An efficient optimization framework for gray-box conservation law simulation

Thesis proposal defense

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Outline

- Background.
- Thesis objective.

- Estimate gradient by twin model.
- Optimization framework.
- Application to turbulent flow optimization.

- Expected contribution.
- Proposed schedule.

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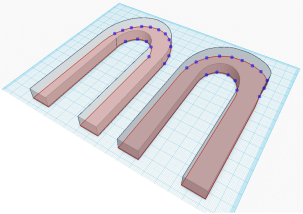
Research background

- Interested in optimization constraint by conservation law simulation.
- Conservation law simulation can be expensive.
- The design space can be high-dimensional.
- Efficient sensitivity (adjoint) analysis may not be available.

A forest of oil wells in California, 1937

Internal cooling of turbine airfoil
Source: http://www.amaterastyo.biz/eng/technologies.html



Design space can be high-dimensional.

Research scope

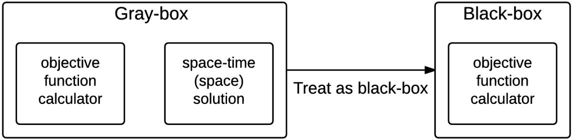
- Gray-box conservation law simulation:
  - adjoint not available.
  - governing PDE and its implementation not available.
  - can output space(-time) solutions.

	PDE and implementation	space(-time) solution	Adjoint
Black-box	✘	✘	✘
Gray-box	✘	✔	✘
Open-box	✔		✔

- High-dimensional design space.
  - large number of parameters required to parameterize the space(-time) dependent design.

Review of optimization methods

- If black-box, use derivative-free optimization,
  (pattern search methods [Tarma03], evolution based methods[Eberhart 10, Davis 10])
  - not require derivative evaluation.
  - not suitable for high-dimension optimization.
- If open-box, use gradient-based optimization,
  (quasi-Newton methods [John 77]: BFGS, L-BFGS, etc.)
  - requires efficient gradient evaluation, generally using adjoint.
  - suitable for high-dimension optimization.
- If gray-box,



Research objective

- Develop a method to estimate the gradient by using the space(-time) solution from the gray-box simulation.
- Formulate an optimization framework that uses the estimated gradient for efficient high-dimensional optimization.
- Given a fixed computational budget, assess how much design objective improvement can be achieved by using the proposed framework.

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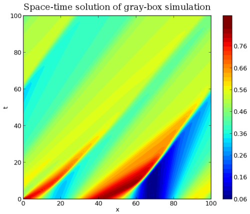
Leverage the space(-time) solution

Estimate the gradient:

- infer the conservation law from the space(-time) solution.
- apply adjoint to estimate gradient.

Example: infer flux $F(u)$ from space-time solution.

$$
\begin{aligned}
&\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c(x) \\
&u(t=0,x) = u_0(x) \\
&u(t,x=0) = u(t,x=1)
\end{aligned}
$$



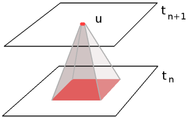
Propose to infer the flux or the source term that reproduce the space(-time) solution. The inferred conservation law is called twin model.

Why is the PDE inferrable?

- The governing PDE is a conservation law. Flux and source terms are functionals.

$$\times \quad \dot{u} = \mathcal{L}(u, c) \quad \checkmark \quad \frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c$$

- The flow quantities only depend on the flow quantities in an older time inside a domain of dependence.



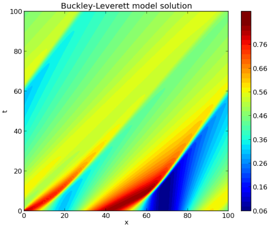
- Space-(time) solution can provide large number of samples.
- The inference can be independent of the design space dimensionality.

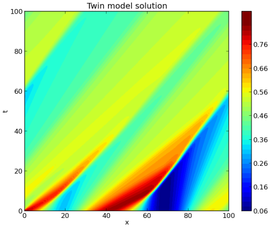
Minimize space(-time) solution mismatch

The inference can boil down to an optimization problem.

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c(x)$$
$$u(t=0,x) = u_0(x)$$
$$u(t,x=0) = u(t,x=1)$$

$$\frac{\partial \tilde{u}}{\partial t} + \frac{\partial \tilde{F}(\tilde{u})}{\partial x} = c(x)$$
$$\tilde{u}(t=0,x) = u_0(x)$$
$$\tilde{u}(t,x=0) = \tilde{u}(t,x=1)$$





$$\min_{\tilde{F}} \left\{ L(\tilde{F}) \equiv \int_t \int_x \|u - \tilde{u}\| \;\, dt\, dx \right\},$$

where $\|\cdot\|$ is a norm to be chosen.

