Construction of Gaussian Surrogate Process Using Numerical and Modeling Error Uncertainty

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Complex System Modeling and UQ

- Complex model UQ based on outputs from ensemble of evaluations (costly simulations) used to fit appropriate surrogate – GaSP, Polynomial Chaos ...
- Effect of numerical error in model evaluation on surrogate construction is unclear but examples show **significant and unpredictable** dependence.
- Numerical error is parameter and output feature dependent!

Proposed Approach

Use *a posteriori* error estimates

The dual weighted *a posteriori* numerical approximation error estimate is used to inform surrogate construction.

Complex System Modeling and UQ

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Numerical Error Estimation

Let:

- $R(U, \alpha) = 0$ is a system of governing equations,
- U is the solution vector, α is the vector of design parameters.

Dual weighted *a posteriori* numerical approximation error estimate needs[1],[2].

- Computation of an approximate residual.

$$R(U, \alpha) - R(U^h, \alpha) = r(U^h, \alpha) \approx r(U^h_H, \alpha)$$

- Computation of an appropriate adjoint.

Complicated for non-linear hyperbolic time dependent systems.

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[1] Becker et al., An optimal control approach to a posteriori error estimation in finite element methods, Acta Numerica, Jan 2003

[2] Nemec et al., djoint-based adaptive mesh refinement for complex geometries, AIAA Paper, 2008

Discrete Adjoint

- The objective is to minimize error in computing functional $\mathrm{J}(U, \alpha) \quad$ subject to $\quad R(U, \alpha) = 0$
- We can only compute $J(U^h, \alpha)$ from a solution of $R(U^h, \alpha)$
- $r(U^h, \alpha) \rightarrow J(U, \alpha) - J(U^h, \alpha)$
- Adjoint ψ relates $r(U^h, \alpha)$ to $\epsilon(U, U^h, \alpha) \equiv J(U, \alpha) - J(U^h, \alpha)$

Discrete Adjoint Cont.

With writing the variation of the functional and governing equation w.r.t design parameters, we will have:

$$\frac{dJ}{d\alpha} = \frac{\partial J}{\partial U}\frac{dU}{d\alpha} + \frac{\partial J}{\partial \alpha}$$

and:

Discrete Adjoint Cont.

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Now,if we replace $\frac{dU}{d\alpha}$ from the second equation into the first equation, we have:

$$\frac{dJ}{d\alpha} = -\frac{\partial J}{\partial U}(\frac{\partial R}{\partial U})^{-1}\frac{\partial R}{\partial \alpha} + \frac{\partial J}{\partial \alpha}$$

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Sensitivity Computation

Assume that n is the size of vector U, and m is the size of vector α:

$$dJ_{scalar} = \underbrace{-\left[\frac{\partial J}{\partial U}\right]_{1\times n}\left[\frac{\partial R}{\partial U}^{-1}\right]_{n\times n}\left[\frac{\partial R}{\partial \alpha}\right]_{n\times m} d\alpha_{m\times 1}}_{\text{scalar}} + \underbrace{\left[\frac{\partial J}{\partial \alpha}\right]_{1\times m} d\alpha_{m\times 1}}_{\text{scalar}}$$

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Above sensitivity can be computed in two ways:

1. Forward mode: first computes $(\frac{\partial R}{\partial U})^{-1}\frac{\partial R}{\partial \alpha}$

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Advantage of Adjoint:

If the number of design parameters are more than the objective functionals, then the computational cost of the adjoint is much lower than the forward method.

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Computing Adjoint

To solve adjoint equation we need Transpose of Jacobian Matrix:

$$\boxed{\left(\frac{\partial R}{\partial U}\right)^T v = \frac{\partial J}{\partial U}^T}$$

TITAN2D uses Godunov finite volume with Euler explicit time scheme, so the descritized form of equations are:

$$U_i^{n+1} = U_i^n - \frac{\triangle t}{\triangle x}\{F^n_{i+\frac{1}{2}} - F^n_{i-\frac{1}{2}}\} - \frac{\triangle t}{\triangle y}\{G^n_{i+\frac{1}{2}} - G^n_{i-\frac{1}{2}}\}$$

$$\left(\frac{\partial R}{\partial U}\right)^T_{m\times m} = K_{ij}$$

where m is the number of time steps, and each K_{ij} is a

Computing Adjoint Cont.

