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Model adaptation for hyperbolic balance laws employing constraint aware neural networks

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Physical phenomena like chemically reacting flows are computationally expensive to simulate due to the interaction between different physics at a wide range of time and length scales. Chemically reacting flows can be described by systems of hyperbolic partial differential equations with stiff source terms. The governing equations can be simplified by assuming chemical equilibrium and then it is possible to replace the full system with a simpler system. We investigate model adaptation for such systems. The model adaptation is carried out between the full system of equations referred to as the complex system and the simple system, which is obtained by projecting the complex system on to the equilibrium manifold. When numerically solving the simple system, to compute the flux a mapping from the state space of the simple system to the state space of the complex system needs to be employed. This involves solving a computationally expensive non-linear system of equations. To further reduce the computational expenses needed when solving the simple system, the mapping employed in the simple system can be replaced by an approximate mapping, which has to be constructed by accounting for the physics behind the mapping. Such an approximate mapping can be constructed employing machine learning techniques like physics based or constraint aware neural networks. Model adaptation is carried out by decomposing the computational domain in space and time and then the complex model is employed where necessary and the simple system, employing the machine learned approximate mapping, where sufficient. The domain decomposition is carried by constructing a posteriori error estimates which take in to account the discretization, modeling errors and errors incurred due to employing the approximate mapping.

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