

An efficient optimization framework for gray-box conservation law simulation

Thesis proposal defense

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May 5, 2015



Outline

- ▶ Background.
- ▶ Thesis objective.
- ▶ Estimate gradient by twin model.
- ▶ Optimization framework.
- ▶ Application to turbulent flow optimization.
- ▶ Expected contribution.
- ▶ Proposed schedule.

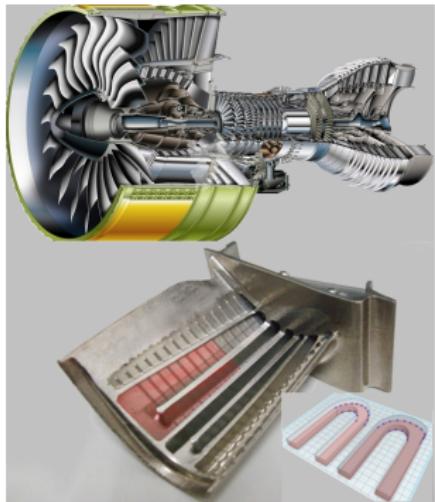
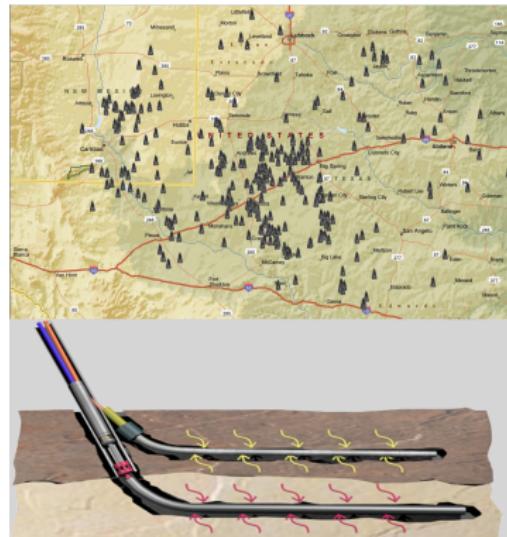


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- Interested in optimization constraint by conservation law simulation.
- Conservation law simulation can be expensive.
- The design space can be high-dimensional.
- Efficient sensitivity (adjoint) analysis may be unavailable.



Internal cooling of turbine airfoil

Source: <http://www.amaterastvo.biz/eng/technologies.html>



► Gray-box conservation law simulation:

- adjoint not available.
- governing PDE and its implementation not available.
- can output space(-time) solutions.

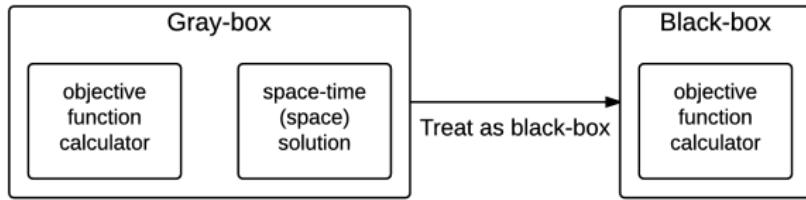
	PDE and implementation	space(-time) solution	Adjoint
Black-box	✗	✗	✗
Gray-box	✗	✓	✗
Open-box	✓		✓

► High-dimensional design space.

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



- If black-box, use **derivative-free optimization**,
pattern search methods [[Tarma03](#)], evolution based methods [[Eberhart 10, Davis 10](#)], etc
 - 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,



- 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 the design objective improvement by using the proposed framework, in a return bend design problem.



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Estimate the gradient:

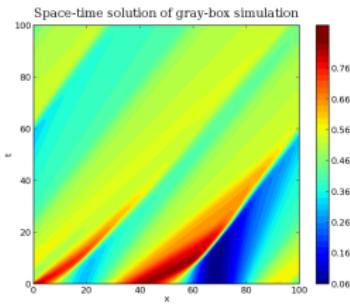
- infer the conservation law from the space(-time) solution.
- apply adjoint to estimate gradient.

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

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c(x)$$

$$u(t=0, x) = u_0(x)$$

$$u(t, x=0) = u(t, x=1)$$



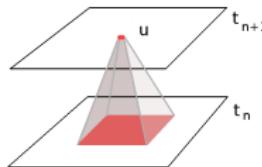
Propose to infer the flux or the source term that reproduce the space(-time) solution. The inferred conservation law is called twin model.