For Euler explicit:

$$K_{i,i} = I \quad \text{and} \quad K_{i,i+1} = \left(\frac{\partial R_p^{i+1}}{\partial U_q^i}\right)^T,$$

- p and q are degrees of freedom
- rest of the components are zero
- depend on the stencil is used. K matrices are also block bounded

$$\left(\frac{\partial R}{\partial U}\right)^T_{m\times m} = \begin{pmatrix} I & K_{1,2} & & & \\ & I & K_{2,3} & \mathbf{0} & \\ & & \ddots & \ddots & \\ & \mathbf{0} & & I & K_{m-1,m} \\ & & & & I \end{pmatrix}$$

Computing Adjoint Cont.

Important conclusion:

To compute adjoint for an explicit system, there is no need to solve a system of equation, and adjoint solution can be found marching backward in time.

$$v_1 + K_{1,2} v_2 = \left(\frac{\partial J}{\partial U}\right)_1^T$$

$$\vdots$$

$$v_{m-1} + K_{m-1,m} v_m = \left(\frac{\partial J}{\partial U}\right)_{m-1}^T$$

$$v_m = \left(\frac{\partial J}{\partial U}\right)_m^T$$

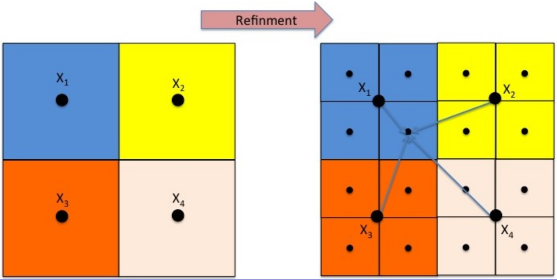
Residual Computation

Recall:

$$R(U,\alpha) - R(U^h,\alpha) = r(U^h,\alpha) \approx r(U_H^h,\alpha)$$

- To compute residual $r(U^h,\alpha)$, we need $R(U^h,\alpha)$ which is expensive.
- But we can find a good approximation for $R(U^h,\alpha)$ from $R(U_H,\alpha)$ which is represented here by $R(U_H^h,\alpha)$.

We approximated $R(U^h,\alpha)$ with bilinear interpolation.



Error Estimation

Let us estimate the error in the objective functional $J(U)$, given the solution on a coarse mesh $J(U_H)$ and our approximate solution $J(U^h, \alpha)$
With Taylor expansion we can write: [3]

$$J(U^h) \approx J(U_H^h) \;-\; \underbrace{(\psi_H^h)^T r(U_H^h)}_{\text{Adjoint correction term}} \;-\; \underbrace{(\psi_h - \psi_H^h)^T r(U_H^h)}_{\text{Remaining term}},$$

where $J(U^h)$ is the functional value on a finer mesh, and all $\Box_H^h$ is the projection of $\Box$ from the coarse mesh to the fine mesh.

[3] Nemec et al., djoint-based adaptive mesh refinement for complex geometries, AIAA Paper, 2008

Error Estimation Cont.

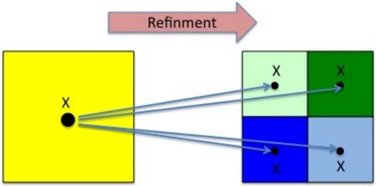
So to compute the error ε

- We have to first find .
- Like $R(U^h, \alpha)$ we can approximate ψ^h with higher order construction.

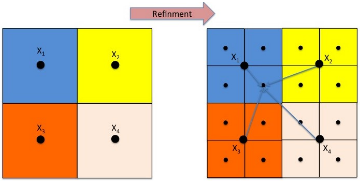
$$J(U^h) \approx J(U_L) - (\psi_L)^T r(U_L) - (\psi_L - \psi_C)^T r(U_L),$$

where $\square_L$, $\square_C$ represent linear and constant reconstruction respectively.

