Universal Differential Equation for Diffusion-Sorption Problem in Porous Media Flow

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Artificial Neural Networks (ANNs) have been widely applied to model hydrological problems with the increasing availability of data and computing power. ANNs are particularly useful to predict dynamic variables and to learn / discover constitutive relationships between variables. In the hydrology field, a specific example of the relationship takes the form of the governing equations of contaminant transport in porous media flow. Fluid flow in porous media is a spatio-temporal problem and it requires a certain numerical structure to solve. The ANNs, on the other hand, are black-box models that lack interpretability especially in their structure and prediction. Therefore, the discovery of the relationships using ANNs is not apparent. Recently, a distributed spatio-temporal ANN architecture (DISTANA) was proposed. The structure consists of transition kernels that learn the connectivity between one spatial cell and its neighboring cells, and prediction kernels that transform the transition kernels output to predict the quantities of interest at the subsequent time step. Another method, namely the Universal Differential Equation (UDE) for scientific machine learning was also introduced. UDE solves spatio-temporal problems by using a Convolutional Neural Network (CNN) structure to handle the spatial dependency and then approximating the differential operator with an ANN. This differential operator will be solved with Ordinary Differential Equation (ODE) solvers to administer the time dependency. In our work, we combine both methods to design an improved network structure to solve a contaminant transport problem in porous media, governed with the non-linear diffusion-sorption equation. The designed architecture consists of flux kernels and state kernels. Flux kernels are necessary to calculate the connectivity between neighboring cells, and are especially useful for handling different types of boundary conditions (Dirichlet, Neumann, and Cauchy). Furthermore, the state kernels are able to predict both observable states and mass-conserved states (total and dissolved contaminant concentration) separately. Additionally, to discover the constitutive relationship of sorption (i.e. the non-linear retardation factor $R$), we regularize its training to reflect the known monotonicity of $R$. As a result, our network is able to approximate $R$ generated with the linear, Freundlich, and Langmuir sorption model, as well as the contaminant concentration with high accuracy.