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ENABLING DIGITAL TWINS THROUGH REDUCED-ORDER AND SURROGATE MODELING

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ABSTRACT

In many engineering applications involving digital twins (DTs), using high-fidelity forward models can render the solution of inverse and control problems computationally intractable. This is typically due to the high-dimensionality and complexity of high-fidelity models, often accompanied by high-dimensional inference parameters and decision spaces. Many-query applications, such as optimization and control, however, require a fast, yet accurate model output response, as well as information about the response uncertainty. Surrogate models and reduced-order models (ROMs) can help make these problems tractable, provided they achieve sufficient accuracy and can be built from a limited number of forward model evaluations. This MS aims at addressing several key challenges that arise in the usage of surrogate models in DT settings:

1. Goal-oriented modeling: Surrogates and ROMs do not necessarily need to reproduce the full spatio-temporal dynamics of the system. Instead, they may only need to capture the control objectives and data assimilation observables accurately. Determining what appropriate methodologies are for the design of such models remains an open challenge.

2. Structure preservation: DTs often simulate system dynamics over extended periods; therefore, the design of corresponding ROMs could exploit physics-based knowledge to preserve important structural properties and invariants, such as energy or mass.

3. Trustworthy neural network surrogates: Neural network representations have shown strong potential as high-dimensional surrogate models, but further work is needed to establish their reliability for dynamical systems, especially when training data is limited.

4. Nonlinear low-dimensional representations: Many surrogate and ROM techniques rely on the existence of an intrinsically low-dimensional parameter-to-output map or solution manifold. However, linear subspace methods may fail to represent this structure efficiently for important problem classes, e.g., advection-dominated flow and transport.

5. Accurate gradient approximation: When surrogates are trained only on samples of high-fidelity input–output maps, and not on their Jacobians, they may approximate gradients poorly. This can, in turn, lead to inaccurate solutions of the optimization problems that underpin data assimilation and optimal control.