Constant reconstruction



Linear reconstruction



Case 1: Burger's Equation

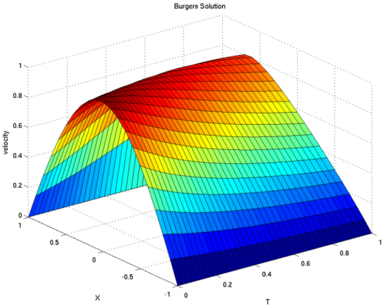
$$
\begin{aligned}
R(x,t) &= \frac{\partial u}{\partial t} + \frac{\alpha}{2}\frac{\partial u^2}{\partial x} = 0, \qquad x \in (-1,1), \quad t \in (0,1),\\
u(x,0) &= \beta \ cos(\frac{\pi}{2}x),\\
u(1,t) &= 0,\\
J &= 0.5 \int_T \int_x u^2 \ dx \ dt,
\end{aligned}
$$

where α and β are uncertain parameters, and are selected from $\mathscr{N}(1, 0.1)$.

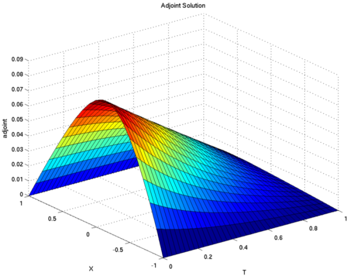
Case 1: Burger's Equation

Results are for a Monte Carlo simulation with 10,000 samples:

