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Sensitivity Analysis Techniques Applied to a Model Shock Problem

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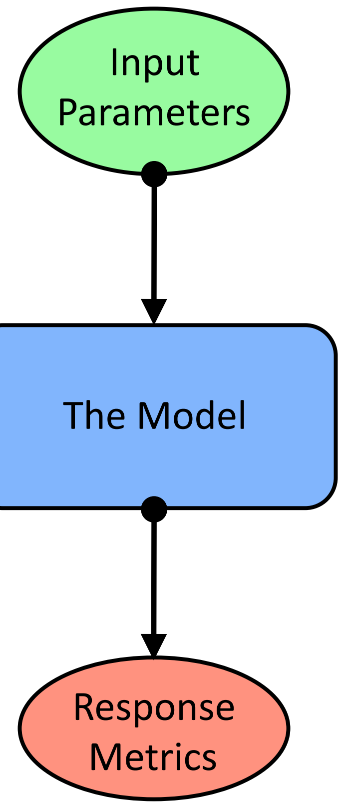
The Sensitivity Analysis Story

- Our problem of interest has 4 inputs and 8 outputs
- Outputs (responses) have different properties:
  - monotonic vs. non-monotonic
  - smooth vs. discontinuous
  - noisy vs. clean
- We examine different SA techniques:

LHS, LP-Tau	} sampling
PCE	} stochastic expansion
SDP, ACOSSO, DACE	} surrogates

- We compute sensitivity indices and compare them to exact values; in particular, we examine performance with respect to sampling resolution



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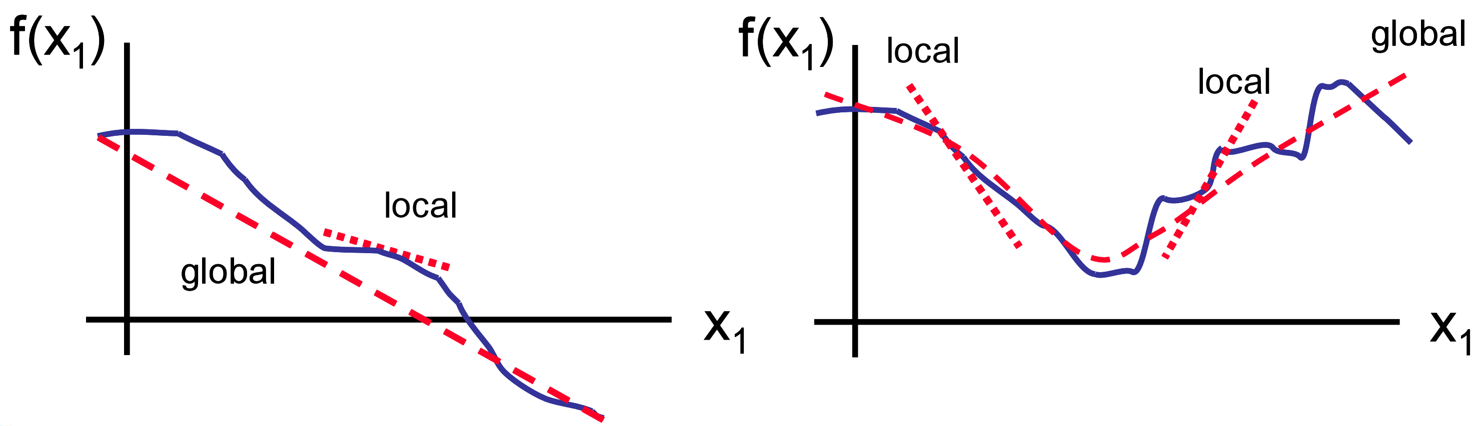
Why Sensitivity Analysis?

- Sensitivity Analysis is a way to rank input variables according to their importance relative to the uncertainty in model output.
- We can determine variables that are important for optimization or UQ, which variables to gather more data on, or which variables to control in an experiment.
- Local: local linear or under-resolved behavior can be misleading.
- Global: can be computationally expensive—meta-modeling can help.



