A regional coupled approach to water cycle prediction during winter 2013/14 in the United Kingdom

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Abstract

A regional coupled approach to water cycle prediction is demonstrated for the 4-month period from November 2013 to February 2014 through analysis of precipitation, soil moisture, river flow and coastal ocean simulations produced by a km-scale atmosphere-land-ocean coupled system focussed on the United Kingdom (UK), running with horizontal grid spacing of around 1.5 km across all components. The Unified Model atmosphere component, in which convection is explicitly simulated, reproduces the observed UK rainfall accumulation (r^2 of 0.62 for daily accumulation), but there is a notable bias in its distribution – too dry over western upland areas and too wet further east. The JULES land surface model soil moisture state is shown to be in broad agreement with a limited number of cosmic-ray neutron probe observations. A comparison of observed and simulated river flow shows the coupled system is useful for predicting broad scale features, such as distinguishing high and low flow regions and times during the period of interest but are shown to be less accurate than optimised hydrological models. The impact of simulated river discharge on NEMO model simulations of coastal ocean state is explored in the coupled system, with comparisons provided relative to experiments using climatological river input and no river input around the UK coasts. Results show that the freshwater flux around the UK contributes of order 0.2 psu to the mean surface salinity, and comparisons to profile observations give evidence of an improved vertical structure when applying simulated flows. This study represents a baseline assessment of the coupled system performance, with priorities for future model developments discussed.

Keywords: (please provide 3-6 keywords). coupled modelling, water cycle prediction, coastal regions of freshwater influence.

1. INTRODUCTION

Winter 2013/14 in the United Kingdom (UK) was notable for the cumulative impacts of a series of successive damaging storms crossing north-west Europe (Kendon et al., 2015; Lewis et al., 2015). Different regions of the UK were substantially impacted by flooding from coastal inundation (Sibley et al., 2015; Wadey et al., 2015), fluvial (Huntingford et al, 2014; Neumann et al., 2015) and groundwater sources (Muchan et al., 2015). Such events provide strong motivation for adopting a more holistic approach to understanding and quantifying the risks to populations and infrastructure from compound flooding from multiple sources and from concurrent hazards (Ciurean et al., 2018; Pilling et al., 2016).

The coupling or linking of different environmental models has long been considered a necessary approach to achieving this more holistic view. This vision was well expressed by Beven (2007; quote below reproduced with kind permission of the author), who invited readers to:

> *"Consider, for flood prediction purposes, the possibility of modelling the subtle (and interdisciplinary) coupling between atmospheric forcing, catchment response, river runoff and coastal interaction with tidally dominated sea levels; capturing these subtleties will require the dynamical coupling of many processes and components from different institutes and different computing systems. Components would be a representation of the coastal seas, the regional atmosphere and the terrestrial surface and subsurface hydrology that would interact through different boundary conditions." (reproduced from Beven, 2007).*

For typical hydrological and risk assessment applications, any coupling of models and data has been achieved by defining linear model chains whereby outputs from one system (e.g. point or distributed observation, numerical weather prediction or climate simulation based data) are fed into a hydrological and/or hydraulic model in order to simulate the land surface response and risk of flood hazard (e.g. Ming et al., 2020; Coxon et al., 2019; Flack et al., 2020). For coastal flood hazards, for example, Couasnon et al. (2020) recently illustrated the need to consider both fluvial and coastal flood drivers in the estimation of compound flood risk at coastal locations at a global scale, with river and coastal surge data obtained from two independent sources, although with both driven by the same ERA-Interim reanalysis of the meteorological forcing.

The vision for the *dynamical coupling* between atmosphere, catchment, rivers and coastal components as set out by Beven (2007) is more closely achieved by adopting a fully coupled approach whereby model components exchange information at run-time via a coupler so that interactions and feedbacks are explicitly simulated. This is well established and illustrated through the evolution of Earth System Models to assess the drivers, sensitivities and impacts of environmental change on global scales (e.g. Sellar et al., 2019). The key challenges for improving how hydrological processes are represented in these systems were discussed by Clark et al. (2015), while Ward et al. (2020) recently addressed the importance of and priorities for better representing the land-ocean interface in Earth System Models.

On regional scales, the development of analogous dynamically coupled Regional Environmental Prediction systems is helping to underpin more whole-system simulations at more catchment and coastal-relevant scales. This is driven by needs to improve short-term hazard prediction (e.g. Rainaud et al., 2017; Zhang et al., 2019) and provision of more integrated longer-timescale assessments of environmental change (e.g. Giorgi et al., 2018). To date, regional coupled systems have tended to be developed with a view to improving either the integration of meteorological and hydrological predictions (e.g. Fersch et al., 2019), or with a focus on better representing the impacts of air-sea interactions on the system through coupling atmosphere and ocean (and occasionally wave) model components (e.g. Thomson et al., 2019; Strajnar et al., 2019). Senatore et al. (2020) bridged these perspectives to some extent in assessing the impact of different sea surface temperature (SST) forecasts used as the lower boundary condition on the hydrological performance of a km-scale regional atmosphere-land simulations focussed on southern Italy. While based on results from only two relatively short case studies, they highlighted differences in precipitation and streamflow simulations when different SST were used. It should also be noted however that a stronger sensitivity was found to the choice of driving model providing lateral atmospheric boundary conditions and many other uncertainties in the water cycle modelling chain were not explored.