Some technical details

- Parameterize the flux or source term
  polynomial, Fourier, wavelet, etc
  - we choose a family of sigmoid functions with various centers.
    $\tilde{F}(\cdot) = \sum_{i=1}^{n} \xi_i s(\cdot)$
- Basis selection
  matching pursuit [Adler 96, Billing07]: forward selection, backward pruning;
  regularization [Stone 77, Schwarz 78, Tibshirani 96]: AIC/BIC, Lasso, elastic net
  - we choose Lasso regularization for basis selection.
    $\min_{\tilde{F}} \left\{ L(\tilde{F}) + \lambda \sum_{i=1}^{n} |\xi_i| \right\}$

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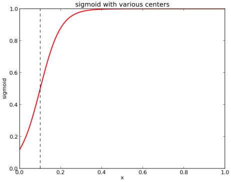

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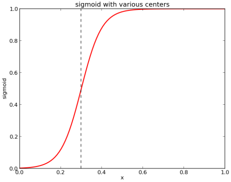

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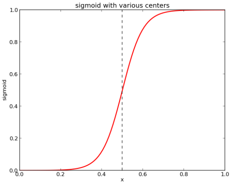

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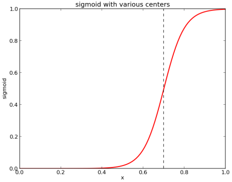

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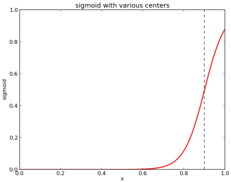

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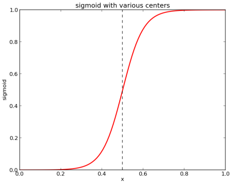

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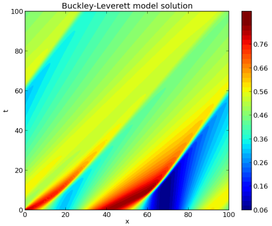
A demonstration of twin model

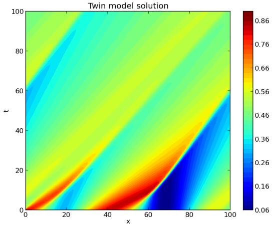
Consider an optimization objective: [Kucuk 06]

$$\min_{c\in\mathbb{R}} \left\{ J(u) \equiv \int_{x=0}^{1} \left| u(x, t=1; c) - u^*(x) \right|^2 \mathrm{d}x \right\}$$

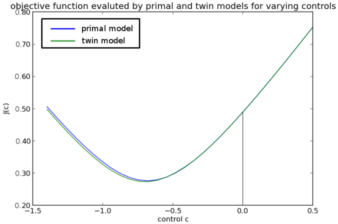
constrained by Buckley-Leverett flow, where c is a constant source term to be optimized. u^* is a given spatial profile.



Gray-box model solution



Twin model solution



J calculated by the two models

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- **Optimization framework. (objective 2)**
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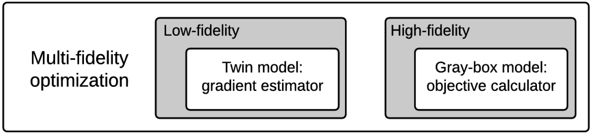
Review of multi-fidelity optimization (MFO)



- MFO methods include
  - pattern search MFO [Booker 99].
  - trust-region MFO [Wild 13, March 12, Robinson 06].
  - Bayesian MFO [Kennedy 01, March 11].
- Choose Bayesian MFO as our optimization framework:
  - uses all high-fidelity model evaluation to find the next design.
  - can fuse sampled data of different types: co-Kriging [Chung 02].
  - the next candidate design is optimal under a Bayesian metric.

Model objective and gradient Bayesianly

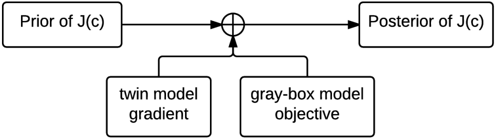
- Gaussian process modeling:
  - $J(c)$: the objective calculated by the gray-box model.
  - $\epsilon(c)$: the error in the objective's gradient calculated by the twin model.
- Relates gray-box model's objective with twin model's gradient:

$$\begin{cases} g(c) = \nabla J(c) + \epsilon(c) \\ \mathrm{cov}\left[\nabla J(c_1), \epsilon(c_2)\right] = 0 \\ \mathrm{cov}\left[J(c_1), \epsilon(c_2)\right] = 0 \end{cases} \qquad \text{for any } c, c_1, c_2\,,$$

where $g(c)$ is the objective's gradient calculated by the twin model.