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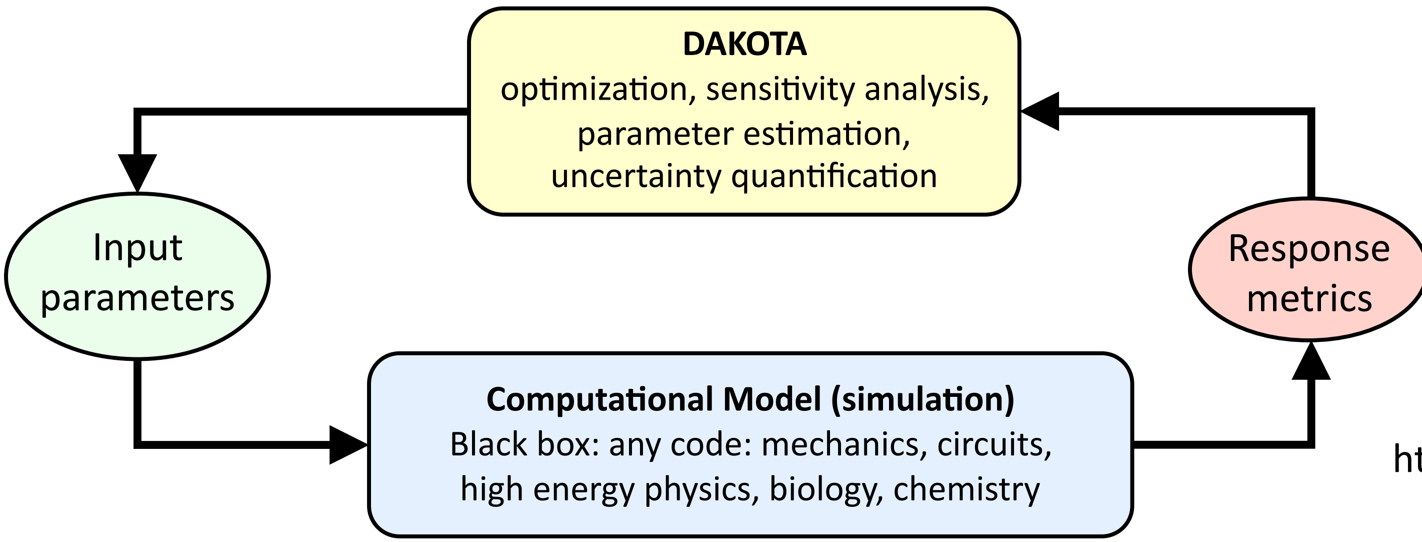
We conduct sensitivity analyses with DAKOTA.



http://dakota.sandia.gov/

- DAKOTA can automate typical "parameter variation" studies with a generic interface to simulation software and advanced methods.
- UQ methods in DAKOTA include:
  - Sampling (LHS, quasi-MC, classical experimental designs, OAs, VBD)
  - Reliability methods (FORM, SORM, AMV+, etc.)
  - Dempster-Shafer Evidence Theory
  - Stochastic expansion methods: Polynomial chaos, stochastic collocation
  - Epistemic-aleatory nested approaches

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Correlation and Variance-Based Decomposition (VBD) are global sensitivity characterizations of uncertainty in model outputs Y.

- Goal: to assess inputs over a hypercube of interest.
- Correlation analysis identifies the strength and direction of a *linear* relationship between input and output.
- VBD identifies the fraction of the variance in the output that can be attributed to an individual variable alone or with interaction effects.
  - Main effect sensitivity S_i is the fraction of the uncertainty in Y that can be attributed to input x_i *alone*

$$S_i = \frac{\mathrm{Var}_{x_i}\left[E(Y|x_i)\right]}{\mathrm{Var}(Y)}$$

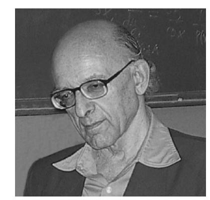
  - Total effect index T_i is the fraction of the uncertainty in Y that can be attributed to x_i *and its interactions with other variables*

$$T_i = \frac{E\left[\mathrm{Var}(Y|x_{-i})\right]}{\mathrm{Var}(Y)}$$

  - Calculation of S_i and T_i requires the evaluation of m-dimensional integrals, approximated by Monte-Carlo sampling.

$$x_{-i} \equiv (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_m)$$

  - *Computationally intensive*, as replicated sets of samples are evaluated: N samples and D inputs → evaluation of $N \times (D+2)$ samples.



I.M. Sobol' developed these ideas

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How sensitivity indices are calculated

$$S_i = \frac{Var(E(Y \mid X_i))}{Var(Y)}$$

- Full Factorial:
  - Take n values of each input variable X_i; the number of samples are a full tensor product of n samples in each input variable, $N = n^d$
  - For each particular value of X_i, calculate the average over the other X_j variables.
    $E(Y \mid X_i = x_{ik})$
  - Calculate the variance of this expectation (variance over n values)
    $Var(E(Y \mid X_i))$
- Approximation in *Sensitivity Analysis in Practice* (Satelli et al. 2004):
  - Calculate two independent sample matrices, A and B, with d (number of inputs) columns and n rows . C_i is constructed by taking the ith column of A and substituting it into B.
  - Y_A, Y_B, and Y_{Ci} are the vectors of responses from evaluating the simulator at the sample values in A, B, or C_i.
  - Total samples is (2+d)*n
  - Requires that n is of order thousands for accuracy

$$f = \frac{Y_A \bullet Y_B}{N}$$

$$estimated\ \mathrm{var}(Y) = \left(\frac{1}{N-1} Y_A \bullet Y_A\right) - f^2$$

$$S_i = \frac{\left(\frac{1}{N-1} Y_A \bullet Y_{c_i}\right) - f^2}{estimated\ \mathrm{var}(Y)}$$

