INTERPOLATING PARAMETERIZED SIMULATION RESULTS


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Motivation

solution, space, time, input parameters

$$u(x,t,s)$$

• Given input parameters, a physical simulation approximates a space/time dependent solution.
• Each solution is computationally expensive, so exhaustive parameter studies (e.g., UQ/SA/optimization) are infeasible.
• Cheaper **reduced order models** enable *guesstimates* for parameter inquiries.

Approximation Model

fixed space/time discretization; truncation; amplitudes

$$\mathbf{x}(s) \approx \sum_{i=1}^{r} \mathbf{u}_i\,\sigma_i\,v_i(s)$$

space-time basis vectors; **unknown** parameter basis functions

Tuning the Approximation

experimental design

$$\begin{bmatrix} \mathbf{x}(s_1) & \cdots & \mathbf{x}(s_n) \end{bmatrix} = \mathbf{X}$$
$$= \mathbf{U}\Sigma\mathbf{V}^T$$

SVD

• The left singular vectors are the space-time basis.
• The singular values give the amplitudes.
• The truncation is determined by examining the decay of the singular values.
• Treat each right singular vector as **samples** from the unknown basis functions.

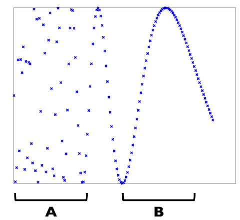
$$\mathbf{V}_{ij} = v_i(s_j)$$

Interpolating the Parameter Basis

$$\{v_i(s_j)\} \longrightarrow v_i(s)$$

• Construct parameter basis functions by interpolating the samples.
• Can use any appropriate interpolation method (e.g., polynomials, radial basis functions, Gaussian process models, piecewise linear, splines, …)

Which section would you rather try to interpolate, ***A*** *or* ***B****?*



Ordered by Increasing Oscillations

• From the SVD, it is natural to expect that the parameter bases will become more oscillatory as the index increases.
• Therefore, we expect the gradient between sample points to increase as the index increases.

"PREDICTABLE"	"UNPREDICTABLE"
$v_1(s),\dots,v_t(s)$	$v_{t+1}(s),\dots,v_r(s)$

For $t = t(s)$ and $\eta \sim N(0,1)$

$$\mathbf{x}(s) \approx \underbrace{\boxed{\sum_{i=1}^{t-1} \mathbf{u}_i\,\sigma_i\,v_i(s)}}_{\text{“predictable”}} + \underbrace{\boxed{\sum_{i=t}^{r} \mathbf{u}_i\,\sigma_i\,\eta_{i-t}}}_{\text{“unpredictable”}}$$

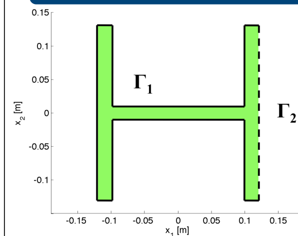
Space-time prediction variance:

$$\mathrm{var}[\mathbf{x}](s) = \mathrm{diag}\left(\sum_{i=t}^{r} \mathbf{u}_i\,\sigma_i^2\,\mathbf{u}_i^T\right)$$

The truncation $t = t(s)$ is the largest τ such that

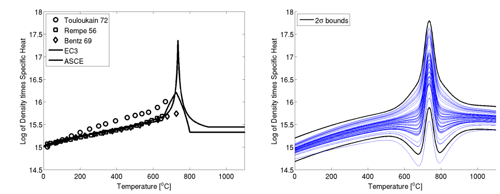
$$\frac{1}{\sigma_1}\sum_{i=1}^{\tau} \sigma_i \left\| \frac{\partial v_i}{\partial s} \right\| < \text{“threshold”}$$

Heat Conduction Example

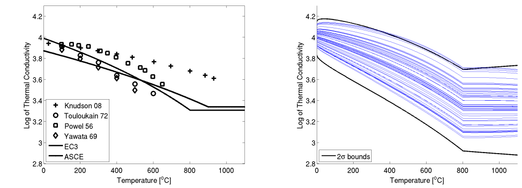


$$\rho c_p \frac{\partial T}{\partial t} = -\nabla\cdot(k\nabla T)$$
$$c_p = c_p(T), \quad k = k(T)$$

Material properties (Kodur, et al. 2010):

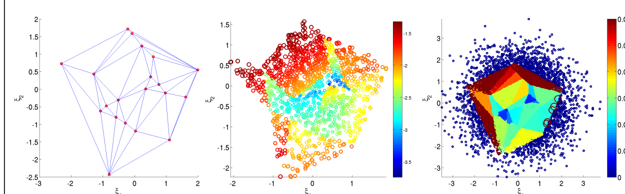


$$\log(\rho c_p(T)) = X(T) + \sigma_X(T)\,G(T,\xi_1)$$



$$\log(k(T)) = Y(T) + \sigma_Y(T)\,G(T,\xi_2)$$

Cross-validation study (piecewise linear interpolation):



LHS Design — Log10 Error — Predictability Measure

• Predictability measure can be used as an importance sampling distribution for refining the ROM.
• To examine a comparison of ROM and the full order model, along with error measures, visit:

www.sandia.gov/~pconsta/samsi_poster.html

National Nuclear Security Administration

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