Velocity

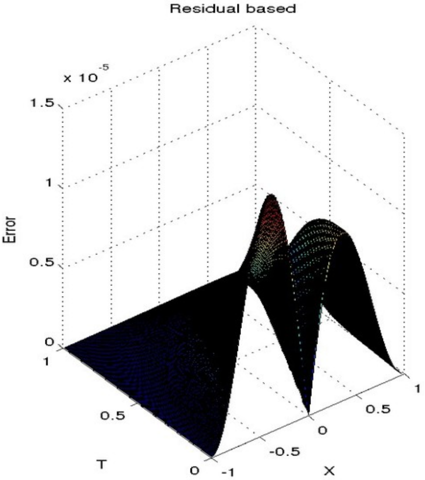


Adjoint



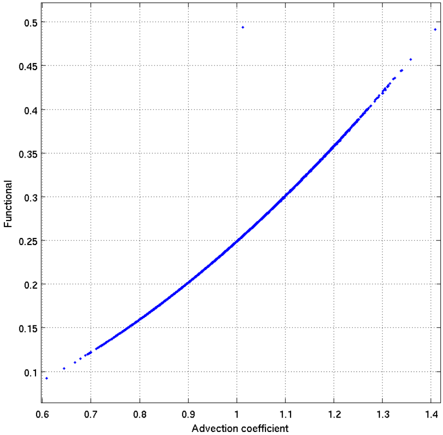
Case 1: Burger's Equation

Computed error



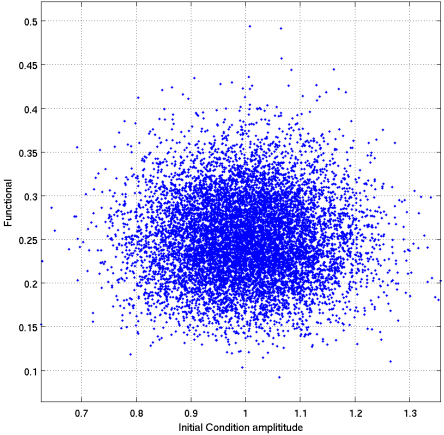
Case 1: Burger's Equation

Functional of interest as a function of advection coefficient



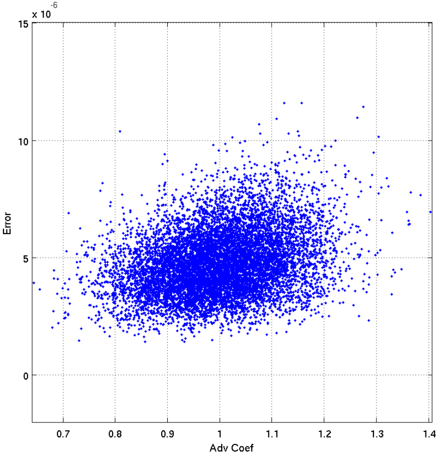
Case 1: Burger's Equation

Functional of interest as a function of initial condition uncertain coefficient



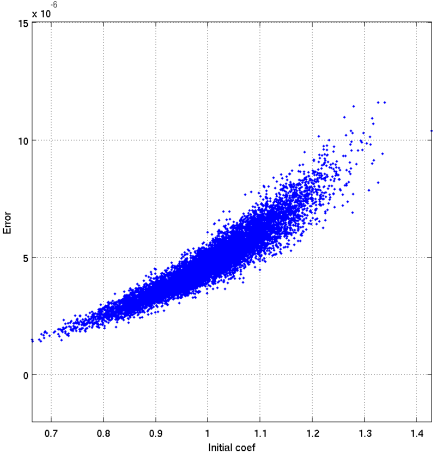
Case 1: Burger's Equation

Error at final stage as a function of advection coefficient



Case 1: Burger's Equation

Error at final stage as a function of initial condition uncertain coefficient



Case 2: Governing Equations

$$U_t + F(U)_x + G(U)_y = S(U)$$

Where:

$$U = (h, hv_x, hv_y)^T$$
$$F = (hv_x, hv_x^2 + 0.5k_{ap}g_z h^2, hv_x hv_y)^T$$
$$G = (hv_y, hv_x v_y, hv_y^2 + 0.5k_{ap}g_z h^2)^T$$

Case 2: Governing Equations Cont.

$$
\begin{aligned}
S &= (0, S_x, S_y)^T \\
S_x &= g_x h - \frac{V_x}{\sqrt{V_x^2 + V_y^2}} \left(g_z h + \frac{h V_x^2}{r_x} \right) \tan(\phi_{bed}) \\
&\quad - h k_{ap} \operatorname{sgn} \left(\frac{\partial V_x}{\partial y} \right) \frac{\partial (g_z h)}{\partial y} \sin(\phi_{int}) \\
S_y &= g_y h - \frac{V_y}{\sqrt{V_x^2 + V_y^2}} \left(g_z h + \frac{h V_y^2}{r_y} \right) \tan(\phi_{bed}) \\
&\quad - h k_{ap} \operatorname{sgn} \left(\frac{\partial V_y}{\partial x} \right) \frac{\partial (g_z h)}{\partial x} \sin(\phi_{int})
\end{aligned}
$$

Case 2: Result

For this case, we considered an inclined plane with the uncertain parameters of:

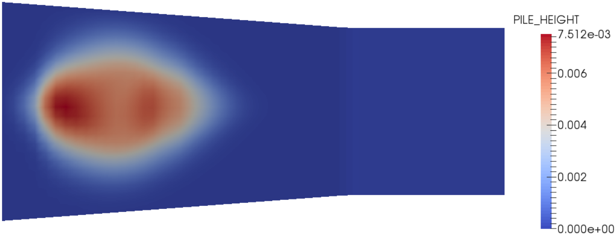
- Initial Volume $\pm 30\%$ *of* $2.64 \times 10^{-4} m^3$
- Bed Friction angle $(23^\circ, 40^\circ)$

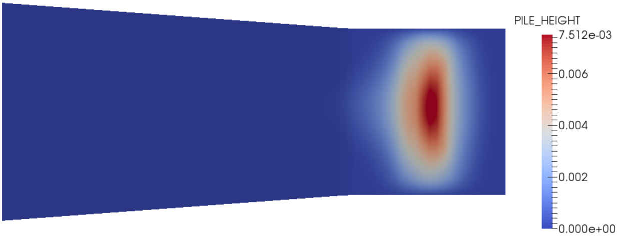
we simulated this process with 256 Latin Hyper cube samples. The functional that we are interested in this case is:

$$J = 0.5 \int_T \int_\Omega h^2 dX dt$$

Case 2: Result

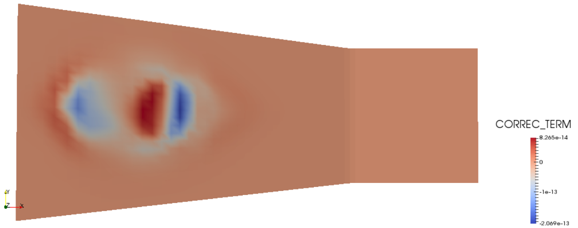
Pile height result for $t = 0.3$ sec and $t = 1$ sec