Durnford et al. (2018) arguably provide the closest realisation to a fully coupled water cycle prediction system on regional scales. The development led by Environment Canada couples interacting regional atmosphere, land surface, river routing and 3-d lake models and provides operational hydrological forecasts on short-to-medium range timescales for the Great Lakes-

St. Lawrence Seaway region of North America. This builds on a detailed analysis of the sensitivity of net basin supply to meteorological forcing and land surface model parameterization conducted by Deacu et al. (2012). Based on an 8-day summer period and longer 4-month evaluation simulations, Durnford et al. (2018) assessed the hydrological performance of the system in terms of simulated precipitation, river flows, lake inflows and water levels, along with more oceanic variables of lake surface currents and temperature. Lake ice forecasts were also illustrated for a winter period. The system was shown to produce reliable results for a 3.5-day forecast, with atmosphere and lake water results considered to be more mature and reliable than those from the river routing model. Critically, it was found that assimilation of observed river flow was required to limit the propagation of precipitation errors into the predicted river flows and downstream to lake quantities.

This paper provides a UK-focussed example of progress towards a more whole-system regional water cycle prediction approach. Results from km-scale fully coupled regional atmosphere-land-ocean model simulations during UK winter 2013/14 are assessed, focussing on its hydrological performance. The following questions are considered:

a) Are km-scale regional simulations of precipitation and soil moisture sufficiently accurate to provide useful forcing for distributed modelling of river flows across UK catchments?

b) How sensitive are regional ocean simulations of the near-coastal region around the UK to the representation and accuracy of input river flows?

c) What do these results imply for future component model development?

The model system and its components are introduced in Section 2. Results are presented in Section 3, with a focus both on broad-scale model performance metrics and the near-coastal impacts of coupling the atmosphere-land system to the regional ocean. The implications of this work are discussed in Section 4 and conclusions briefly drawn in Section 5.

2. DATA AND METHODS

This study assesses the performance of a km-scale regional atmosphere-land-ocean coupled prediction system focussed on the UK for simulations during the 4-month period covering winter 2013/14 between 30 October 2013 and 28 February 2014. Simulations use the UK coupled system and model grids detailed by Lewis et al. (2018) and Lewis et al. (2019). Hourly mean variables are exchanged between model components using the OASIS3-MCT coupling libraries (Valcke et al., 2017) each hour through the simulation. All simulations are free running with no data assimilation applied to any component. Relevant aspects of each model component are briefly summarised below.

2.1 Atmosphere model component

The atmosphere component of the coupled system uses the Unified Model (UM; version 11.1) code, implicitly coupled to the JULES (Joint UK Land Environment Simulator; Best et al., 2011; version 5.2) land surface model. Both components use the RAL1 science configuration documented by Bush et al. (2020). The variable resolution model grid is defined in rotated polar coordinates, with regular 1.5 km horizontal grid spacing in a central region focussed on the UK and stretching to 4 km spacing towards the outer domain edge (Figure 1). At this resolution, atmospheric convection is represented explicitly by the model dynamics rather than being parameterized. Lateral boundary conditions are applied hourly. These are provided by the first 24 h of operational global-scale Met Office numerical weather prediction (NWP) simulations archived from the time of the experiment, available then at a resolution of order 25 km. Simulations are initialised by interpolating the operational global analysis valid for 00Z on 30 October 2013 to the regional grid.

[Insert Figure 1]

2.2 Land surface and river flow model component

The RAL1 configuration of JULES has 4 soil layers to a depth of 3 m and surface land use heterogeneity is accounted for by defining the fractions of 9 possible tiles of vegetation (broadleaf trees, needle-leaved trees, temperate C3 grass, tropical C4 grass and shrubs) and non-vegetated land-use (urban areas, inland water, bare soil and land ice) types for each grid cell (Lewis et al., 2018). The Brooks and Corey formulation for soil hydraulic conductivity (Cosby et al., 1994) is used, based on the mapped soil sand, silt and clay fractions used in the operational regional NWP configuration (Bush et al., 2020). Sub-grid-scale heterogeneity of soil moisture is computed using the Probability Distributed Model (PDM; Moore, 2007). The configuration used in this study adopts the PDM optimisations recommended by Martinez-de la Torre et al. (2019), developed from assessments of JULES simulations focussed on 13 UK catchments at 1 km resolution driven by 30-years of an observation-based meteorological forcing. The main difference relative to the use of PDM in the RAL1 land surface model configuration used for operational NWP (Bush et al., 2020) is the introduction of a terrain slope-dependent formulation for the ratio between S_0, the minimum storage below which there is no surface saturation, and S_{max}, the maximum allowed storage in a grid cell. This ratio is illustrated in Figure 1a) for the 1.5 km variable resolution grid used in this study. This parameterization constrains the surface runoff production to wetter periods over flatter regions and enhances it over steeper regions relative to the standard and non-spatially varying PDM parameters used in RAL1. Saturation excess generates surface runoff (Clark and Gedney, 2007) while free drainage from the base of the soil column is treated as sub-surface runoff.

Accumulated surface and sub-surface runoff can be routed in JULES using the River Flow Model (RFM) implementation the kinematic wave equation solution (Bell et al., 2007; Dadson et al., 2011). Water storages in each grid cell are computed and outflows routed to the downstream grid cell defined by a pre-calculated flow direction map linking adjacent points in the domain. Appendix B of Lewis et al. (2018) provides further details. Note that no optimisation or calibration of the river routing wave speed parameters has been attempted in this study, with values listed in Table C3 of Lewis et al. (2018) used for this initial assessment. A river routing timestep of 30 min is used, while the atmosphere and land models have a timestep of 1 min. River routing is performed for the UK and Ireland only, with no flow directions defined for other land areas in the model domain to avoid the variable grid resolution of the land (and thereby river network) grid in these regions.

2.3 Ocean model component

The UK coupled system uses NEMO (Nucleus for European Modelling of the Ocean; version 3.6; Madec et al., 2020) to simulate the 3-d ocean state across the North-West European shelf with tidal and meteorological forcing. The AMM15 science configuration (Graham et al., 2018; Tonani et al., 2019) is used. The NEMO ocean grid has the same domain as the atmosphere, with regular 1.5 km horizontal spacing throughout (Lewis et al., 2019). The model bathymetry is based on European Marine Observation and Data Network

(EMODNET), with a minimum possible ocean depth of 10 m set in the absence of coastal wetting and drying. Daily lateral boundary conditions from a 1/12 ° operational ocean forecasting system for the North Atlantic are applied, and initial conditions for 30 October 2013 are provided by the long-term AMM15 hindcast simulation described by Graham et al., (2018).

