In the first year of the project, we are focused on attaining the first object to develop a computational Bayesian framework for uncertainty quantification. The framework considers various sources of uncertainty in data, model structures, model parameters, and driving forces (e.g., natural changes related to climate change and human-induced engineering remediation). The framework is implemented using Bayesian network. In the network, model components (deterministic and stochastic) are separated into network nodes, and relations between the components are represented by network edges, which are also pathways of uncertainty propagation. To evaluate the developed method, a Bayesian network was developed for model scenarios of flooding and precipitation, groundwater flow and reactive transport problems. Contribution of different uncertainty sources to predictive uncertainty was quantified.

Uncertainty quantification within the network is conducted using the state-of-the-art sparse grid methods, which are computationally efficient and can be integrated with the Bayesian network seamlessly. The sparse grid methods can alleviate the problem of curse-of-the-dimensionality of conventional Monte Carlo methods by selecting a small number of sparse grid points (in parameter space) to evaluate statistical moments of quantities of interest. On the other hand, the sparse grid methods can also be used to develop a surrogate of the original model, a polynomial-like interpolation that is fast to evaluate. We have applied the sparse grid methods to groundwater flow and reactive transport problems. Since reactive transport problems are more challenging because of model nonlinearity, more advanced sparse grid methods are necessary such as high-order stochastic collocation method with adaptive schemes.

To thoroughly evaluate the developed methods, a synthetic problem of hexavalent uranium (U(VI)) reactive transport was developed based on data and information at the Naturita UMTRA site. The synthetic problem considers three geological settings, three kinds of boundary conditions, and nine geochemical reactions. We are conducting uncertainty quantification using conventional methods, and the results will be used to evaluate computational efficiency and accuracy of the sparse grid methods. The computational tool will be used to the real-world modeling at Naturita to gain insights into groundwater reactive transport modeling.