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

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

- 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

twin model

The inference can boil down to an optimization problem.

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = c(x)$$

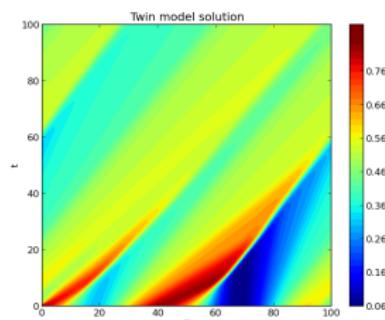
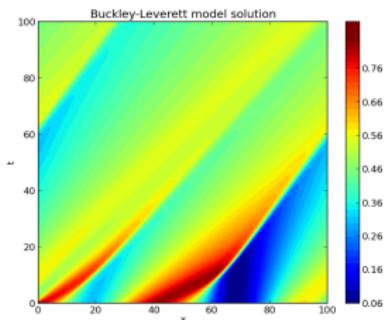
$$u(t=0, x) = u_0(x)$$

$$u(t, x=0) = u(t, x=1)$$

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

$$\tilde{u}(t=0, x) = u_0(x)$$

$$\tilde{u}(t, x=0) = \tilde{u}(t, x=1)$$



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

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



- ▶ 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.

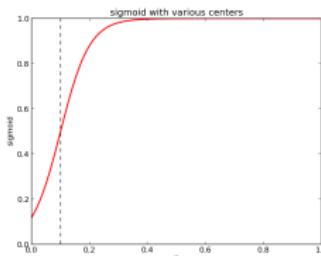
$$\min_{\tilde{F}} \left\{ L(\tilde{F}) + \lambda \sum_{i=1}^n |\xi_i| \right\}$$



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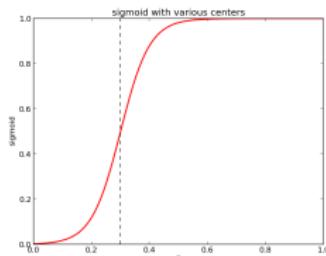
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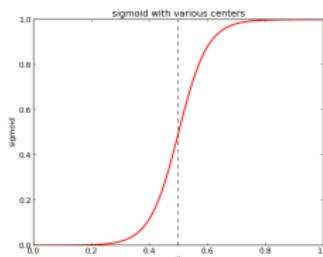
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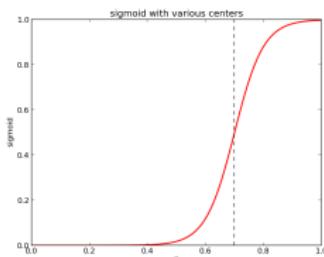
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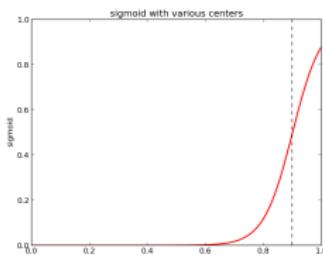
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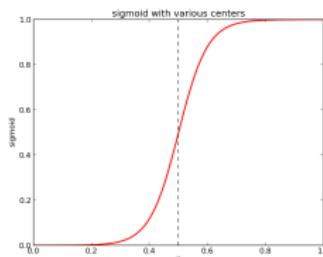
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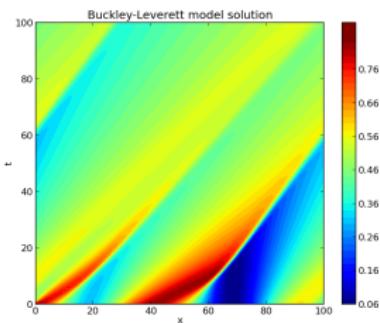
A demonstration of twin model

twin model

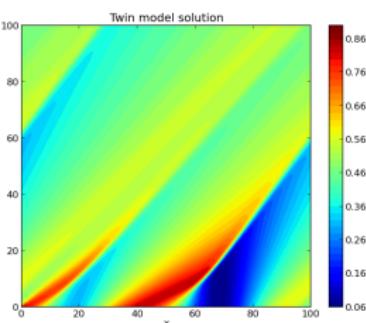
Consider an objective: [Kucuk 06]

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

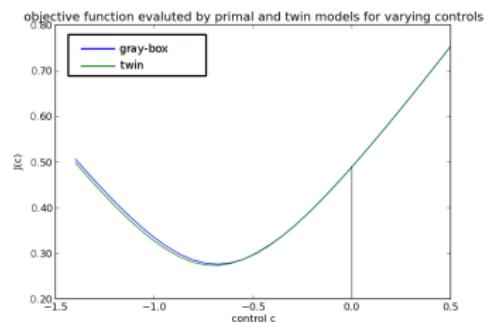
constrained by Buckley-Leverett flow, where c is a constant source term to be optimized. u^* is a given spatial profile.



