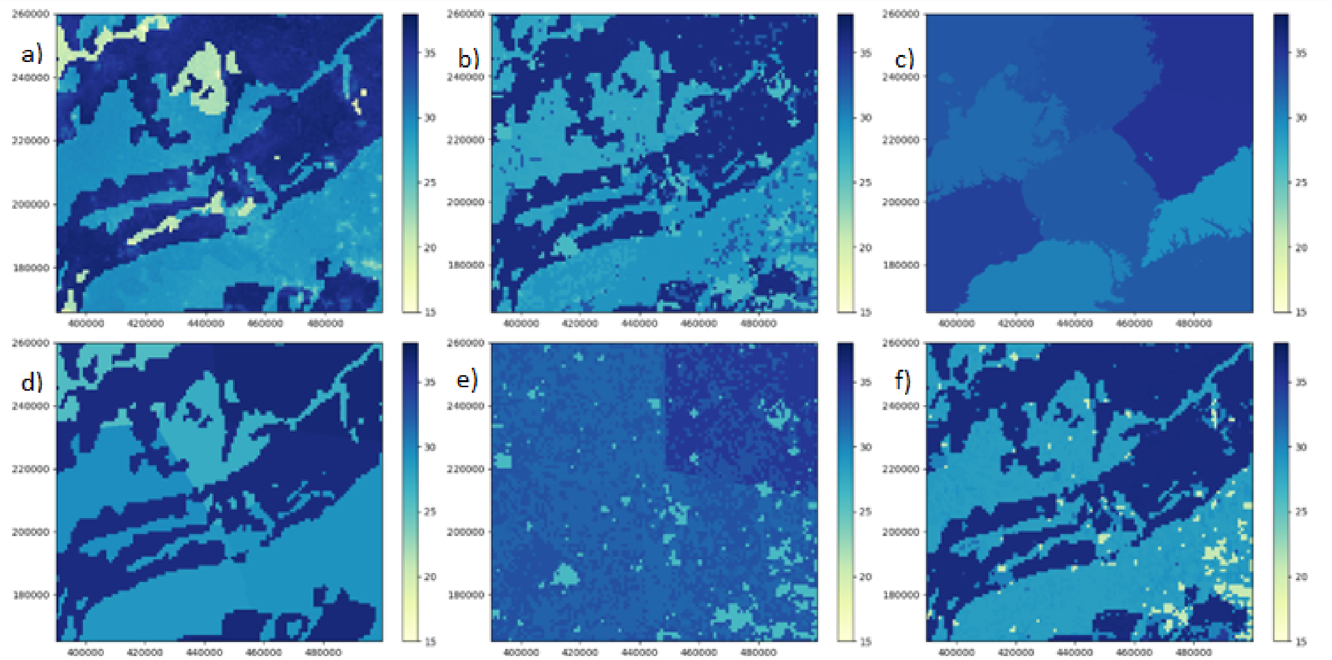

Figure 4. JULES top layer soil moisture (kgm^{-1}) snapshots over the whole domain for different modelling approaches . Panel a shows gridded soil moisture (10450 grid cells), other panels show JULES clustered results for N = 10 and the following clustering characteristics: b) latitude, longitude, elevation, slope, soil type, land cover; c) latitude, longitude, elevation; d) latitude, longitude, soil type; e) latitude, longitude, land cover and f) land cover and soil type

3.1.2 Soil moisture comparison with observations

In figure 3 we showed qualitatively that the 1000 LRU simulation with all clustering covariates appears to match the gridded JULES soil moisture patterns well. We will refer to output from this simulation as ‘1000 LRU’. In this section we compare time series soil moisture predictions from the 1000 LRU simulation with those from the gridded simulation and with soil moisture observations from the COSMOS-UK network (see figure 1 for locations of instruments.) In order to make this comparison we have translated 4-layer JULES soil moisture outputs in kgm^{-1} to volumetric water content expressed as a fraction, and averaged over the COSMOS-UK observation depth. We use the method outline in Cooper et al. (2021a) for this. Figure 5 shows daily averaged soil moisture observations in the simulation period from each of three COSMOS-UK instruments (chimn, sheep, waddn) as solid black lines. The dotted blue line is daily averaged JULES 1000 LRU output and the red line shows the JULES gridded equivalent.

