Unleashed numerical daemons in our pub: Is poor numerical implementation of hydrologic models hurting the Predictions in Ungauged Basins initiative?

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Much of the research in the PUB initiative is focused on the analysis and interpretation of model results in well instrumented watersheds, in order to inform appropriate model structures and parameter values for use in ungauged basins. However, many of the models used in PUB share a common characteristic: poor numerical implementation. It is likely that many published conclusions, including (i) parameter sensitivity, optima and uncertainty estimates, and, more disconcertingly, (ii) the interpretation of hydrologic model output to gain insights into internal catchment dynamics, including the relative significance and behavior of different processes, may be questionable due to numerical artifacts introduced by unreliable time stepping schemes. Such lack of attention to numerical schemes has almost certainly hindered progress in the PUB initiative.

Here, we comprehensively evaluate several classes of time stepping schemes in terms of numerical fidelity, computational efficiency, and impact on model sensitivity analysis, calibration and prediction. Extensive numerical experiments are carried out using 8 distinct time stepping algorithms and 6 different conceptual hydrological models, applied in the densely gauged experimental Mahurangi catchment as well as in 12 MOPEX basins with diverse physical characteristics and hydroclimatic regimes. Results show that numerical errors of uncontrolled time stepping schemes, which remain widely used in hydrology, routinely dwarf the structural errors of the model conceptualization. This has serious implications for model analysis and predictive use, including inconsistent inferences of parameters and internal states even if the calibrated streamflow predictions are similar. Even when numerical errors allow "getting the right result for the wrong reason", they make the model unduly fragile in predictive mode, as evidenced in validation tests.

The extensive analyses in this paper indicate that these deformations are not rare isolated instances, but affect virtually any model structure, in any catchment, and under common hydroclimatic conditions. Erroneous or misleading conclusions of model analysis and prediction arising from numerical artifacts in the model implementations are intolerable, especially given that robust numerics are accepted as mainstream in other areas of science and engineering. From the range of simple methods investigated in this work, the fixed step implicit Euler method and the adaptive explicit Heun method emerge as good practical choices for the majority of simulation scenarios. We hope that the vivid empirical findings from this study will encourage the Hydrologist to seriously address model numerics, preventing them from obscuring our quest for more meaningful model interpretation and prediction.