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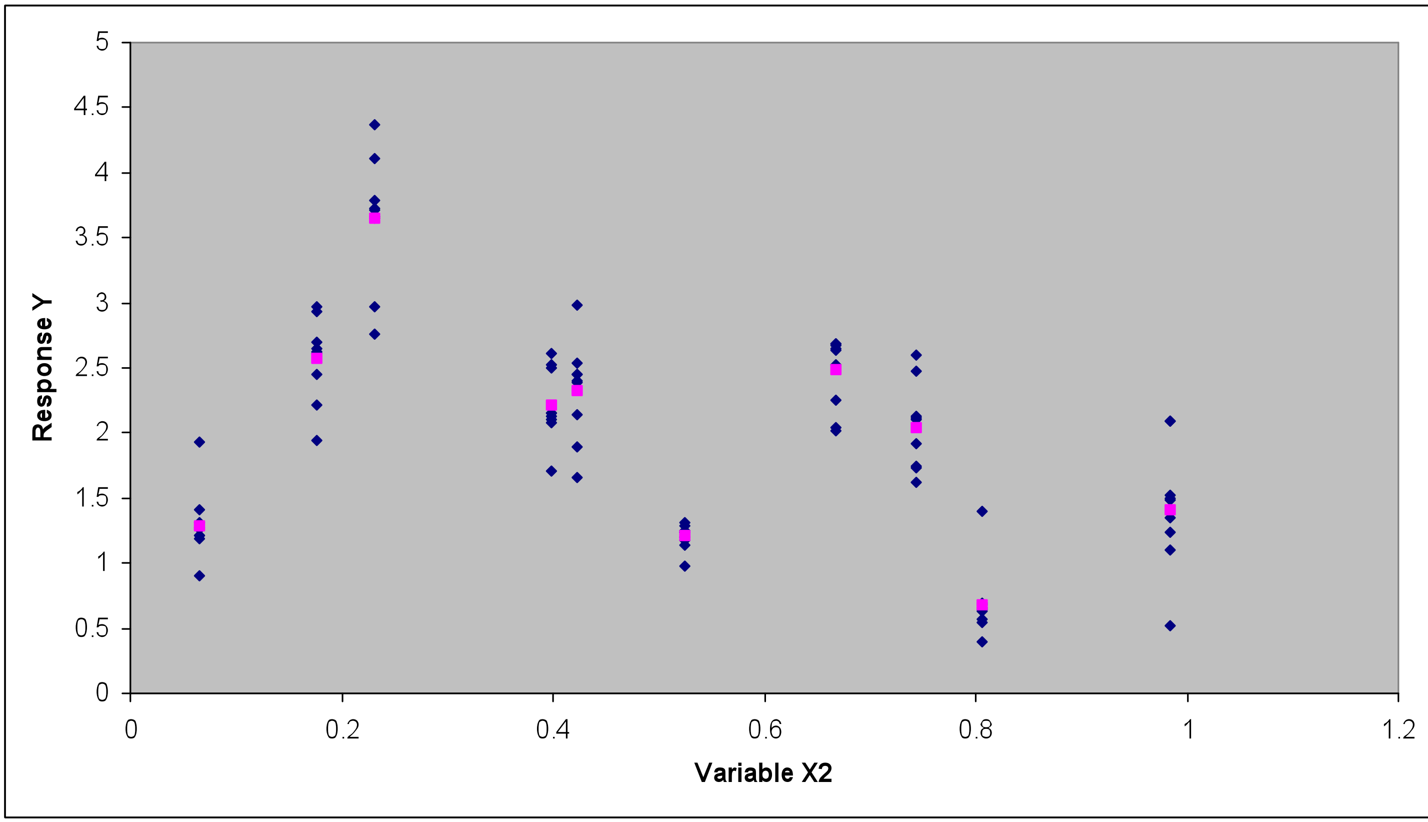
Variance-Based Decomposition: a notional example.

- Main effects indices S_j identify the fraction of uncertainty in the output attributed to X_j alone
- Total effects indices T_j corresponds to the fraction of the uncertainty attributed to X_j and its interactions with other variables



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Meta-models (Response Surfaces) provide an alternative to sampling-based VBD.

- Build the meta-model using some of the data
  - This is feasible for moderately high dimensional data
- Calculate additional matrices to be analyzed using the meta-model and compute VBD indices
- Meta-models can also be used, e.g., to generate confidence intervals of the computed indices *(measure of convergence)*
- There are different approaches to constructing these surrogates:
  - Stochastic expansions (polynomial chaos, stochastic collocation)
  - "Regression" surfaces (regression and smoothing)

Other response surface models provide alternatives to sampling-based approaches.