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Figure 6 shows corresponding Kling-Gupta Efficiency (KGE) metrics, and components, for the timeseries shown in figure 5. The KGE metric describes how well a model timeseries matches equivalent observations (Gupta et al. (2009); Knoben et al. (2019). The ideal value of KGE = 1 corresponds to a perfect match between model and observations; KGE >= -0.41 indicates some skill in the model. The value of the KGE is given by

$$KGE = 1 - \sqrt{(1-r)^2 + (1-\alpha)^2 + (1-\beta)^2}, \tag{1}$$

where

$$\alpha = \frac{\sigma_{model}}{\sigma_{obs}} \tag{2}$$

and

$$\beta = \frac{\mu_{model}}{\mu_{obs}}. \tag{3}$$

In equations (2) and (3), μ_{model} and μ_{obs} represent the mean values of the modelled and measured soil moisture time series respectively; σ_{model} and σ_{obs} are the corresponding time series standard deviations. The correlation coefficient between the model and the observation time series is represented by r; a value of r = 1 would indicate perfect correlation, r = -1 indicates anti-correlation, and r = 0 indicates no correlation between the model and observations. Equation (2) shows that the value of α is a measure of how closely the spread in the modelled soil moisture values matches that of the observations, with α = 1 corresponding to perfect matching of these quantities. The β component of the KGE is a measure of bias between the model and observations, with β = 1 indicating zero bias.

Figures 5 and 6 show that all the JULES runs are skilful in replicating COSMOS-UK soil moisture at the instrument locations (KGE » -0.41). The overall KGE metric is higher for JULES 1000 LRU than JULES gridded at two of the three sites, whereas the gridded run shows better performance at the Waddesdon (waddn) site. The values of beta are less than one for all the simulations, indicating an overall dry bias in the JULES runs. The values of alpha are all also less than 1, and this means that the modelled soil moisture variance is in all cases lower than the observed equivalent. The correlation coefficients are high for all simulations (>0.79), and higher for JULES gridded than JULES 1000 LRU. Slightly lower correlation coefficients for the clustered runs are likely due to averaging out of the meteorological drivers over the grid cells in the LRU approach.

3.2 Routed river flow

The results in section 3.1.2 are informative but only relevant at three specific locations in the domain. In this section we aggregate JULES water flux outputs to the scale of catchments of various sizes and examine whether we can use our LRU approach to match observed river flow gauge data at 26 gauges in the domain. In order to do this we took daily averaged surface and subsurface runoffs from the JULES gridded simulation and the JULES 1000 LRU simulation and used and used them as inputs to RFM in UniFhy (Hallouin et al. (2022); Hallouin and Ellis (2021)) to create daily river flow time series.

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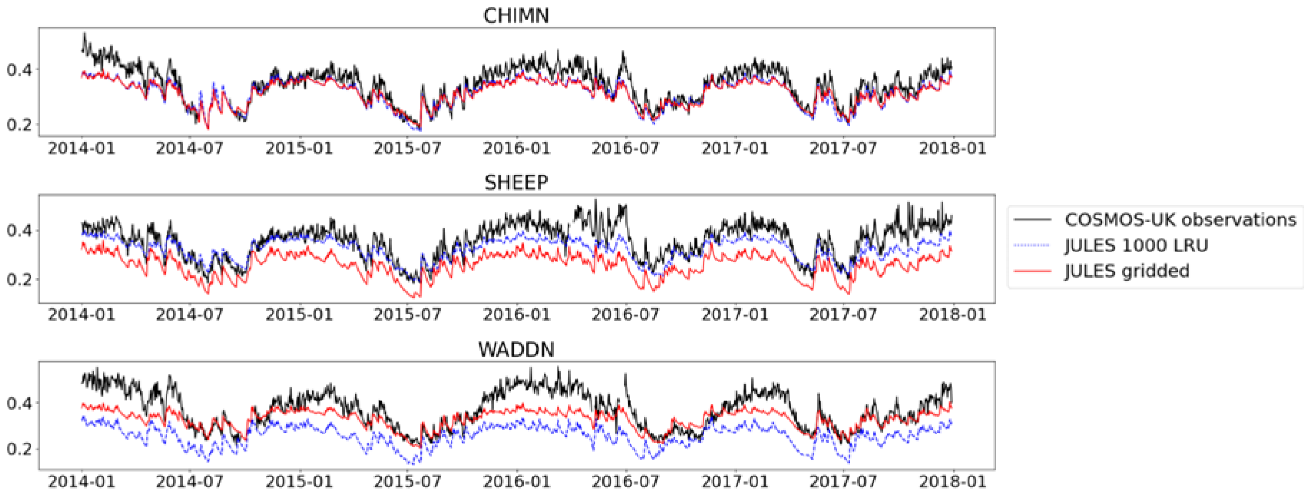