For the first time, the sensitivity of the ocean component to the use of coupled river flow simulations is assessed. Typically, for example in operational application of AMM15 and UK regional coupled research published to date, a climatological river discharge is used (Tonani et al., 2019). Figure 1a) shows 232 locations within the model domain where a daily climatology of river flows has been defined. For UK coastal points, these are based on National River Flow Archive gauge observations over the period 1980-2014 while around other coastlines data are based on a pre-existing climatology averaged across 1950-2005. There is a clear imbalance between the number of discharge points around the UK relative to other areas in the model domain. For each discharge location, a river depth is specified, and a freshwater flux is applied to all ocean model levels above that depth. The climatology therefore represents some typical freshwater flux for a given day of the year, aiming to capture the main discharge locations and magnitude to establish representative near-coastal salinity and density structures.

In contrast the coupled system enables simulated river flows, representative of current conditions, to discharge into the ocean and explicitly link land to ocean processes. As the ocean and atmosphere/land grids have their own defined land-sea masks, a one-dimensional coupling approach has been defined using OASIS whereby JULES coastal outflow locations are identified, numbered, and paired with the nearest NEMO inflow points on the ocean grid. Figure 1b) shows 842 connection points between the UK and Ireland river routing grid and discharge points on the ocean grid. Given that coupled river flows are only computed for UK and Ireland rivers in this implementation, the NEMO code was modified to use a runoff coupling mask to distinguish between regions where the coupled rivers should be used while continuing to use the daily climatology elsewhere in the model domain.

2.4 Experimental design

This study focuses on an assessment of the performance on the UK coupled system during winter 2013/14 for simulating precipitation and its impact through the land surface and hydrological system. Three different approaches to representing river discharge into the ocean component of the coupled system are then considered, summarised in Table 1. In the fully coupled approach (CPLriv), hourly mean JULES simulated river discharge at coastal points around the UK and Ireland are mapped to the nearest NEMO ocean grid points, with climatological discharge applied elsewhere. CPLclim uses the same atmosphere-land-ocean coupled configuration but applying the climatological river discharge everywhere. In CPLnoriv, discharges around UK and Ireland are set to zero through the simulations, with climatological discharge still applied elsewhere, providing an upper bound on the magnitude of the impact of river flow quality on ocean simulations.

[Insert Table 1]

3. RESULTS

3.1 Precipitation

The spatial and temporal evolution of monthly accumulated precipitation across the UK between November 2013 and February 2014 is shown in Figure 2. The HadUK-Grid 1 km gridded rainfall product based on gauge observations (Perry and Hollis, 2005) indicates a relatively dry November but notably and increasingly wet conditions relative to climatology across much of the UK from December onwards (see Figure 3, Kendon et al., 2015 for anomaly maps). Qualitatively, the broad spatial distribution and monthly evolution of the CPLriv precipitation in Figure 2e)-h) is in good agreement with observations. That CPLriv can reproduce observed climatological features is encouraging given that the system has no data assimilation for any component.

[Insert Figure 2]

Differences between HadUK-Grid and CPLriv in Figure 2i)-l) highlight the tendency for the convective-scale Unified Model simulation to underestimate precipitation over upland areas across western UK while overestimating rainfall in the drier regions further east. Smith et al. (2012) described the considerable benefit of simulations at these resolutions for improving the representation of orographic precipitation enhancement relative to coarser-scale model grids in which local terrain gradients are smoothed out and convection is explicitly parameterized. However, these results are consistent with errors in the precipitation over orography highlighted more recently by Chen et al. (2019) for long-duration Unified Model simulation using a similar configuration to that used in this study.

Time series in Figure 2(m) compare water-day mean HadUK-Grid precipitation for England, Scotland and Wales land areas with the equivalent simulated quantity from CPLriv. This shows good agreement through winter 2013/14 with a correlation coefficient of 0.62. This provides confidence that the UK coupled system provides a robust simulation of winter precipitation, though noting spatial errors in the representation of orographic effects, which will be important in the context of hydrological simulation.

3.2 Land surface hydrological response

The partitioning of precipitation falling on the surface through winter 2013/14 between evaporation and runoff components is shown in Figures 3 and 4. Surface runoff represents the largest flux and responds directly to precipitation as expected. December was notably wet in western Scotland and February was wettest in south-western England and Wales. The sub-surface response is more complex. Mean results for November (Figure 3e) are particularly dry over much of the UK and Ireland, but excessive runoff is apparent in some areas of Scotland and persist through the winter. As discussed by Gomez et al. (2020), the anomalously wet regions are potentially a feature of the initial soil moisture conditions interpolated from the global model analysis available for the valid time of these simulations. Mean sub-surface runoff features in November are particularly smooth, indicative of an extended period of spin-up to more convective-scale forced conditions on the 1.5 km resolution model grid. Hydrological results for November should therefore be treated with caution. Later in winter, the sub-surface runoff increases, particularly on western slopes of upland regions. This spatial distribution is driven by the slope-dependent PDM configuration introduced by Martinez-de la Torre et al. (2019).

[Insert Figure 3]

[Insert Figure 4]

The mean simulated volumetric water content (VWC) fraction in the upper (0 - 10 cm below surface) and lowest (1 – 3 m below surface) JULES soil layers is shown in Figure 4. There is a clear contrast in timescales between the upper layer being driven by instantaneous precipitation, also reflected in the surface runoff, and the lower layer driven by the accumulated precipitation over time, reflected in the sub-surface runoff evolution. The initial condition and spin-up issues highlighted in Figure 3 are not apparent in the spatial averages shown in Figure 4. By the end of February 2014, the lowest soil level holds as much water as the upper layer, and the magnitude of surface and sub-surface runoff components are more similar.