- SDP = State-Dependent Parameter Regression
  - SDP modeling* is a class of non-parametric smoothing, first suggested by Young§, that is similar to smoothing splines and kernel regression approaches but is performed using recursive (non-numerical) Kalman filter and associated fixed interval smoothing.
  - Good for additive models, and flexibile in adapting to local discontinuities, strong non-linearity, and heteroskedasticity.
- ACOSSO = Adaptive COmponent Selection and Smoothing Operator
  - ACOSSO† is a multivariate smoothing-spline approach (COSSO‡) that is augmented by a weighted (w_j), scaled (λ) penalty function:

$$\hat{f} = \min_{f \in \mathcal{F}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \left(Y_i - f(x_i) \right)^2 + \lambda \underbrace{\sum_{d=1}^{D}}_{D = \text{\# inputs}} w_d \left\| P^d f \right\| \right\}$$

  - ACOSSO is thought to perform best for a reasonably smooth underlying response.
- DACE = Design and Analysis of Computer Experiments
  - Gaussian Process emulator for the data

§ Young, P. C. "The identification and estimation of nonlinear stochastic systems," in *Nonlinear Dynamics and Statistics*, A. I. Mees et al., eds., Birkhauser, Boston (2001).

* Ratto, M., Pagano, A., Young, P. C., "State dependent parameter meta-modelling and sensitivity analysis," *Comput. Phys. Comm.*, **177**, pp. 863–876 (2007).

† Storlie, C.B., Bondell, H.D., Reich, B.J., Zhang, H.H., "Surface estimation, variable selection, and the nonparametric oracle property," *Stat. Sinica,* to appear (2010).

‡ Y. Lin,Y., and H. Zhang, H., "Component selection and smoothing in smoothing spline analysis of variance models," Ann. Stat., **34**, pp. 2272–2297 (2006).

Stochastic Expansion Methods provide one alternative to sampling-based VBD.

- Stochastic expansion methods — Polynomial Chaos Expansion (PCE) or Stochastic Collocation (SC) — produce functional representations of stochastic variability.
- Sudret* (i) demonstrated that the sensitivity indices are explicit functions of the stochastic expansion, and (ii) derived the PCE case.
  - *NOTE*: Once the PCE is obtained, sensitivity indices are calculated *explicitly*, i.e., without sampling
- Tang§ derived the sensitivity indices as analytic functions of SC.
- Both of these techniques have been implemented in DAKOTA.
- This approach is *very efficient*, since the calculation of sensitivity indicies does *not* require more function evaluations in addition to those used to construct the stochastic expansions.

* Sudret, B., "Global Sensitivity analysis using polynomial chaos expansion," *Rel. Engr. & Syst. Safety*, **93**, pp. 964–979 (2008).

§ Tang, G., Iaccarino, G., Eldred, M.S., "Global Sensitivity Analysis for Stochastic Collocation Expansion," paper AIAA-2010-2922 in *Proceedings of the 12th AIAA Non-Deterministic Approaches Conference*, Orlando, FL, 12–15 April 2010.

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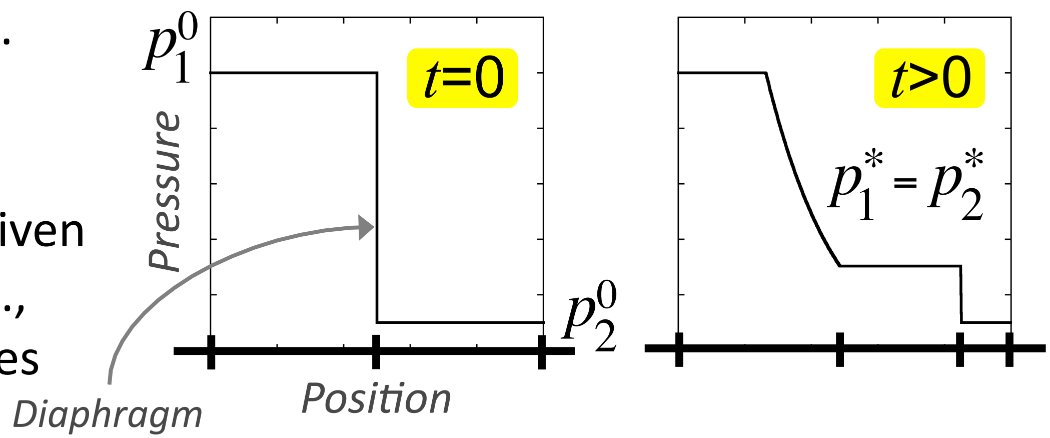
An archetypal case for 1-D compressible flow is the experimental “shock tube” configuration.

- For 1-D compressible, inviscid, non-heat-conducting flow, the state U and flux f are given by

$$U = [\rho,\ \rho u,\ \rho E]^{\mathsf{T}} \qquad\qquad f = [\rho u,\ \rho u^2 + p,\ \rho E u + p u]^{\mathsf{T}}$$

where $E = \boxed{e} + \boxed{\tfrac{1}{2}u^2}$ *Specific internal energy (SIE)* *Specific kinetic energy*

- An example is an experimental shock tube for gas dynamics.
  - Conservation laws = PDEs.
  - Constant, uniform initial conditions.
  - For $t > 0$, the solution is given by a set of self-similar (i.e., functions of x/t only) waves



- This is a specific case of the so-called Riemann problem.