Figure 5. Soil moisture (volumetric water content) time series at three COSMOS-UK sites over the period 2014 to 2017(inc). The solid black line is COSMOS-UK daily soil moisture observations, the dotted blue line is equivalent soil moisture at the instrument location from JULES 1000 LRU; the red line is soil moisture from the 1km JULES gridded simulation (10450 grid cells).

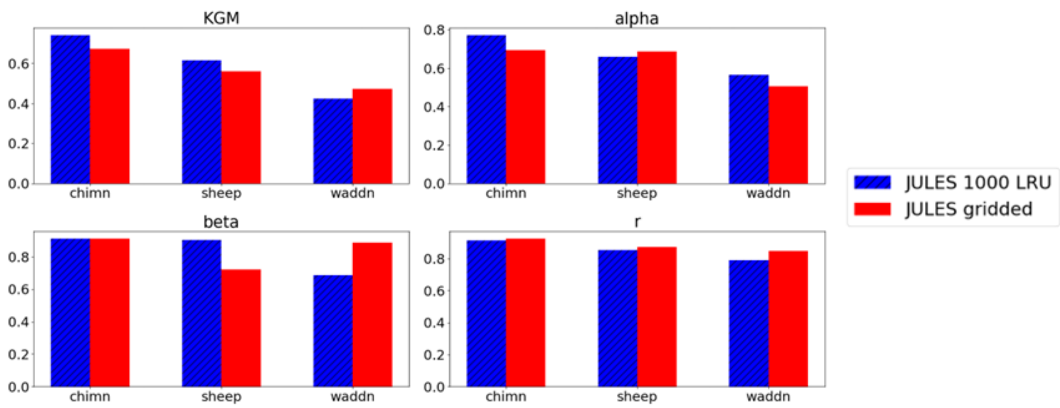

Figure 6. KGE and components, showing goodness of fit of JULES modelling approaches to COSMOS-UK soil moisture data at three COSMOS-UK sites (chimn, sheep and waddn); corresponding time series are given in fig 5. Red bars correspond to the gridded approach (10450 grid cells) and the blue bars correspond to 1000LRUs. The ideal value of each metric is 1.

We routed the JULES 1km runoff at 1km resolution, using river routing parameters from the CHESS-land dataset, and refer to river flow generated using the JULES gridded simulation as 'JULES gridded'. We produced river flow for the JULES 1000 LRU configuration at two different river routing resolutions: 50m and 1km. The underlying grid resolution for the JULES LRU configurations is 50m, and since we have river routing parameters at 50m from the IHDTM, we can route the runoffs at this high

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resolution in UniFHy. We refer to 50m river flows from the JULES 1000 LRU simulation with all clustering covariates used as 'JULES LRU'. However, river routing at 50m is much more computationally expensive than routing at 1km. We therefore also aggregated the 50m runoff values from JULES 1000 LRU to the same 1km grid used for the gridded JULES runs and put these through the same 1km routing model; we refer to these river flow simulations as 'JULES LRU regridded'.

