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Simulation-based inference as a paradigm for scientific machine learning in the cryosphere and beyond

Brian Groenke[1,2,5], Kristoffer Aalstad[7], Norbert Pirk[7], Sebastian Westermann[7], Jakob Zscheischler[5,6], Guillermo Gallego[2,4], and Julia Boike[1,3]
[1]Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Permafrost Section, Potsdam, Germany (brian.groenke@awi.de)
[2]Technical University of Berlin, Department of Electrical Engineering and Computer Science, Berlin, Germany
[3]Humboldt University of Berlin, Geography Department, Berlin, Germany
[4]Einstein Center for a Digitial Future, Berlin, Germany
[5]Helmholtz Centre for Environmental Research, Department of Computational Hydrosystems, Leipzig, Germany
[6]Technical University of Dresden, Department of Environmental Sciences, Dresden, Germany
[7]University of Oslo, Department of Geosciences, Oslo, Norway

Mechanistic or dynamical models based on governing equations are ubiquitous throughout science and engineering. Such models, also referred to as “simulators”, are typically characterized by a forward mapping from some set of inputs or parameters to one or more output quantities of interest. In many cases, the inputs required for the forward model are either unknown or represent approximations of unresolved processes. Bayesian inference provides a natural framework for constraining this model uncertainty using observed data. Such a framework is especially valuable in cryospheric application domains such as permafrost research, where direct observations of many quantities of interest, e.g. subsurface temperature and soil moisture, are only sparsely available. Mechanistic models based on known physics therefore play an indispensable role in filling these gaps. However, virtually all methods for Bayesian inference require repeated evaluation of the forward model which is often computationally challenging, especially for dynamical systems. As a result, computational requirements of statistical inference very quickly become intractable even for systems of only moderate complexity. The burgeoning field of “simulation-based inference” (SBI) aims to leverage modern computational methods from machine learning (ML) and data assimilation (DA) to overcome these challenges and facilitate large scale uncertainty quantification in complex scientific models. In this work, we show how SBI can be seen as a unifying theoretical framework that bridges the gap between existing DA methods (e.g. variants of the ensemble Kalman filter) and full-fledged Bayesian inference with the goal of facilitating hybrid statistical-physical modeling of complex systems. We present a novel set of software tools for making SBI more accessible to researchers along with benchmarks of several methods drawn from both the ML and DA literature. Two of these benchmarks are based on use cases from Arctic land surface modeling: degree day approximation of snowmelt and geothermal inversion of historical climate change from boreholes in Arctic permafrost. We highlight the contributions that SBI can make to solving such inverse problems and discuss further potential

applications in the cryosphere and beyond.