One of the challenges inherent in any assessment of the simulated land surface response to precipitation has been the limited observations of components of the terrestrial water cycle at scales relevant to the model grid. The COSMOS-UK cosmic−ray soil moisture observing system (Evans et al., 2016) was first established in 2013 and has since expanded to 52 sites across the UK. During winter 2013/14 an initial 4 sites were active across a small part of southern England (Figure 1b). Cosmic-rays are used to derive an estimate of soil moisture representative of a horizontal area of about 0.12 km^2 (order 20-times smaller than the model grid area of 2.25 km^2) and a nominal observation depth of order 20 cm, but which varies in time by order 5-10 cm.

[Insert Figure 5]

Quantitative comparison of simulated and observation-derived VWC in Figure 5 should be treated with some caution given that the model and COSMOS-UK represent different vertical and horizontal scales, and that grid box mean diagnostics represent considerable surface heterogeneity within each model grid, even at 1.5 km resolution. The variability of model data within a 5 x 5 neighbourhood of grid points surrounding each location is considered, highlighting the regions surrounding Chimney Meadows (Figure 5b) and Wytham Woods (Figure 5c) to be considerably more heterogenous than those surrounding Sheepdrove (Figure 5a) and Waddesdon (Figure 5d). Comparing more qualitatively to the COSMOS-UK observations, CPLriv simulations are in relatively close alignment to observed VWC and well capture a gradual decrease in VWC during November followed by a relatively abrupt increase during mid-December. There is lower variability in VWC in both model and observations during January and February. The model timeseries show less day-to-day variability than COSMOS-UK and lower VWC than observed at 3 of the 4 locations. Yang et al. (2020) and Yang et al. (2014) reported systematic under-estimation of VWC in observation-forced JULES simulations during southern hemisphere winter and attributed this to the lack of lateral soil water flow in the JULES model. Blyth et al., (2019) found that JULES simulated evaporation tended to be excessive compared with flux tower observations, also consistent with these results. A third process deficiency consistent with this bias is a tendency for there to be insufficient infiltration of precipitation into the JULES soil column (e.g. Mueller-Quintino et al., 2016; Largeron et al., 2018; Martinez-de la Torre, 2019).

There is remarkably good qualitative agreement between CPLriv and COSMOS-UK at Sheepdrove (Figure 5a). The lack of variability in VWC between adjacent model grid points in the 5 x 5 neighbourhood may indicate this to be a less hydrologically complex location (Cooper et al., 2020), and given the site is at 170 m altitude in the Chiltern Hills, there may be a more limited role for lateral flows here. It is also possible that the authors were simply fortunate with compensating errors in both model and observation at this location!

The comparison to COSMOS-UK provide reassurance that the JULES land surface model configuration in CPLriv provides representative simulations of soil moisture through this period. This analysis indicates that a more extensive assessment of the simulated JULES soil moisture state at km-scales for more recent periods would be of considerable value, making use of the more extensive and multi-annual COSMOS-UK observations available today in order to better characterise, understand and improve the representation of soil moisture processes. This analysis could usefully form the basis for further optimisation of land surface parameters, and assessment of the variability and accuracy of VWC on each land surface tile within a land model grids.

3.3 River flow

Relative to diagnostics of soil moisture processes, river discharge is a well observed part of the terrestrial water cycle. Figure 6 shows a first-order check on the typical magnitude of simulated and observed flows through the study period across parts of the river routing network, indicating generally good distinction between higher and lower flow regions in CPLriv. Daily mean river flow gauge observations are provided by the UK National River Flow Archive (NRFA). Summary bias and Nash-Sutcliffe efficiency (NSE) metrics for the simulated river flow in CPLriv between December 2013 and February 2014 are compared with observations at 154 gauges in Figure 7. This set of gauges includes the 146 UK Benchmark Network sites (UKBN2; Harrigan et al., 2018), selected to favour relatively natural flow regimes and good hydrometric data quality, together with those of the 13 catchments assessed by Martinez-de la Torre et al. (2019) not included in UKBN2.

[Insert Figure 6]

[Insert Figure 7]

Given that the system is driven by simulated precipitation, most land surface parameters have been optimised for NWP applications, and no tuning has been applied for river flow parameters, Figure 7a) is encouraging in that the simulated flows have small biases relative to most gauge locations (104 locations where the bias is within 10 m^3s^{-1}). More substantial biases can be seen in south-eastern England where CPLriv flows are overestimated relative to observations. This is characterised as a groundwater dominated region – a process not represented in the free drainage approach of the JULES configuration used in these simulations. Batelis et al. (2020) described the application of a new groundwater flow boundary parameterization in JULES which may improve flow simulations in such regions. CPLriv can also be seen to overestimate flows in central Scotland, which are likely attributable to excessive sub-surface runoff and a poorly initialized soil moisture state.

While a NSE value of 1 represents a perfect simulation of the observed time series, a NSE value of zero indicates that the simulation provides no better prediction of the observed time series than the observed mean, and might be considered a minimal requirement of a useful river flow simulation. This target is only met for 69 (order 45%) of the 154 gauges considered, with 13 locations having a summary NSE value greater than 0.5. Figure 7b) shows that the locations with best NSE values tend to be where observed flows are largest, and therefore typically of most interest from the perspective of the broad scale hydrological response in CPLriv.