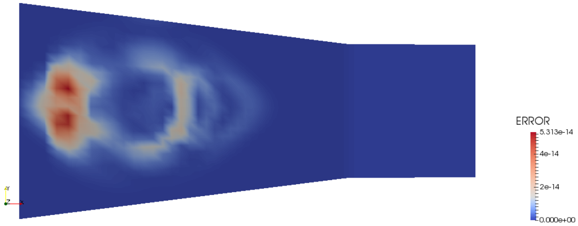




Case 2: Result

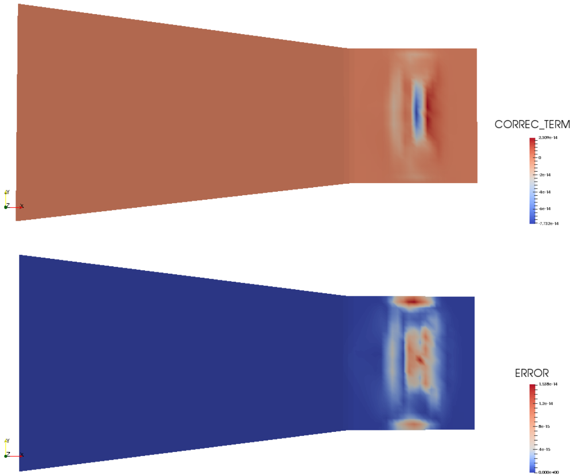
Correction term and Error for incline at $t = 0.3$ sec





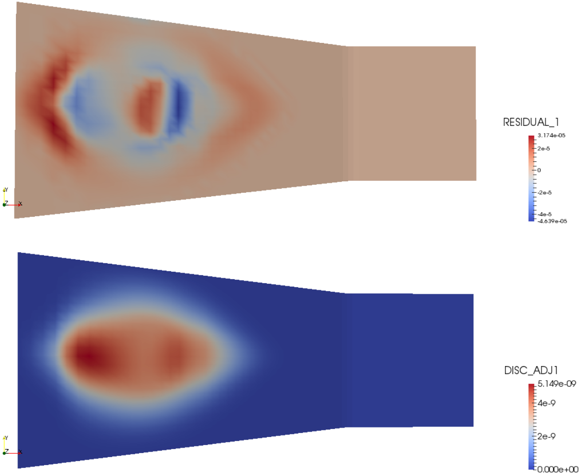
Case 2: Result

Correction term and Error for incline at $t = 1$ sec



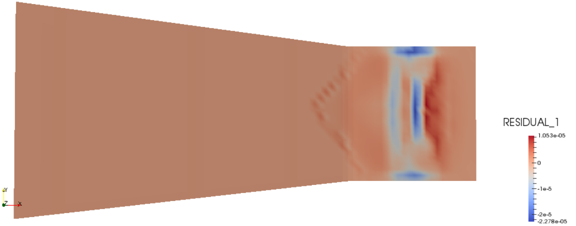
Case 2: Result

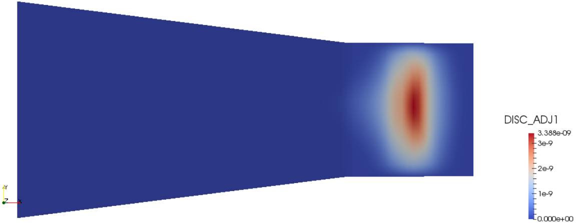
Residual and Adjoint result at $t = 0.3$ sec



Case 2: Result

Residual and Adjoint result at $t = 1$ sec





Summary

Simple approximations of residual and adjoints lead to a usable numerical error estimate that informs the surrogate construction.