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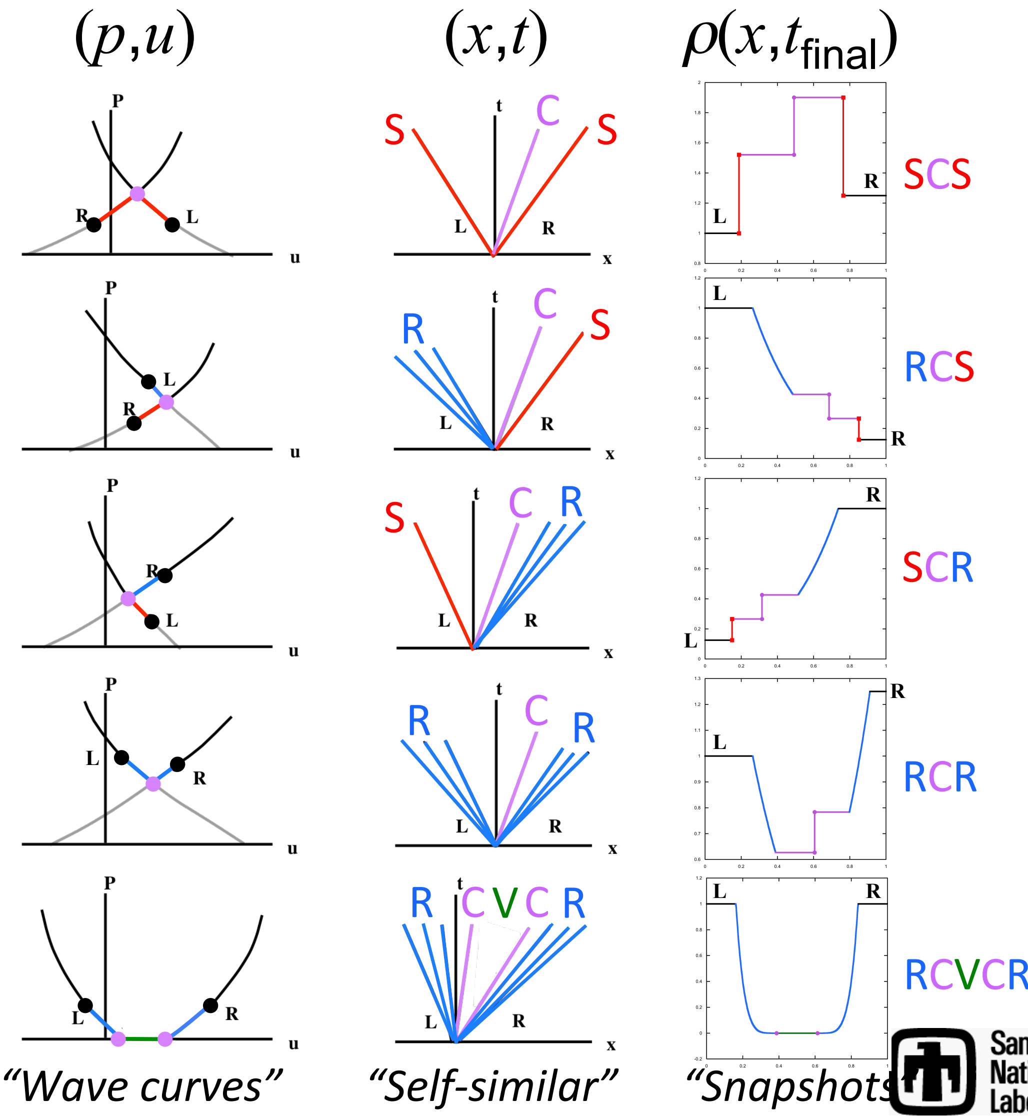
The Riemann problem can have *very different* solutions, depending on the initial conditions.

- There are five basic solutions for the 1D gas dynamics equations with an ideal gas EOS*.
  - These depend on the relative pressures and velocities in the ICs
- S = Shock

  C = Contact

  R = Rarefaction

  V = Vacuum/Void



*R. Menikoff, *Applications of Non-Reactive Compressible Fluids*, LANL Report LA-UR-01-273 (2001)