Figure 8 provides a more direct illustration of the simulated and observed daily mean flows through winter 2013/14 for four of the gauges considered by Martinez-de la Torre et al. (2019). The Tamar, Tay and Severn gauges are among the locations where CPLriv has largest low bias relative to observations (Figure 7a) while CPLriv is biased high at Thames, attributable in part to missing groundwater storage. For reference, results from observation-driven hydrological model simulations of Grid-to-Grid (G2G; Bell et al., 2018; Bell et al.,

2007) and DECIPHeR (Coxon et al., 2019) are shown. These indicate plausible best simulated results. DECIPHeR is a 100-member ensemble, illustrating the potential range of hydrological model solutions for a given observed input. Both G2G and DECIPHeR are driven by 1 km^2 gridded daily precipitation fields derived from rain gauge observations. G2G was driven by a corrected monthly potential evaporation derived from 5 km^2 gridded temperature observations (Rudd et al., 2017), while as described by Coxon et al. (2019), the DECIPHeR ensemble was driven by daily potential evapotranspiration data derived at 1 km^2 by Robinson et al. (2017). The G2G model underpins operational flood forecasting in the UK and has therefore been optimised to represent peak flow conditions across a wide range of UK hydrological regimes (Pilling et al., 2016). Unlike JULES or G2G grid-based routing, DECIPHeR represents a different model architecture that uses hydrological response units to represent land heterogeneity and a semi-distributed approach to flow routing (Coxon et al., 2019).

The CPLriv flows vary too slowly with time compared to observations and G2G or DECIPHeR, although the variability on weekly to monthly timescales is consistent. For 3 of the 4 locations presented in Fig. 8, the slower variability of CPLriv simulated flows contributes to an under-prediction of peak flows. Results are often but not always within the range of possible solutions provided by the DECIPHeR observation-driven ensemble. Further tuning and improvement of the CPLriv flow results is outside the scope of this study, but this initial analysis of the coupled system flows gives some confidence that there are opportunities for improvement through more careful assessment of the appropriate land surface and flow parameters required for simulations driven by UM meteorology. For example, Largeron et al. (2018) found that changes to the JULES infiltration could lead to much more responsive river flow simulations. This research should assess the impact of future system changes across temporal scales of interest (e.g. Weedon et al., 2015).

3.4 Discharge to ocean

Coupled modelling approaches enable terrestrial hydrological simulations to directly impact the near coastal ocean. The time series of accumulated river discharge into the ocean around UK and Ireland coastlines in CPLriv (Figure 9) is consistent with previous results for precipitation, soil moisture and river flow variables of the system, declining through November and early December 2013 before reaching maxima over a period of around 3 weeks in late December to mid-January 2014 and again in February. This is consistent with the evolution of the UK National Runoff Series (UKNRS), an observation-derived estimate of the discharge from England, Scotland and Wales coastlines. This is calculated as described by Marsh et al. (2015) by accumulating the total observed runoff from NRFA gauged catchments and using simulations of the G2G model to account for flows from remaining ungauged catchments. G2G data accounts for around 37% of the England-Wales-Scotland outflow product. CPLriv results are up to 50% lower than UKNRS during the December/January peak and, consistent with Figure 8, show less day-to-day variability than the UKNRS reference. Figure 9 also shows the equivalent discharge in the climatological river flows used to force the ocean in CPLclim simulations. CPLriv total values only begin to exceed CPLclim during February whereas the relatively stationary winter climatology is likely an overestimate of the observed coastal discharge during the first part and an underestimate during the later part of winter 2013/14. In the context of a first evaluation of a more coupled approach to the UK water cycle however, Figure 9 provides further reassurance that the order of magnitude of discharge from CPLriv and its temporal variability are broadly representative.

[Insert Figure 9]

3.5 Coastal ocean response

The sensitivity of the coupled NEMO ocean surface salinity to the freshwater flux imposed at the coastline is summarised in Figure 10. Monthly mean salinity difference maps show the extent of regions of freshwater influence around the UK and Ireland. CPLriv is generally less fresh than CPLclim, consistent with the relatively reduced discharge (Figure 9). Largest differences, exceeding 2 psu, due to lower flows in CPLriv are apparent for outflow regions from the Thames (consistent with Figure 7b), Bristol Channel (associated with lower flows from the river Severn; Figure 7c) and Humber Estuary (fed by the rivers Ouse and Trent; Figure 6b). Timeseries of region mean surface salinity in Figure 10e) show that the CPLnoriv ocean surface becomes increasingly saline with time, reaching a mean difference of nearly 0.2 psu over the 4-month simulation period. This exceeds the CPLriv and CPLclim variability during the period. CPLnoriv becomes well mixed through the ocean depth, resulting in considerably less temporal variability due to tidal and meteorological forcing than CPLriv or CPLclim. By default, river discharge is applied in NEMO with zero salinity (i.e. fresh water). This is a simplifying assumption and additional source of uncertainty. Sensitivity to input salinity and parameterizations of estuarine mixing processes should be explored in future.

[Insert Figure 10]

The mean SST response (Figure 11) is typically within 0.1 K around the UK coastline, with more complex and less coherent spatial patterns of SST differences due to the river forcing than for salinity. Figure 11e) indicates that the SST sensitivity (even for CPLnoriv results) is considerably smaller than the magnitude near-coastal SST simulation errors. Those errors can be mainly attributed to missing ocean model processes such as coastline wetting and drying or meteorological or tidal forcing errors (Tonani et al., 2019). Analysis of SST results at some coastal buoys around the UK (not shown) does indicate more localised responses to differences in river forcing associated with the representation of specific storms in CPLriv and their absence in CPLclim. While outside the scope of this paper, and noting sensitivities are within the observational error, this provides some encouragement that near-coastal simulations can be improved through further optimisation of the river flows in CPLriv.

[Insert 11]

The sensitivity of simulated vertical profiles of ocean salinity and temperature through winter 2013/14 at the L4 buoy location off the south-west England coast (Figure 1) is shown in Figure 12 and 13 respectively. Vertical ocean profile observations are provided by CTD sensor measurements operated weekly by Plymouth Marine Laboratory (Smyth et al., 2009).

