Space mapping techniques for complex PDE systems

Oliver Lass

Fachbereich Mathematik und Statistik
Universität Konstanz

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Motivation

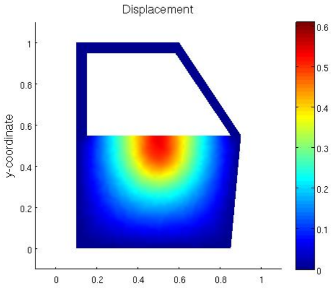
Model for Lithium Ion Battery:

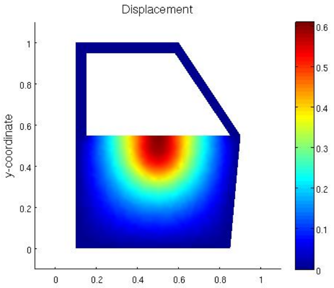
$$
\begin{aligned}
&-\nabla\cdot(\kappa(c)\nabla\Phi_e) - S_e(\Phi_s-\Phi_e,c) = 0\\
&-\nabla\cdot(\sigma\nabla\Phi_s) + S_e(\Phi_s-\Phi_e,c) + f = 0\\
&(\varepsilon_e c)_t - \nabla\cdot\left(D\nabla c\right) = S_c(\Phi_s-\Phi_e,c)\\
&+\ \text{Neumann boundary conditions}\\
&\int_\Omega \Phi_e\,\mathrm{d}\mathbf{x} = 0 \quad \text{(uniqueness)}
\end{aligned}
$$

Parameter estimation:

- Reduce optimization effort with little loss in accuracy
- Combine with current simulation tools

Example





Solution to

$$\text{(left plot)} \quad -\operatorname{div}\left(2(1+n)\lambda(\mathbf{x})\,|\nabla u(\mathbf{x})|_2^{2n}\,\nabla u(\mathbf{x})\right) = g(\mathbf{x})$$
$$\text{(right plot)} \quad -\operatorname{div}\left(2(1+n)\lambda(\mathbf{x})\nabla u(\mathbf{x})\right) = g(\mathbf{x})$$

for a constant parameter $\lambda = 0.5$

Problem

- Control problem for partial differential equation

$$\text{minimize } J(u,y) \text{ over } (u,y) \in W \times U$$
$$\text{subject to } A(y,u)y + C(y,u) = 0 \text{ in } \Omega$$

- Assuming unique solution of state equation
- Reduced form given as

$$\text{minimize } J_{red}(u) = J(y(u),u) \text{ over } u \in U$$

Models

Fine model:

$$\text{minimize } g \text{ over } x \in X$$

- Accurate but expensive model g
- Gradients of g are assumed not to be available

Coarse model:

$$\text{minimize } \hat{g} \text{ over } \hat{x} \in \hat{X}$$

- Cheap model $\hat{g}$
- Gradients of $\hat{g}$ are assumed to be available

Surrogate Optimization - Space Mapping

Idea:

- Replace fine model $g(x)$ with the cheaper coarse model $\hat{g}(\hat{x})$
- Link the two models by the Space Mapping $\hat{x} = P(x)$
- It follows

$$g(x) \approx (\hat{g} \circ P)(x) \text{ for all } x \in \mathcal{A} \subseteq X$$

- In the Surrogate Optimization use $\hat{g} \circ P(x)$ instead of $g(x)$, i.e.,

$$\text{minimize } g_P(x) = \hat{g}(P(x)) \text{ over } x \in X$$

Definition (first approach):

$$P(x) = \operatorname{argmin} \left\{ \frac{1}{2}[\hat{g}(\hat{x}) - g(x)]^2 \,|\, \hat{x} \in \hat{X} \right\}$$

if $S(x) = \{\hat{x} \in \hat{X} \,|\, \hat{g}(\hat{x}) = g(x)\}$ is empty

$$P(x) = \operatorname{argmin} \left\{ \frac{\alpha}{2} \|\hat{x} - x\|_2^2 \text{ s.t. } \hat{g}(\hat{x}) = g(x) \,|\, \hat{x} \in \hat{X} \right\}$$