Figure 7 shows a hydrograph for one of the gauges in the domain; this is daily flow observations at the Thames at Reading for February 2014 to December 2017 (JULES output water flux timeseries from January 2014 were used as the RFM hydrological model spin up period). In each panel, the black dotted line is gauged observed flow from the National River flow Archive (NRFA). The top panel also shows modelled river flow from the JULES gridded simulation in red; the bottom panel shows the equivalent output for JULES LRU in blue. We note that the hydrographs for the different modelling approaches look quite different; the gridded outputs are flashier than the observed flows - i.e. the model shows more short term variability than the observations. The JULES LRU output looks much smoother than the JULES gridded output, but misses or underestimates many of the peaks in the observed hydrograph. The clustering approach necessarily involves averaging of meteorological inputs such as precipitation, and this might be the reason that the clustered river outputs fail to capture some extremes.

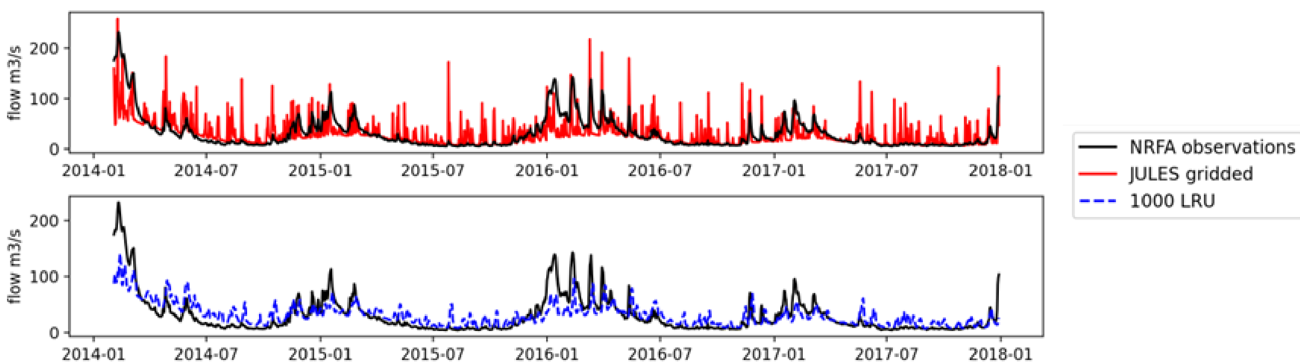

Figure 7. Hydrograph for the Thames at Reading (domain catchment outlet) for February 2014 to December 2108 (inc). The black line shows daily NRFA observed river flow on each panel. The top panel also shows river flows generated from JULES gridded, while the bottom panel shows river flows generated from the JULES 1000 LRU simulation.

We used python functions in the software package evalhyd (Hallouin and Bourgin, 2023; Hallouin et al., 2023b, a) to calculate a number of standard metrics for our modelled river flows, using observed flow data at 26 gauging stations in our domain as ground truth. The resulting KGE metrics and components (which use equations 1 to 3) are shown in figure 8. For each boxplot, produced using matplotlib.pyplot.boxplot, the notch shows the median value of the metric for a particular JULES configuration across 26 gauges. The coloured box extends from the first quartile to the third quartile of the metric distribution values, and the whiskers extend from each box by 1.5 times the inter-quartile range. Metric values past the end of the whiskers are shown with empty circles. Panel a of figure 8 shows that the JULES LRU configuration (red) has the highest median KGE score of the three simulations, outperforming both the JULES gridded (blue) and JULES regridded (green) approaches. Panel b shows that the JULES LRU approach gives higher correlation coefficients than the JULES gridded approach, and that some of the improvement in median correlation persists into the JULES regridded simulations. In panel c we see that the median alpha values for the JULES gridded and JULES LRU simulations are similar, and panel d shows that the median value of beta is closest to the ideal value of 1 for the JULES LRU simulation; this indicates reduced bias compared to both the gridded and regridded approaches. Figure 8 shows that the 1000 LRU approach matches river observations better than the standard gridded approach, i.e., we can generate improved river flows for a lower computational cost in the land surface part of the simulation. However, some of this improvement is very likely due to the increased resolution of river routing, which has a high computational cost. The JULES regridded simulation removes this effect, and comparing the green and blue boxes in 8 shows that the JULES regridded approach gives similar overall KGE results to the original gridded approach, while still benefiting from a ten fold reduction in compute resource.