[Insert Figure 12]

[Insert Figure 13]

Results for 9 December (Figure 12a and 13a) show some indications of the ocean state at depth spinning up from a common initial condition with climatological river inputs. The CPLclim profile matches the observed inversion relatively well, but is overall too fresh by around 0.25 psu, consistent with a relatively high river discharge relative to observations through November and December. The CPLriv and CPLnoriv results by contrast are well mixed throughout and more closely match observed salinity in the upper 20 m. The CPLnoriv salinity remains relatively constant through this period and tends to be too saline (and too cool) even at 50 m depth and completely misses the observed near-surface freshwater induced inversion. CPLriv and CPLclim have more similar profiles, but there are encouraging signals that the shape of CPLriv salinity profiles better match observations than CPLclim and have closer agreement to observed near-surface values. Such differences may be particularly important when assimilating profile information for example (King et al., 2019), and merits a more rigorous assessment of the impact of simulated river inputs in a full ocean assimilation experiment in near future. The temperature profiles in Figure 13 also show clear structural differences between simulations, consistent with the differences in salinity, although the magnitude of differences between CPLriv and CPLclim is typically within 0.1 K to 0.2 K.

4. DISCUSSION

This study provides a first assessment of the hydrological performance of a whole system simulation of the water cycle using a UK-focussed regional coupled system at km-scale. In common with the evidence provided by Durnford et al. (2018), the vision for a more integrated approach to water cycle prediction is a technical reality. A free-running km-scale coupled simulation of the UK water cycle across atmosphere, land and ocean components has been demonstrated and run successfully, producing broadly representative results across those components for winter 2013/14.

These results highlight that many limitations and scientific challenges remain to be overcome before the system could be applied with confidence for hazard prediction applications across timescales. This study is therefore considered to provide a baseline of system performance from which to build through future enhancements. As demonstrated by Deacu et al. (2012) in the Canadian context, and advocated by Flack et al. (2019) in the context of UK predictions, system improvements should be realised with an end-to-end assessment to avoid building dependence on either compensating errors or necessary bias or calibration corrections through a modelling chain. These CPLriv simulations will need to be revisited to demonstrate the impact of future developments. Further evaluation experiments will also be required to cover a broader range of climatological conditions, including those associated with convectively dominated intense summer rainfall and prolonged dry periods.

While the simulated precipitation in CPLriv is representative of observations at national scale, there are clear biases in its distribution even on monthly timescales with relatively low accumulation over steeper terrain across western UK and too much rainfall propagating further east. While the benefit of km-scale resolution atmosphere modelling for improving the representation of orographic rainfall has been well established (e.g. Roberts et al., 2008; Smith et al., 2015), this study shows lower skill for precipitation over steep terrain than indicated for operational regional NWP results for the UK at 1.5 km resolution by Smith et al. (2015). The west-east bias pattern is however consistent with the results for winter precipitation of a regional climate (i.e. non-assimilating) application of the UM over Scotland at this scale by Chan et al. (2018). This merits further investigation and improvement, both to identify the role of data assimilation in the better operational NWP performance and to assess whether there are additional influences such as changes to model physics, domain extent or global boundary conditions which impact precipitation biases. An experiment is proposed to assess the land surface response to parallel free-running and assimilative NWP meteorology driving JULES over a prolonged period, to better understand the extent to which simulated river flows are degraded by the absence of assimilation in CPLriv at present.

The CPLriv hydrological configuration effectively translates the recommendations of Martinez-de la Torre et al. (2019), obtained from an assessment of observation-driven JULES simulations (1991-2000) at 13 gauges of interest, to a national-scale system driven by a regional atmosphere model, and set on a different model grid with different soil ancillary information to match the configurations used in regional NWP for the UK. Martinez-de la Torre et al. (2019) presented river flow simulations biased low relative to observations (typically between -30% and -10% bias) with NSE metrics in the range 0.59 to 0.85. In common with Martinez-de la Torre et al. (2019), key land surface processes for improvement remain a balance between:

- Reducing excessive evaporation (Blyth et al., 2019),
- Enhancing infiltration of precipitation into the soil column (Largeron et al., 2018),
- Addition of lateral and sub-surface flows in the land model (e.g. Batelis et al., 2020).

A number of these enhancements are being currently delivered and coordinated through the Hydro-JULES programme (https://hydro-jules.org/). Hydro-JULES research is also deriving improved land surface parameters through a data assimilation framework using the COSMOS observations (Cooper et al., 2020; Pinnington et al., 2020). Enhancements to be delivered from Hydro-JULES can now be readily applied and demonstrated in the UK coupled system and CPLriv experiments should be repeated to assess their impact within an integrated system.

The recent development of a UK regional soil moisture analysis for NWP by Gomez et al. (2020) provides opportunities to explore the impact of improved soil moisture updating on system performance. Several authors have highlighted the value of river flow assimilation for improving both river flow and soil moisture (e.g. Warrach-Sagi and Wulfmeyer, 2010; McMillan et al., 2013; Sun et al. 2016; Tian et al., 2019). This will be of benefit in the UK context, but there are first order model biases that are worth addressing as a more immediate development priority. As advocated by Clark et al. (2015), there also remain opportunities to improve the river flow parameterization, for example by implementing a 1-D diffusive wave solution.

There is also a strong requirement to move to the assessment of land surface and river flow simulations in probabilistic terms. Work is in progress to run the UK coupled system in ensemble mode, with the atmosphere component driven by the MOGREPS-UK operational NWP ensemble (Porson et al., 2020). Driving regional river flow predictions with an ensemble of precipitation input, and introducing stochastic and parameter perturbations in the land surface and river routing components offers many opportunities to better understand the propagation of uncertainty through the system, as well as consider appropriate design of regional coupled ensemble systems when coupling a range of potential flow solutions with ensemble ocean model components.

