Slides Outline

Sections

1. Research background.
2. Twin model.
3. Optimization with twin model.
4. Application to a turbulent flow optimization.

Research background

1. Motivation:
   - Optimization based on conservation law simulation.
   - Design space is high dimensional.

   Example: optimization of turbulent return bend geometry. (picture)
2. Many conservation law simulators are gray-box. What is gray-box / black-box / open-box. (table, merge PDE+implementation)
3. Research scope:
   - conservation law.
   - gray-box simulation.
   - high-dimension design.
4. If open-box, review of gradient-based.
5. In reality, not open-box. Treat as black-box, review of gradient-free. Curse of dimensionality. However, not take advantage of space-time solution.
6. When lower-fidelity models are available, can save overall computation time by multi-fidelity optimization. High-fidelity model is the gray-box simulator; low-fidelity model can be constructed by surrogate methods.
7. Review of surrogate methods.
   - physics-based surrogates: use the physics of the underlying system, such as
     - coarser discretization: *require simulator's PDE.*
     - reduced order model (POD, DEIM, balanced truncation): *require simulator's PDE.*
     - simplified physics (RANS, dual porosity, thin airfoil theory).
   - functional surrogate: use the sample value of objective function, such as
     - radial basis function approximation.
     - polynomial approximation.
     - neural network.

   Narrative: functional surrogate not suitable in my research scope because design space is high-dimensional. Focus on physics-based surrogate.
8. Physics-based surrogates can be adaptive.
   - Adaptive discretization: *require simulator's PDE.*
   - Goal oriented reduced order model: match observations, *require simulator's PDE*
9. Research objective.
   - Develop a method for inferring a surrogate conservation law from the space-time solution of an gray-box simulation.
   - Assess how much computation saving can be achieved using the proposed method in a return bend optimization problem.

Twin model

1. Adaptive physics-based surrogate that reproduces the space-time solution.

   - does not require simulator's PDE, instead infer a convervation law PDE.
   - PDE is inferred by matching the gray-box simulation's space-time solution.

   Example problem: infer Buckley-Leverett equation flux function.

2. Benefits of matching space-time solution

   - Small domain of dependence (low dimensional inputs)
   - Large number of samples
   - Dimension independent of design

   Time independent is a special case. Pseudo-time marching until convergence.

3. Functions can be parameterized. Infer twin model is an inverse problem.
   Review of inverse problems, two viewpoints.

   - Statistical estimation.
   - Parameter identification.

   Twin model is an open-box, use adjoint for parameter identificaiton.

4. Formulation. Time dependent. General: not same grid, different weight.

5. Formulation. Time-independent. General.

6. Candidate basis (Questions)

   - polynomial
   - Fourier
   - wavelet

   How about adaptive basis selection (supervised: peceptron basis selection. unsupervised: e.g. vector quantization.)

7. Numerical example: twin model with fixed structure

8. Numerical example: prediction of objective functions about one training.

9. Basis selection: for time-dependent and time-independent twin models

   - regularization-based methods
   - test-based methods

10. Basis selection: for time-dependent twin models. Reduce to linear basis selection scheme by

    - Solve twin model with restart.
    - Finite difference approximation.

    (picture: basis selection)

Optimization with twin model

1. General optimization statement.
2. Review of multi-fidelity optimization schemes. Provably convergent.
   - pattern search
   - Trust region
   - Bayesian
3. Review of Bayesian MFO. Include Bayesian optimization flowcharts.
4. Advantages of Bayesian MFO
   - Uses all high-fidelity evaluations to choose the next design to evaluate.
   - Balances exploration and exploitation. Done by appropriate acquisition function of the posterior. Expected improvement formulation.
5. Propose to use twin model's gradient and gray-box simulation objective function in Bayesian multifidelity framework. (flowchart)
6. Model twin model gradient and gray-box objective function. Posterior can be obtained by coKriging. Hyperparameters can be estimated by MLE.
7. Flowchart (full optimization procedure)
8. Demonstration: high-dimensional optimization with noisy gradient.
9. Discussion on convergence of non-constraint optimization. Proposed theorem.
10. Constraint optimization. Two types of constraints (their names in existing literatures?)
    (a) Type 1: require solution of PDE simulation.
    (b) Type 2: not require solution of PDE simulation.

    Only interested in type 1.
11. Constraint optimization. Constraint expected improvement formulation.

Application to a turbulent flow optimization

1. Problem description. Optimize return bend geometry to minimize pressure drop. Low Mach number, incompressible. (picture) Interested in ensemble average quantities.

2. Candidate PDE models for turbulent flows. Two categories:

   - PDEs for ensemble average quantities. They satisfy a conservation law PDE. But the PDE is not closure: modelling Reynolds stress is an open problem. RANS models. Low-fidelity.
   - PDEs for instantaneous quantities. Such as LES, DNS. Costly to solve. Generally no adjoint? High-fidelity.

3. Propose to construct a twin model for the ensemble average quantities. Train the twin model by high fidelity simulation's time-averaged space-time solution. (flowchart)

4. Review of RANS models.

   - Models based on Boussinesq hypothesis: eddy viscosity.
     - algebraic models.
     - one-equation models. (transport equation)
     - two-equation models. (transport equation)
   - Reynolds stress modelling.

   Focus on two-equation models for its ability to capture more complex turbulent phenomenons.

5. Twin model can be applied to infer PDE for eddy viscosity. For example $k - \omega$ models. The rhs of PDEs for for k and ω are adaptive.

6. Future work.

   - Implement LES in OpenFoam, serving as gray-box simulation.
   - Implement a RANS model with adjoint.
   - Still an open problem how to parameterize the rhs of twin model. As a first step, consider the constants in the $k - \omega$ model as variables.
   - Assess computational savings, and optimal solution quality given limited computation budget.

Miscellaneous

1. Expected contributions
   - Enable adjoint gradient computation even if the governing conservation law is not available.
   - Demonstrate that efficient gradient-based optimization is possible, even if the underlying simulator does not implement an adjoint.
   - Demonstrate my method's superiority in a high-fidelity turbulent flow optimization with a high-dimensional design space.
2. Proposed schedule
   - **Completed:**
     - Course work.
     - Formulation of twin model and its inference.
     - Basis selection for time-dependent twin model.
     - Optimization framework using twin model.
     - Demonstration of twin model in a 1D example.
   - **To be complete:**
     - **2015 Apr**: Write proposal defense slides. Wrap up the proof of theorem **??**.
     - **2015 May**: Defend proposal. Demonstrate the complete algorithm on a the 1D Buckley-Leverett example.
     - **2015 Jun**: Setup an LES solver for the return bend testcase in OpenFoam, write a RANS solver with adjoint for the return bend.
     - **2015 Jul**: Hold a committee meeting for progress report.
     - **2015 Jul-Oct**: Implement optimization on the return bend example.
     - **2015 Aug-Nov**: Write thesis.
     - **2016 Jan**: Defend thesis.
3. Major and minor programs of study, courseworks
4. References