CAMI Retreat 2012

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Applications of Optimal Control of Systems Governed by Partial Differential Equations

Outline

- Early Motivations
  - State Estimation
  - Program Validation
  - Optimal Operation
- Program Validation
- State Estimation for a Model problem
- Information Content of Measurements in Nonstandard Flow BVPs

Experience

- state estimation for gas pipelines
- optimal operation of gas pipelines
- advection reaction diffusion equations
- contaminant tracking in air and water
  - Results of Volkan Akcelik (CMU) George Biros (U Penn) Andrei Draganescu (UMBC) Omar Ghattas (U Texas), and Judy Hill (Sandia)

Program Validation

- Gaining confidence in a discrete model by comparison with experiment
- Experimentalist/Modeler relationship
- When do an experiment and a simulation to agree?
  - choice of metric is crucial
  - stable aspects of unstable problems

Working Definition
Experiment/Model Agreement

Given a metric and a tolerance, a model and an experiment agree if there are inputs from a plausible set that can drive the model so that it is within tolerance of the experiment.

- Input errors include modelling errors
- Optimization of a function of millions or billions of variables, where each function evaluation is a hero calculation is daunting

State Estimation for Model Problem

$$
\begin{aligned}
\partial_t u + A(t)u &= 0 \text{ on } \Omega \times (0,\infty) \\
u &= 0 \text{ on } \partial\Omega \times (0,\infty) \\
u &= w \text{ on } \Omega \text{ at } t = 0
\end{aligned}
$$

$$A(t)u = -\sum_i \partial_i \left(\sum_j a_{ij}(x,t)\partial_j u + b_i(x,t)u \right) + c(x,t)u$$

Solution operator

$$S(t)w = u(\cdot, t)$$

Inverse Problem

$$\min_{w \in L^2} \mathcal{J}_\epsilon(w)$$

$$\mathcal{J}_\epsilon(w) = \frac{1}{2\epsilon}\|S(T)w - f\|^2 + \frac{1}{2}\|w\|^2$$

Numerical Approximation

Finite Element Space

V_{h_0} piecewise linears in H_0^1 based on triangles

$V_{h/2}$ comes form V_h by Goursat refinement

for $h = h_0/2^j$

Discrete Galerkin Equations

$$< d_t U^m, \phi > + a(t_m, U^m, \phi) = 0 \text{ for } \phi \in V_h$$

$$d_t U^m = (U^m - U^{m-1})/k$$

$$t_m = mk \text{ where } k = k(h) = k_0 h^2/T$$

$$U^0 = \pi_h w, \text{ where } \pi_h = L^2 \text{ projection}$$

Discrete Solution Operator

$$S^h(t_m)w = U^m$$

Discrete Optimization Problem

$$\min_{W \in V_h} \mathcal{J}_\epsilon^y(W)$$

$$\mathcal{J}_\epsilon^h(w) = \frac{1}{2\epsilon}\|S^h(T)W - f\|^2 + \frac{1}{2}\|W\|^2$$

Aside: Gradient Computation

This is simple mathematics from the 19th century, but it is instructive to examine it in this context.

- c controls – possible size $N_c = 1e9$
- u solution – possible size $N_u = 1e13$
- $G(c,u) = 0$ is discrete PDE – size N_u
- $J(c,u)$ is "cost functional" to minimize
- $\mathcal{J}(c) = J(c,u)$ where $G(c,u) = 0$

$$0 = G_c \delta c + G_u \delta u$$

$$\delta u = -G_u^{-1} G_c \delta c$$

$$\delta J = \left(J_c - J_u G_u^{-1} G_c \right) \delta c$$

$$\nabla \mathcal{J} = J_c - J_u G_u^{-1} G_c$$

$$\nabla \mathcal{J} = J_c - (G_c^T G_u^{-T} J_u^T)^T$$

$G_c^T G_u^{-T} J_u^T$ is $(N_c \times N_u)(N_u \times N_u)(N_u \times 1)$

What & Why

We will use multigrid to attack this problem

Why would one use multigrid on a compact perturbation of the identity?

The goal is to solve the problem in one iteration

Two Level Scheme

$$(H_\epsilon^h)^{-1} \sim M_\epsilon^h = (H_\epsilon^{2h})^{-1}\pi_{2h} + (I - \pi_{2h})$$

$$\left| \frac{< M_\epsilon^h W, W >}{< H_\epsilon^h W, W >} - 1 \right| \leq \frac{Ch^2}{\epsilon}$$

Punchline: For the multilevel version the total work is about four times the forward solution.

Computational work of Ghattas et al.

These results are for a variation of the model problem in which one uses “weather station “-like data instead of end-time data.

Non Standard BC's for Flow Problems

In flow problems with inlets and outlets we usually study boundary value problems with specified flows on the boundary. These are never known. With Optimal Control one can compute (regularized) solutions that match other conditions, such as measured pressures and total flow.

How stable are such problems?

In some ways these are like analytic continuation from discrete data – Stability will depend on global assumptions.