The impact of modifying the river discharge from the land into the coastal ocean around the UK has been quantified for winter 2013/14. While differences between CPLriv and CPLclim ocean results demonstrate some sensitivity, this analysis also highlights that the exact details of the river flow simulation are of second order importance to other coastal ocean processes. It will be interesting to revisit this analysis when the CPLriv discharges are not biased low relative to observations, and to undertake more detailed analysis of the impacts for specific case studies of coastal flooding and tidal locking in a multi-hazard context. Assessing the sensitivity of the near-coastal ocean to river discharge is also hampered by the limited availability of in-situ salinity observations around the UK coast, with the L4 profile observations presented here being a very rare and valuable resource. A brief comparison between CPLriv salinity results with SMOS satellite derived salinity products derived by Olmedo et al. (2020) proved inconclusive due to limited data availability in the near-coastal regions where river discharges were impacting ocean simulations.

Finally, it is worth revisiting the vision for more dynamical coupling of the water cycle in the context of Earth System processes at regional scales. These extend beyond physical couplings between components into provision of capabilities to deliver forecasts and assessments of environmental changes on biogeochemical processes, and ultimately to include the role of anthropogenic influence on these. The modelling framework presented here provides a good basis from which to advance coupling to marine and terrestrial biogeochemistry models and inform questions of water quality and marine health. This vision was well characterised again by Beven (2007), as follows:

> *Built on the fluxes within those models, air and water pollutant transport models and biogeochemical models could, additionally, be implemented locally within the regional scale domain. Each component should be able to assimilate data transmitted from field sites and to assess the uncertainty in the predictions. Such an integrated system should operate both in real time, assimilating data and boundary conditions from larger scale models and displaying the 'current state of the environment', as well as providing the potential to update model predictions into the future under different scenarios."*

5. CONCLUSIONS

A km-scale regional coupled simulation system has been presented with results showing broadly representative predictions of precipitation, soil moisture, river flow and coastal ocean state for free-running simulations focussed on the UK for winter 2013/14. Four specific questions were set out in Section 1.

a) Are km-scale regional simulations of precipitation and soil moisture sufficiently accurate to provide useful forcing for distributed modelling of river flows across UK catchments?

For winter 2013/14, a west-east bias in accumulated precipitation simulations has been identified, with rainfall too low over upland areas of western UK and too much rainfall advected further east. This assessment has been unable to determine how limiting these biases are for modelling of river flows across the UK – in practice there are too many processes within the coupled hydro-meteorological modelling chain. For the time of interest in this study, there were relatively few in-situ observations of soil moisture state, although the direct comparison presented shows moderately good agreement between simulations and observations where available. There are opportunities to further improve the simulated river flow results presented, and this study provides a necessary baseline of the hydrological performance of the UK km-scale regional coupled system.

b) How sensitive are regional ocean simulations of the near-coastal region around the UK to the representation and accuracy of input river flows?

Dynamically coupled prediction systems enable new insight to be gained on the 'hydrological response' of the near-coastal ocean to hydro-meteorological processes. For winter 2013/14, the near coastal salinity can be modified by more than 2 psu in regions impacted by river discharge around the UK coast. On average, the impact on temperature is considerably smaller, and the sensitivity to river flows shown to be of second-order importance relative to other sources of near-coastal ocean errors.

c) What do these results imply for future component model development?

This study demonstrates the feasibility of a vision for more dynamically coupled systems to provide useful predictions at scales relevant to catchment and coastal processes. Development priorities have been identified for further improving the quality of these predictions. These remain a balance between model physics enhancements across components – e.g. reducing precipitation biases, improving land surface model representation of evaporation and infiltration processes; addition of missing processes, notably of lateral and sub-surface water flows in the land surface model; and a move to more assimilative and probabilistic modelling frameworks. These developments will provide a strong basis for further exploration to more biogeochemical aspects of the Earth System at regional scales in future.

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DATA AVAILABILITY

Coupled model data used in this study amount to several Tb, archived to tape storage at the Met Office. These data can be readily shared with interested collaborators on contacting the lead author. Details on obtaining the model codes used to produce these results are set out in the Appendices of Lewis et al. (2019).

Details and links to freely access the HadUK-Grid precipitation data are available from https://www.metoffice.gov.uk/research/climate/maps-and-data/data/haduk-grid/datasets.

COSMOS-UK observation data are available from https://cosmos.ceh.ac.uk/. NRFA river flow observation data are available from https://nrfa.ceh.ac.uk/. L4 ocean observations are accessible via https://www.westernchannelobservatory.org.uk/data.php. G2G model data are available from https://doi.org/10.5285/f52f012d-9f2e-42cc-b628-9cdea4fa3ba0 and the DECIPHeR ensemble flow simulations from https://doi.org/10.5285/d770b12a-3824-4e40-8da1-930cf9470858.

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TABLES

Run Name	UK + Ireland river discharge	Rest of domain river discharge
CPLriv	JULES simulation, OASIS coupled	AMM15 climatology
CPLclim	AMM15 climatology	AMM15 climatology
CPLnoriv	Zero flows	AMM15 climatology

Table 1: Summary of coupled simulations assessed

FIGURE LEGENDS

Figure 1: (a) Map of coupled model domain extent (black surrounding box). Shaded colours illustrate the S_0/S_{max} slope-dependent PDM parameter for each land grid point. Line contours show the ocean model bathymetry, with solid contours drawn every 50 m in locations where the ocean depth is shallower than 250 m and dashed contours every 500 m where the ocean is deeper. Red circles indicate the location of climatological river outflow points in the ocean model. (b) Zoom of the UK and Ireland region of the model domain (red box in (a)) with shading illustrating the upstream number of grid cells of the river routing grid. The locations of gauge observations on the rivers Tay, Severn [Sev], Thames [Thm] and Tamar [Tam] are shown by black open circles. The location of the L4 ocean buoy off the south-west England coast is shown as a pink cross. The location of Sheepdrove [1], Chimney Meadows [2], Wytham Woods [3] and Waddesdon [4] COSMOS-UK soil moisture cosmic probe observation sites are indicated by green crosses. Red circles show the location of climatological outflow points in the ocean model (as in (a)). Blue diamonds indicate the location of ocean model river outflow points in the coupled system. Other sub-regions considered in the study are highlighted for reference.