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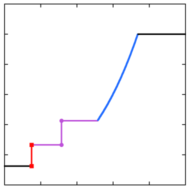
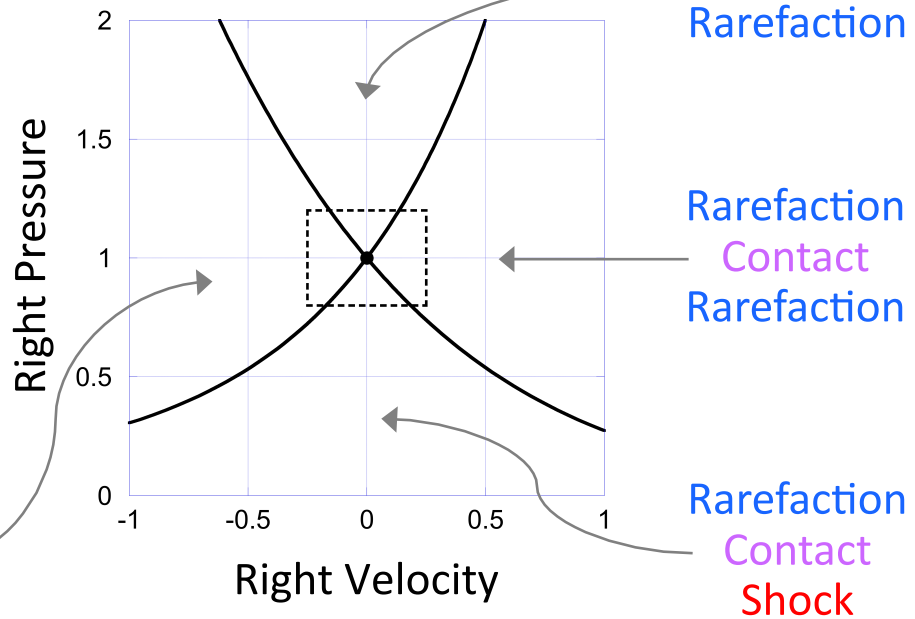
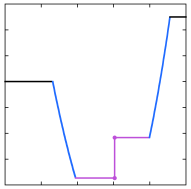
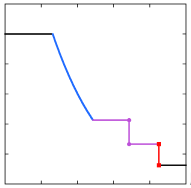
We focus on sensitivity analysis for a single problem, related to the well-known Sod problem.

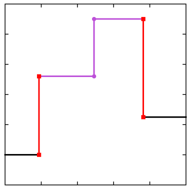
- Initial state: $(\rho,p,u,\gamma) = \begin{cases} (1.0,\ \ 1.0,\ 0.0,1.4), & -0.5 \le x < 0.5 \quad \text{“Left”} \\ (0.125,1.0,0.0,1.4), & 0.5 < x \le 1.5 \quad \text{“Right”} \end{cases}$
- Fix the left state; vary the right state; consider fixed $t_{\text{final}} = 0.2$
- The solution structure varies significantly near the initial point (•).
- Evaluate the sensitivity near that point.











Sod G., : “A Survey of Several Finite Difference Methods for Systems of Nonlinear Hyperbolic Conservation Laws”, *J. Comput. Phys.*, **27**, pp. 1–31 (1978).

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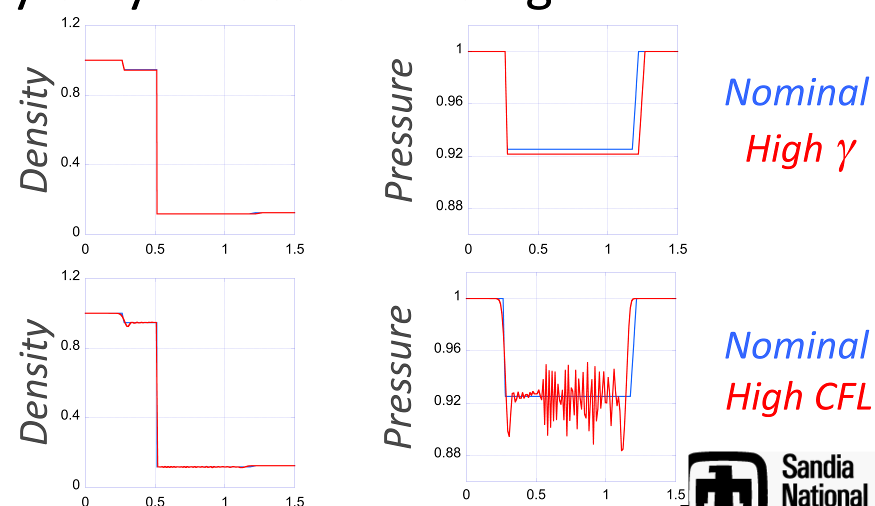
We fix the final time and the left state, but vary both the right state and a numerical parameter.

		Input	Why?
Right	X_1	Initial pressure on right	Uncertainty in initial condition
Right	X_2	Initial velocity on right	Uncertainty in initial condition
Right	X_3	Polytropic index γ on right	Uncertainty in material model
	X_4	CFL parameter: $c_s \, \Delta t / \Delta x$	Numerical parameter

- From the self-similar nature of the solution, only one state need be varied, not both: hence, we vary only values on the right.
- Higher pressure, higher γ $\rightarrow$ higher sound speeds and faster wave propagation
- 0 < CFL < 1 $\rightarrow$ stable
  CFL > 1 $\rightarrow$ unstable



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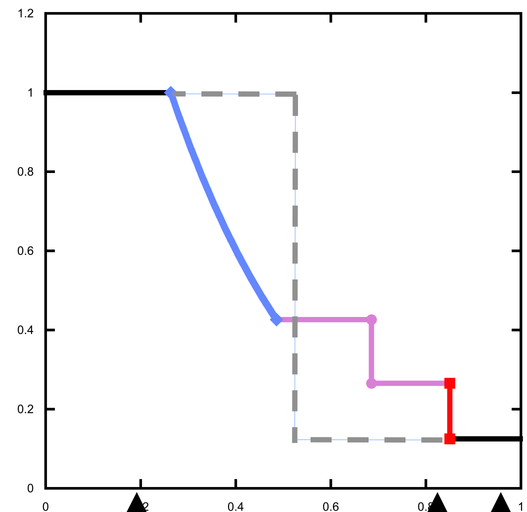
Most of our responses are from probes

- A probe measures some quantity at some location
  - We measured at one location on the left and two on the right of the initial interface location
  - We record the value at the end of the simulations, t=0.2



X=0.35
Y5, Y6, Y7

X=1.16
Y2, Y3, Y4

X=1.4
Y1

- Defining the responses requires a lot of thought; intuition about the physics is not enough

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We consider specific characteristics of the solution as the output variables.