In figure 9 we show more standard river flow metrics - again calculated using the evalhyd package. Panel a shows the Nash Sutcliffe Efficiency (NSE) for the three JULES approaches at the same 26 gauges as in fig 8; panels b, c and d show the mean absolute error (MAE), mean absolute relative error (MARE) and root mean square error (RMSE) respectively between modelled and measured daily flow. Figure 9 shows that the JULES LRU approach again gives the best results of the three approaches, with the the highest median NSE value, and the lowest median MAE, MARE and RMSE values. The NSE results show that the JULES LRU simulations result in a skillful forecast (NSE > 0), at 24 of the 26 gauge locations, compared to 17 skillful forecasts for JULES gridded and skill at 20 gauges for JULES regridded.

Overall our experiments show that the JULES LRU routed at 50m gives the best match to data. However, the computational expense involved at routing at this high resolution is high. JULES gridded and JULES regridded results are broadly similar, indicating that it is possible to save computational resource at the JULES land surface modelling stage and then route at lower resolution to match the skill of a gridded approach.

4 Conclusions

We have shown that it is possible to successfully use a clustering technique to simulate soil moisture and river flow in a test domain using JULES. We showed that the choice of clustering covariate is important when reproducing spatial patterns in soil moisture; the most important covariates are likely to vary by geographical location, and depend on the scale of the domain of interest. We found that soil moisture time series could be reproduced at three locations in the domain with skill very similar to that for gridded runs. We also found that we could better match observed river flows at 26 gauges in the domain using JULES LRU water flux outputs routed at 50m than the standard 1km gridded JULES routed at 1km (0.47 median KGE vs 0.23 median KGE); correcting for river routing resolution gave similar performance to the gridded approach (0.21 median KGE). Our results suggest much potential for reducing computational expense in land surface modelling, which would enable ensemble runs to be performed at much lower cost. Such ensemble are commonly used for sensitivity studies as well as some data assimilation techniques. Another advantage of this type of clustering approach is that it enables use of higher resolution datasets in LSMs where available. For example, a combination of high resolution land cover information coupled with a clustering approach could be a good way deal with sub-grid heterogeneity, and provide an alternative to land cover tiling approaches.

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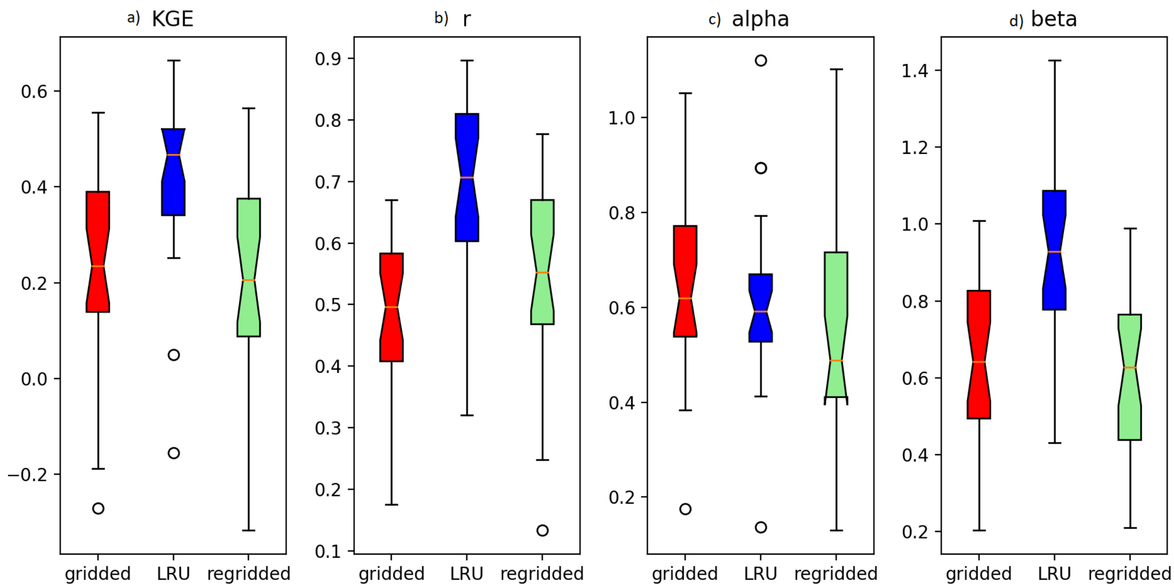

Figure 8. Aggregated KGE metric and components r, alpha and beta for routed JULES outputs at 26 NRFA gauges across the catchment. The red box shows results for JULES gridded, the blue box shows the results for JULES LRU and the green box shows the results for JULES regridded.