if $S(x)$ is not empty

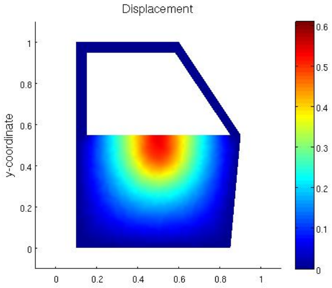
Space Mapping

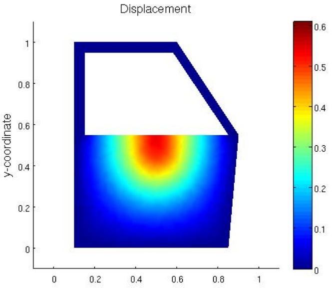
Definition (second approach):

$$P(x) = \operatorname{argmin}\left\{\frac{\alpha}{2}\|\hat{x} - x\|_M^2 + \frac{1}{2}[\hat{g}(\hat{x}) - g(x)]^2 \,|\, \hat{x} \in \hat{X}\right\}$$

with α a smoothing parameter

Space Mapping (Example)





Solution to

$$\text{(left plot)} \quad -\operatorname{div}\left(2(1+n)\lambda(\mathbf{x})\,|\nabla u(\mathbf{x})|_2^{2n}\,\nabla u(\mathbf{x})\right) = g(\mathbf{x})$$

$$\text{(right plot)} \quad -\operatorname{div}\left(2(1+n)\mu(\mathbf{x})\nabla u(\mathbf{x})\right) = g(\mathbf{x})$$

for a constant parameter $\lambda = 0.5$ and $\mu(\mathbf{x}) = P(\lambda(\mathbf{x}))$

Surrogate Optimization

$$\text{minimize } g_P(x) = \hat{g}(P(x)) \text{ over } x \in X$$

with

$$P(x) = \operatorname{argmin} \left\{ \frac{\alpha}{2} \|\hat{x} - x\|_M^2 + \frac{1}{2} [\hat{g}(\hat{x}) - g(x)]^2 \mid \hat{x} \in \hat{X} \right\}$$

Gradient of g_P given as

$$\nabla g_P(x) = P'(x)^\top \nabla \hat{g}(\hat{x})$$

- Requires gradient of the fine model
- Approximate gradient by Broyden's formula

Broyden's Update

Local linearization of P

$$P(x + \Delta x) \approx P(x) + P'(x)\Delta x$$

Secant's equation

$$B\Delta x_k = \Delta P_k$$

with $\Delta P_k = P(x_k + \Delta x_k) - P(x_k)$.

Good Broyden's update:

$$B_{k+1} = B_k + \frac{\Delta P_k - B_k \Delta x_k}{\|\Delta x_k\|_2^2} \Delta x_k^\top$$

Broyden's Update

Local linearization of $\hat{g}$

$$\hat{g}(P(x_k + \Delta x)) \approx \hat{g}(P(x_k)) + (P'(x_k)^\top \nabla \hat{g}(P(x_k)))^\top \Delta x$$

Secant's condition

$$\nabla \hat{g}_k^\top B \Delta x_k = \Delta \hat{g}_k$$

with $\Delta \hat{g}_k = \hat{g}(P(x_k + \Delta x_k)) - \hat{g}(P(x_k))$.

Modified Broyden's update:

$$\widetilde{\Delta P_k} = \Delta P_k + \sigma_k \frac{\Delta \hat{g}_k - \nabla \hat{g}_k^\top \Delta P_k}{\|\nabla \hat{g}_k\|_2^2} \nabla \hat{g}_k$$

$$B_{k+1} = B_k + \frac{\widetilde{\Delta P_k} - B_k \Delta x_k}{\|\Delta x_k\|_2^2} \Delta x_k^\top$$

References

- M.H. Bakr, J.W. Bandler, K. Masden, and J. Søndergaard. *An introduction to the space mapping technique*. *Optim Eng*, 2(4):369-384, 2001.
- L.N. Vicente. *Space Mapping: Models, Sensitivities, and Trust-Regions Methods*. *Optimization and Engineering*, 4(3):159-175, 2003.
- M. Hintermüller and L.N. Vicente. *Space mapping for optimal control of partial differential equations*. *SIAM J. on Optimization*, 15(4):1002-1025, 2005.
- O. Lass, C. Posch, G. Scharrer, and S. Volkwein. *Spase mapping techniques for a structural optimization problem governed by the p-Laplace equation*. Submitted, 2009.

Thank you
for your Attention!