Figure 2: Maps of (a-d) observed and (e-h) CPLriv simulated monthly accumulated precipitation for November and December 2013, and January and February 2014. Figures a)-d) show the HadUK-Grid 1 km x 1 km gridded gauge observed precipitation product (Perry and Hollis, 2005). Figures e)-h) show the accumulated precipitation computed from the CPLriv hourly mean rainfall rate. (i-l) Monthly accumulation differences between CPLriv and HadUK-Grid precipitation computed on the HadUK-Grid grid. (m) Time series comparing the CPLriv simulated and HadUK-Grid observed daily mean (water day 0900-0900) precipitation across England, Scotland and Wales land points through the period.

Figure 3: Maps of monthly mean (a-d) surface evaporation, (e-h) surface runoff and (i-l) sub-surface runoff rate simulated by CPLriv for November and December 2013, and January and February 2014 respectively. Note colour bar scales are different for each variable.

Figure 4: Timeseries of spatially averaged simulated (a) soil evaporation, (b) surface runoff, (c) volumetric soil moisture content of the upper (0 - 0.1 m depth) soil level (solid) and lowest (1 - 3 m depth below surface) soil level (dashed), (d) sub-surface runoff across

England, Scotland and Wales land points in the CPLriv coupled system during winter 2013/14.

Figure 5: Timeseries showing CPLriv simulated total volumetric water content in the top 2 soil levels (to depth 35 cm below surface) through November 2013 to February 2014. Plots (a) – (d) are for points marked 1 – 4 in Figure 1 respectively. The mean value in a 5 x 5 neighbourhood of grid points nearest each location is shown as a solid line, with 1 standard deviation about that value shaded. The minimum and maximum model values in the neighbourhood are shown as dashed line time series. Also plotted are available daily mean COSMOS-UK cosmic-ray derived volumetric water content estimations for each location (Stanley et al., 2020). The mean typical depth for which these observations are considered appropriate through the period for each site is listed in each figure legend.

Figure 6: Maps of mean simulated river flow speeds between November 2013 and February 2014 for selected sub-regions of the UK (see Figure 1). Mean observed flows for the same period at gauges in the National River Flow Archive (NRFA) UK Benchmark (UKBN2) dataset are plotted using the same colour scale as shaded square symbols.

Figure 7: Summary of (a) Bias [MODEL-OBS] and (b) Nash-Sutcliffe Efficiency (NSE) metrics comparing observed and simulated river flow at selected National River Flow Archive (NRFA) locations. Only data from December 2013, January 2014 and February 2014 are included here to avoid any spin up impacts at the start of the simulation period. The size of circles is representative of the maximum observed flow during the period. In (b), green shaded circles show where NSE >= 0, with shading indicated by the colour scale. Yellow filled circles show where -1 <= NSE < 0, orange unfilled circles where -10 < NSE < -1 and red unfilled circles where NSE values less than -10 are computed for the evaluation period.

Figure 8: Timeseries of observed (black dashed) and simulated (red) daily mean (0900-0900) river flow at selected gauge locations from those assessed by Martinez-de la Torre et al. (2019) between November 2013 and February 2014. Mean bias (model – obs) and Nash-Sutcliffe Efficiency metrics, computed from 1 December 2013, are listed. River flows from the G2G in dark blue (Bell et al., 2018) and DECIPHeR in grey (Coxon et al., 2019) hydrological models driven by the same observed precipitation and observation-based potential evaporation are also shown as a reference. As DECIPHeR is a 100-member

ensemble dataset, the ensemble mean is plotted along with maxima and minima simulated daily flows.

Figure 9: Timeseries of accumulated discharge from land to ocean around England, Scotland and Wales coastlines during winter 2013/14 in the CPL simulations (red), as assumed in the AMM15 ocean model climatology (blue) and a UK National Runoff Series estimated from gauge observations by the National River Flow Archive (black dashed line; Marsh et al., 2015).

Figure 10: Monthly mean differences of (a-d) sea surface salinity simulated by CPLriv and CPLclim through winter 2013/14. (e) Timeseries of average sea surface salinity in the region with bathymetry shallower than 250 m around UK and Ireland coasts simulated by CPLriv, CPLclim and CPLnoriv configurations.

Figure 11: Monthly mean differences of (a-d) sea surface temperature simulated by CPLriv and CPLclim through winter 2013/14. (e) Timeseries of average bias [model – observation] between simulations and observed SST by near-coastal buoys in the region with bathymetry shallower than 250 m around UK and Ireland coasts for CPLriv, CPLclim and CPLnoriv configurations during January and February 2014.

Figure 12: Vertical profiles of observed and simulated ocean salinity at the L4 ocean buoy location (see Figure 1) on (a) 9 December, (b) 17 December 2013, (c) 14 January, (d) 20 January, (e) 29 January, (f) 10 February 2014. Daily mean profiles are computed from 5x5 grid points nearest to the observation point, with 1 standard deviation indicated by error bars.

Figure 13: Vertical profiles of observed and simulated ocean temperature at the L4 ocean buoy location (see Figure 1) on (a) 9 December, (b) 17 December 2013, (c) 14 January, (d) 20 January, (e) 29 January, (f) 10 February 2014.