		Output	Why?
Right	Y_1	Specific internal energy, x = 1.4	Coupled physics
Right	Y_2	Mass density, x = 1.16	Wave speed
Right	Y_3	Kinetic energy, x = 1.16	Physics diagnostic
Right	Y_4	Time of 1st $\Delta\rho$, x = 1.16	Experimental diagnostic
Left	Y_5	Mass density, x = 0.35	Wave speed
Left	Y_6	Kinetic energy, x = 0.35	Physics diagnostic
Left	Y_7	Time of 1st $\Delta\rho$, x = 0.35	Experimental diagnostic
	Y_8	CPU time	Computational diagnostic

- Shock-Physics analysts think of the problem in these terms

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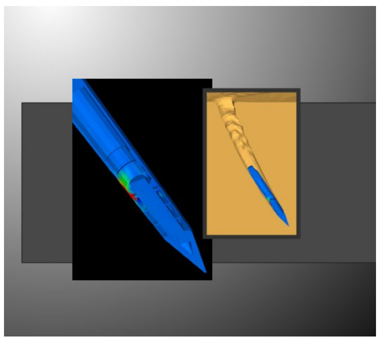
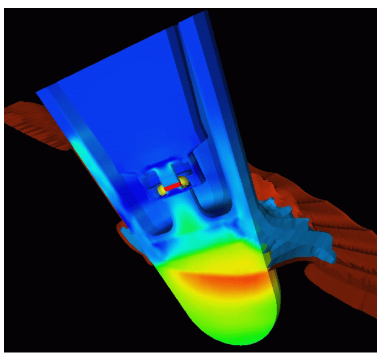
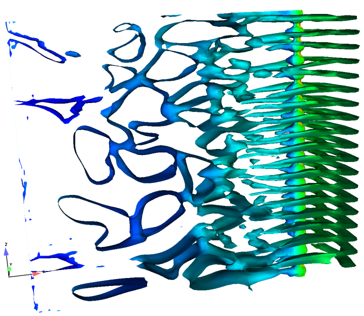
We simulate this problem with the ALEGRA multi-physics code.

Shock and Multi-physics







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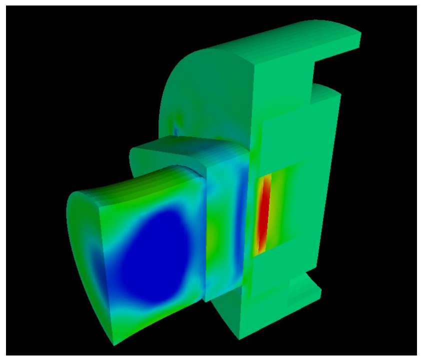
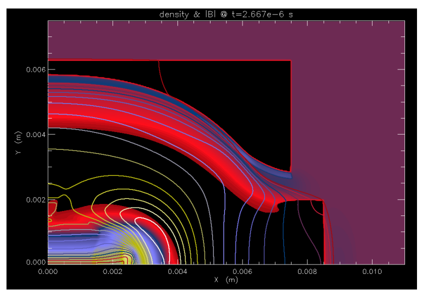
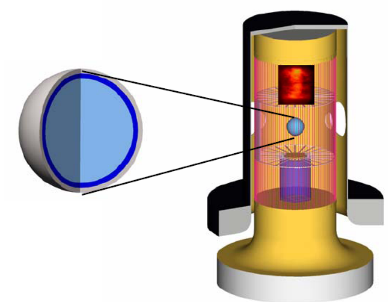
HEDP Theory and ICF Target Design





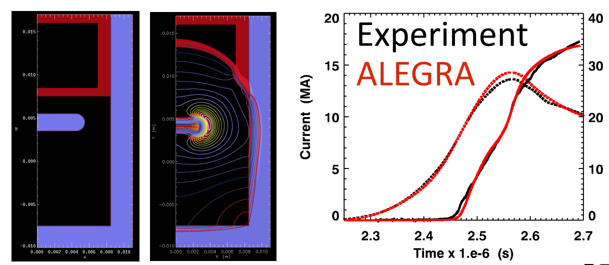


Overview

- The ALEGRA suite of applications models shock and high energy environments for solids, fluids, and plasmas using a multi-material arbitrary Lagrangian-Eulerian (ALE) multi-physics methodology.
- ALEGRA applications run on large, parallel, message-passing architectures in 2-D and 3-D geometries.