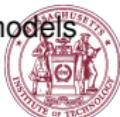
Gray-box model solution



Twin model solution



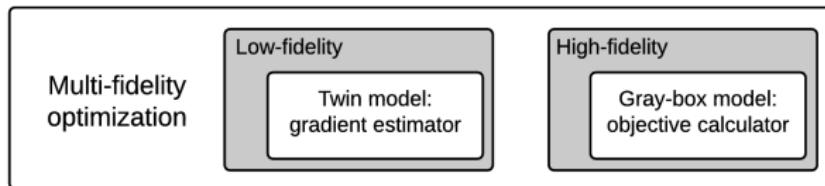
J calculated by the two models



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- 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.



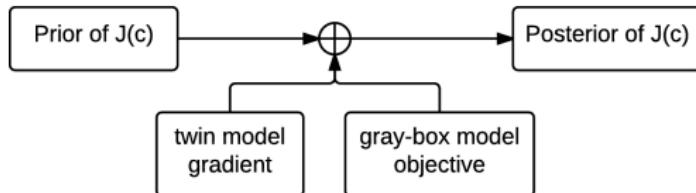
- Gaussian process modeling:
 - $J(c)$: the objective calculated by the gray-box model.
 - $\epsilon(c)$: the error in the objective's gradient calculated by the twin model.
- Relate gray-box model's objective with twin model's gradient:

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

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



- ▶ Update $J(c)$ Bayesianly

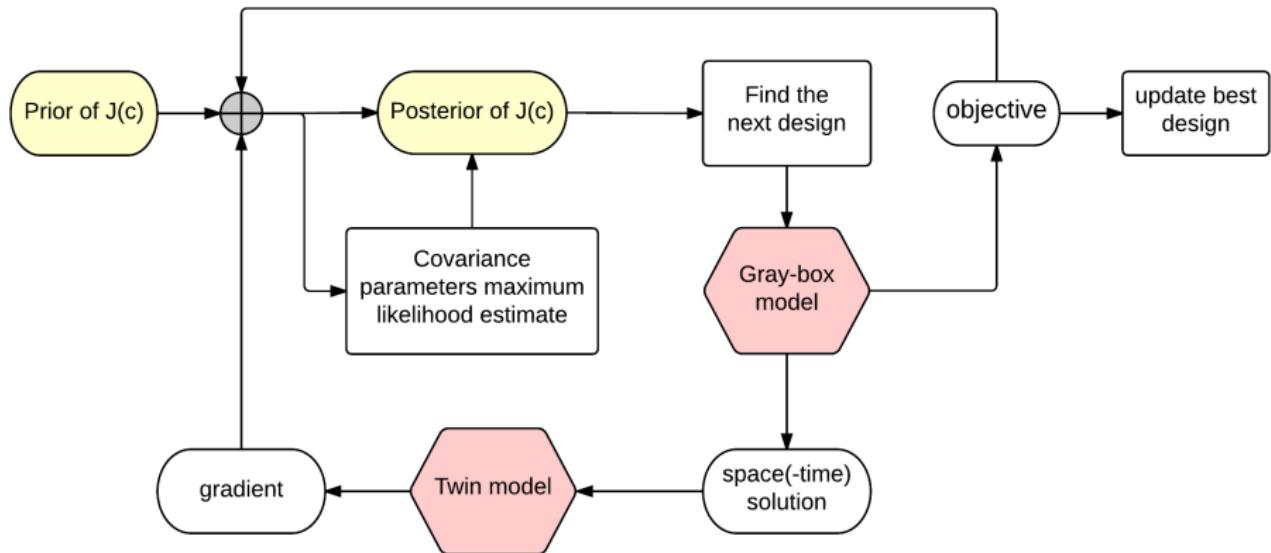


- ▶ Find the next design to evaluate the gray-box model [Snoek 12]
 - ▶ Define “improvement”: $\max \{J(c_{best}) - J(c), 0\}$.
 - ▶ Choose the next design as the maximizer of the expected improvement.



