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Interactive comment on "A parallel workflow implementation for PEST version 13.6 in high-performance computing for WRF-Hydro version 5.0: a case study over the Midwestern United States" *by* Jiali Wang et al.

Doherty (Referee)

johndoherty@ozemail.com.au

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The authors describe modifications that they made to PEST to enhance its use on a HPC. They then describe use of their modified PEST in calibration of a complex surface water model.

While I found the paper interesting, I found that it was lacking in information in some respects. For example nothing is said about the interface that they constructed between parallel PEST and the run management software that they employed. Nor was

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any reference made to PEST settings. While I agree with the authors that use of inversion methods that can parallelize model runs and handle the estimation of many parameters employed by a complex model is a much-needed addition to the arsenal of surface water modelling, I think that many more advances could be made than the authors have made. In particular, there was no mention of the use of Tikhonov regularisation to accommodate parameter nonuniqueness at the same time as it promulgates uniqueness through obtaining a set of parameters that "make sense" from an expert knowledge point of view. This, I think, is one of the strongest arguments for use of gradient-based, highly parameterized methods in regional surface or land use model calibration, that is the ability to not just accommodate nonuniqueness, but to turn the "wiggle room" engendered by nonuniqueness into formulation of an inverse problem that can actually make regionalization and transportability of parameters a reality.

The authors use a simple objective function. This may be ok for some inverse problems. However as they point out, some of the smaller flows (in terms of location in space and location in a single flow time series) are not as well fitted as they could be. Perhaps weights should be a function of flow – and of location. Perhaps other important aspects of the flow time series should be made more visible to PEST through formulation of separate, targetted objective function components to ensure that these aspects of the time series are also well fit.

The authors make a big deal out of their modifications to parallel PEST so that it is HPC-friendly. Actually, I think that the BEOPEST version of PEST has similar capabilities. The original version of BEOPEST used both MPI and TCP/IP for communication between master and slaves (now called manager and workers). Now only TCP/IP is used. One of the reasons that BEOPEST's capabilities exceed those of parallel PEST in the HPC environment (actually on any network) is that the manager does not need to write model input files and read model output files across the network. This makes run management must faster, more secure, and able to take place in a greater variety of network environments.

In summary, I think that what the authors have done is good. However I also think that the potential for regional surface water model calibration and uncertainty analysis in a HPC environment still remains largely untapped. Some of this potential will be realised with use of singular value decomposition to ensure numerical stability when inverse problems are ill-posed, use of Tikhonov regularisation to ensure parameter sensibility and transportability under the same conditions, and more creative formulation of the objective function than the authors have done.

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