Further benefits to JULES outputs are likely achievable by taking a full HydroBlocks - like approach, i.e. allowing water to move between LRUs; an alternative approach might be to use vector schemes for river routing. Exploring this capability for use with JULES will be an avenue for future research.

Code and data availability. JULES source code, instructions for access and running are available from the JULES FCM repository: https://code.metoffice.gov.uk/trac/jules/wiki/WaysToRunJules. The specific configurations and namelists used to run the experiments in the paper are available at https://code.metoffice.gov.uk/trac/jules with the suite id: u-cq437. JULES and unifhy outputs created for this paper, as well as information on how to download configurations, datasets and code used can be found in Cooper et al. (2023).

Author contributions. All authors contributed to initial experiment design and analysis of results. EC set up and ran the simulations, with significant input from RE for the UniFHy runs. EC wrote the manuscript, with input from all authors

Competing interests. The authors have no competing interests

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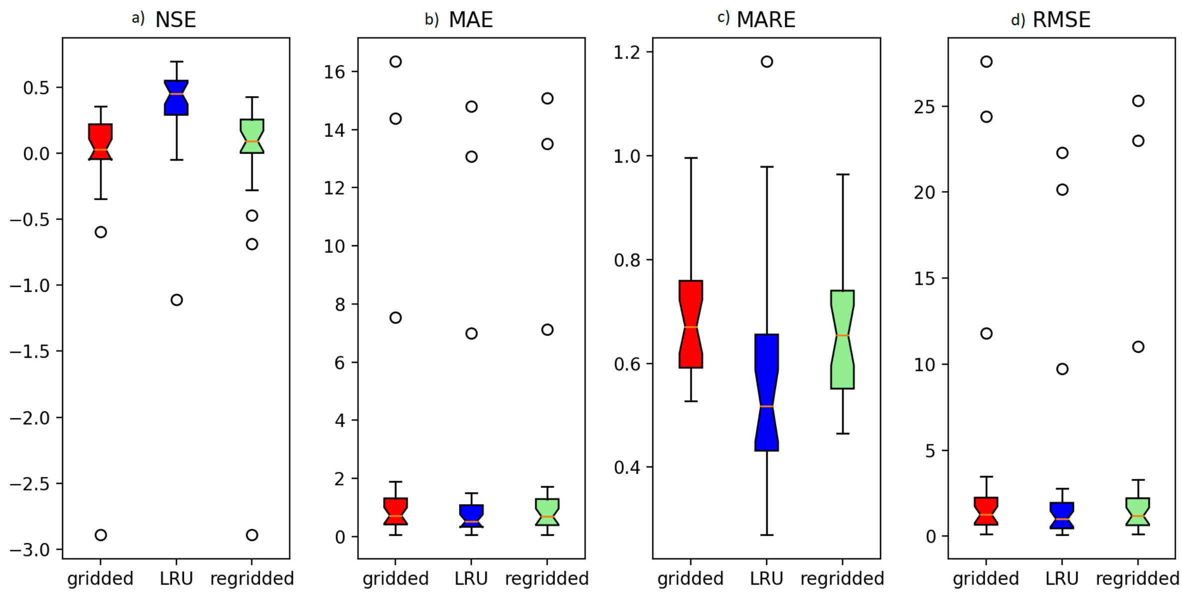

Figure 9. Aggregated NSE, MAE, MARE and RMSE metrics for routed JULES outputs at 26 NRFA gauges across the catchment.The red box shows results for JULES gridded, the blue box shows the results for JULES LRU and the green box shows the results for JULES regridded.

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