Optimization framework

optimization



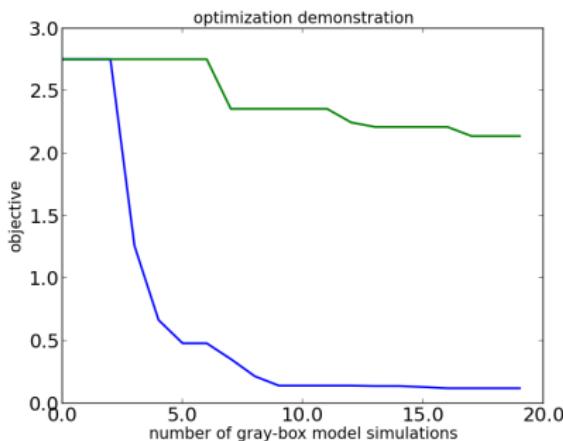
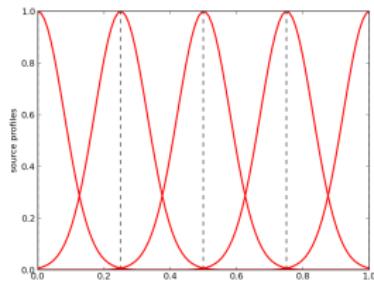
A demonstration of optimization

optimization

- ▶ Source parameterized by 5 design variables.
- ▶ Optimization problem:

$$\min_{c \in \mathbb{R}^5} \left\{ J(u) \equiv \int_{x=0}^1 |u(x, t = 1; c) - u^*(x)|^2 dx + \lambda \sum_{i=1}^5 c_i^2 \right\},$$

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

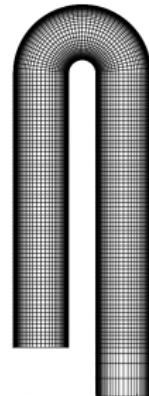
application

- 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>



- Flow is turbulent and incompressible, $Re \sim 40,000$, $Mach \sim 0.05$
- 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



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- Develop an efficient method to estimate gradients when the governing PDE is unavailable.
- Provide an optimization framework based on gray-box conservation law simulation for 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.



► Completed

- Course work.
- Formulation of twin model and its inference.
- Development of twin model optimization framework.
- Demonstration of optimization on a 1-D flow testcase.

► To be completed

- May 15': Setup an 2-D LES solver for the return bend testcase in OpenFoam.
- Jun 15': Setup a RANS solver with adaptive eddy viscosity in python.
- Jul-Oct 15': Optimize return bend geometry.
- Aug 15': Hold a committee meeting to report progress.
- Sep-Nov 15': Write thesis.
- Jan 16': Defense.



Thank you!



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References VII



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Discussion of optimization convergence 1

backup

Theorem

The design sequence is dense.

Assume

- ▶ $\mathcal{X} \in \mathbb{R}^n$, $\|\cdot\|$ be the L_2 norm defined on \mathcal{X} .
- ▶ \mathcal{H} and \mathcal{H}' be two reproducing kernel Hilbert spaces of functions on \mathcal{X} , with kernels $K(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ and $K'(\cdot, \cdot) : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ respectively.
- ▶ There exist $k : \mathbb{R}^+ \cup \{0\} \mapsto \mathbb{R}$ and $k' : \mathbb{R}^+ \cup \{0\} \mapsto \mathbb{R}$, such that K and K' satisfies $K(x, y) = k(\|x - y\|)$ and $K'(x, y) = k'(\|x - y\|)$ respectively, for $\forall x, y \in \mathcal{X}$.
- ▶ k and k' has the Fourier transforms \hat{k} and \hat{k}' respectively. They satisfy the asymptotic properties $\hat{k}(u) = \Theta(|u|^{-n-2\nu})$ and $\hat{k}'(u) = \Theta(|u|^{-n-2\nu'})$, as $|u| \rightarrow \infty$, with $\frac{1}{2} < \nu < \infty$ and $\nu' = \nu - 1$. (Θ is the asymptotic big Θ notation.)

Then all functions in \mathcal{H} are differentiable.

In addition, let

- ▶ $f \in \mathcal{H}$.
- ▶ $\epsilon = (\epsilon_1, \dots, \epsilon_n)^T$, $\epsilon_i \in \mathcal{H}'$, $i = 1, \dots, n$. ϵ_i is independent of ϵ_j for $i \neq j$.
- ▶ $g = \epsilon + \nabla f$.