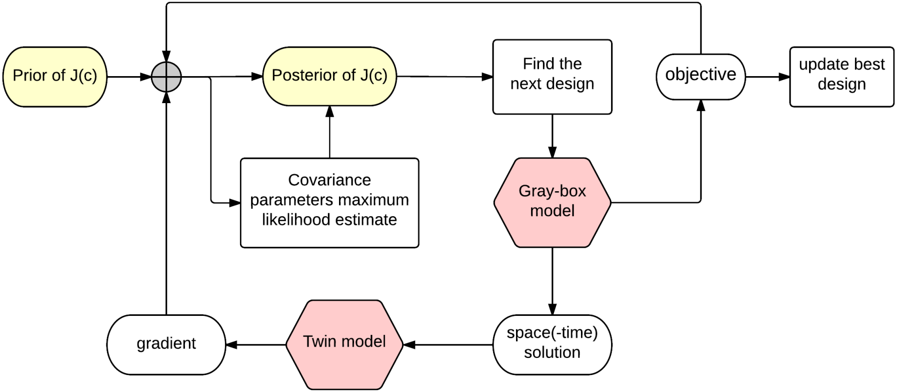
Perform Bayesian optimization

- Update $J(c)$ Bayesianly



- Find the next design to evaluate the gray-box model [Snoek 12]
  - Define "improvement": $\max\{J(c_{best}) - J(c), 0\}$.
  - Choose the next design as the maximizer of the expected improvement.

Optimization framework

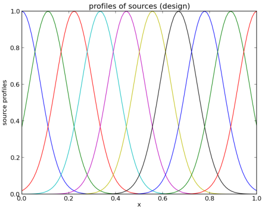


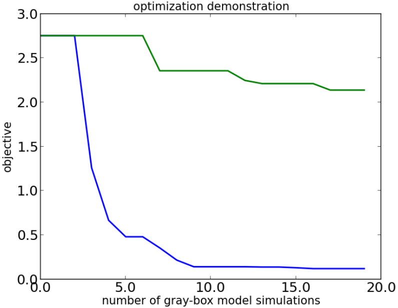
A demonstration of optimization

- Source parameterized by 10 design variables.
- Optimization problem:

$$\min_{c\in\mathbb{R}^{10}} \left\{ J(u) \equiv \int_{x=0}^{1} \left| u(x,t=1;c) - u^*(x) \right|^2 \mathrm{d}x \right\},$$

where $u^*(x) = u^*(x, t=1; c^*)$, u^* generated by gray-box model.





github.com/septfleur/twinmodel.git

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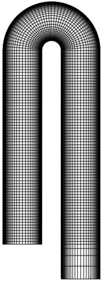
Optimize return bend geometry

- Optimize the geometry of an internal cooling hole in turbine airfoil to minimize the time averaged pressure loss. [Coletti 13]
- Model as a 2-D return bend problem.
- Design space can be high-dimension.

Internal cooling of turbine airfoil
Source: http://www.amaterastyo.biz/eng/technologies.html



Apply twin model optimization framework

- Flow is turbulent and incompressible, *Re* $\sim 40,000$, *Mach* ~ 0.05
- Candidate simulation models:
  - Time averaged quantities:

    RANS models: Reynolds stress models, eddy viscosity models (e.g. mixing length models, $k-\omega$ models), etc [Wilcox 98]
  - Space-time dependent quantities:

    LES, DNS, etc
- Apply twin model optimization framework:
  - Gray-box model: time averaged quantities of LES simulation.
  - Twin model: a RANS model with adaptive eddy viscosity modelling.

Candidate models for turbulent flow

Optimization by twin model

Infer PDEs for eddy viscosity

Future work for turbulent flow optimization

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Expected contributions

- Develop an efficient method to estimate gradients when the governing PDE is not available.
- Provide an optimization framework based on gray-box conservation law simulation in high-dimensional design problems.
- A demonstration of the twin model optimization framework in a high-dimensional turbulent flow optimization, showing superior objective function improvement given a fixed computational budget.

Proposed schedule

[Autor, 90]

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References VII

Discussion of optimization convergence

Exploit twin model more than its gradient?

Extension to constraint optimization