Suppose an infinitely long sequence is generated by the following strategy:

$$\begin{aligned} x_{s+1} &= \arg \max_{x \in \mathcal{X}} \mathbb{E} \left[\max (f(x) - f(x_s^*), 0) \mid \mathcal{S} \right] \\ x_s^* &= \arg \max_{x \in \{x_1, \dots, x_s\}} f(x) \\ \mathcal{S} &= \left\{ \{x_1, \dots, x_s\}, \{f(x_1), \dots, f(x_s)\}, \{g(x_1), \dots, g(x_s)\} \right\} \end{aligned}$$

Then the sequence $\{x_1, x_2, \dots\}$ is dense in \mathcal{X} for $\forall x_1 \in \mathcal{X}$.

- Mostly interested in improving the objective given a limited computational budget, when the design is far from optimal.
- Gray-box simulation can be so expensive that only a small number of evaluations are feasible.
- When the design is close to the optimal, the optimization framework degenerates to DFO.
- A convergence proof helps complete the theory, but may offer little practical value in realistic problems.



- ▶ Proposed framework collocates (in the design space)
 - gray-box objective evaluation.
 - twin model training.
 - twin model gradient evaluation.
- ▶ May benefit from non-collocated optimization framework, for example
 - perform a sub-optimization (gradient-based) using twin model in a trust-region.
- ▶ However, twin model is **not** a “dispensable” asset in terms of evaluation cost.



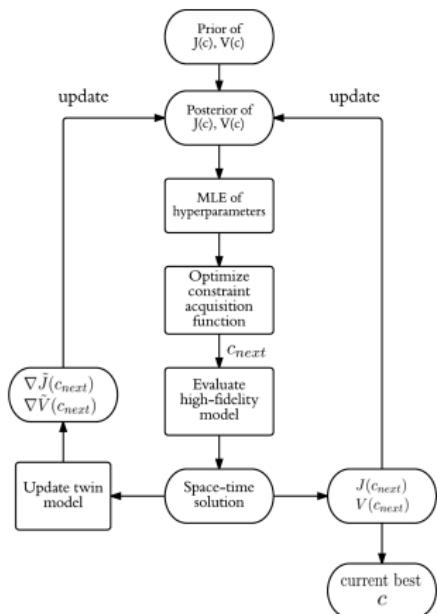
► Categorize constraints:

- constraint evaluation that requires PDE simulation.
- constraint evaluation that not requires PDE simulation.

► Constraint expected improvement:

$$\mathbb{E} \left[\max (J(c) - J(c_s^*), 0) \mid \mathcal{S} \right] \cdot \mathbb{P}[V(c) \leq 0 \mid \mathcal{S}],$$

► Constraint twin model optimization framework.



Basis selection without PDE solve

backup

For time dependent twin model,

$$Err_G = \frac{1}{T} \sum_{i=1}^N \sum_{k=1}^T (\tilde{u}_{ik} - u_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i|$$

$$Err_L = \frac{1}{T} \sum_{i=1}^N \sum_{k=1}^T (\tilde{u}'_{ik} - u_{ik})^2 \Delta t_k |\Delta \mathbf{x}_i|$$



Theorem

Global-local error

Consider the timestepwise mapping of the twin model

$$G : \mathbb{R}^n \mapsto \mathbb{R}^n, \tilde{u}^i \rightarrow G\tilde{u}^i = \tilde{u}^{i+1}, \quad i = 1, \dots, n.$$

If G is a Lipschitz continuous mapping with constant α

$$\|Gx - Gy\|_{L_2} \leq \alpha \|x - y\|_{L_2}$$

then

$$Err_G \leq (1 + \alpha + \dots + \alpha^{n-1}) Err_L.$$

If $\alpha < 1$, then

$$Err_G < \frac{1}{1 - \alpha} Err_L$$

► Aerospace computational engineering

- 2.25 advanced fluid dynamics
- 16.920 numerical methods for PDE
- 6.437 inference and information
- 16.322 statistical estimation and control
- 18.335 introduction to numerical methods
- 16.940 numerical methods for stochastic modeling
- 6.438 algorithms for inference

► Finance

- mas.665/15.375 development ventures
- 15.450 analytics of finance
- 15.s26 special seminar in management
- 15.401 finance theory I (P/D/F)