ALEGRA Applications

- Armor Design and Analysis
- Shaped Charges & Explosively Formed Penetrators
- Railgun Design and Analysis
- Magnetohydrodynamics (MHD)
- Z-pinch, Inertial Confinement Fusion
- Isentropic Compression Experiments/Magnetic Flyers



Isentropic Compression: Magnetic Flyer Predictions vs Expt

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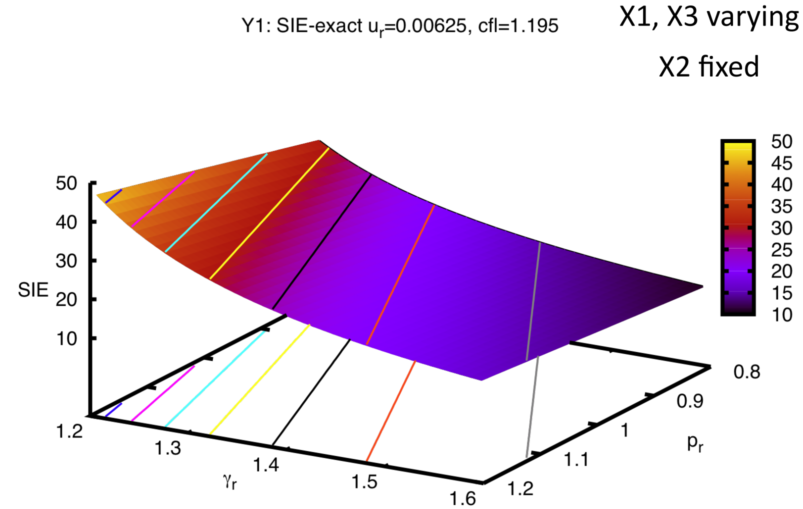
Y1: SIE at x = 1.4
Output surface slice for the Exact Model

- Y1 is a simple output we use as a test
- No waves reach this probe location so the SIE remains at its initial value
  - The initial value is a function of X1 and X3 only



- Surfaces shown were generated with an exact Riemann solver ("Exact Model"), not the simulation code.

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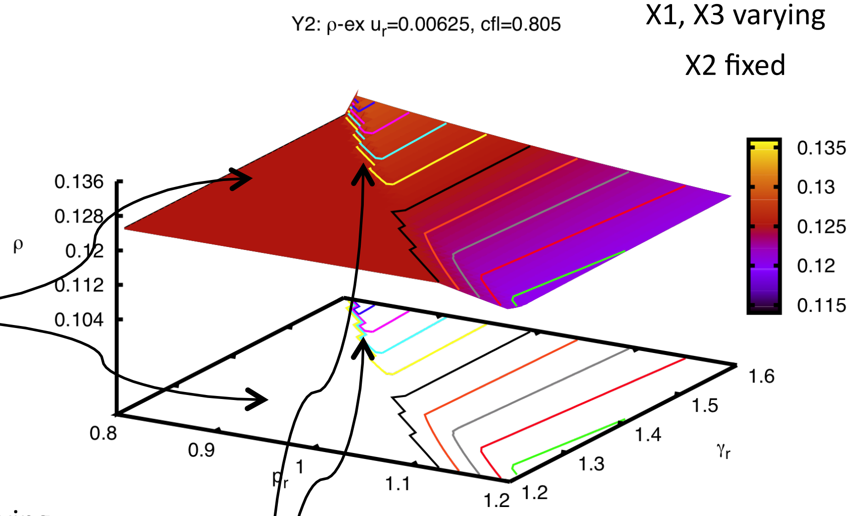
Y2: ρ at x = 1.16
Output surface slices for the Exact Model

X1, X3 varying

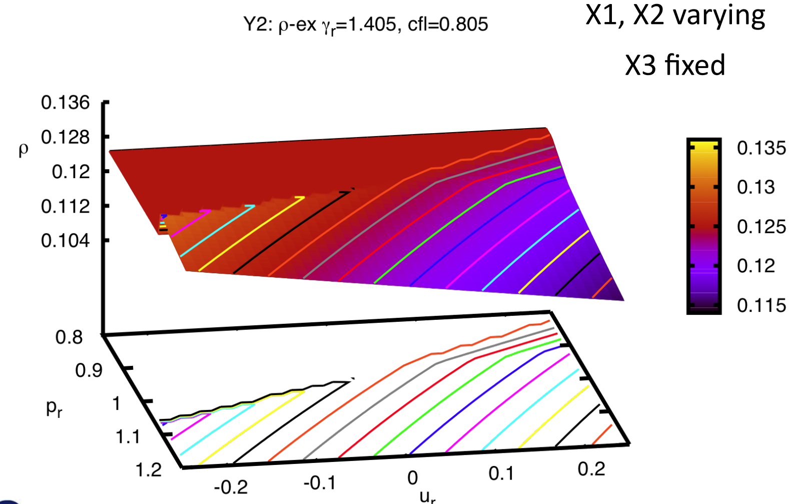
X2 fixed



Flat plateaus indicate no waves have reached this location

X1, X2 varying

X3 fixed



Sharp jumps indicate shocks

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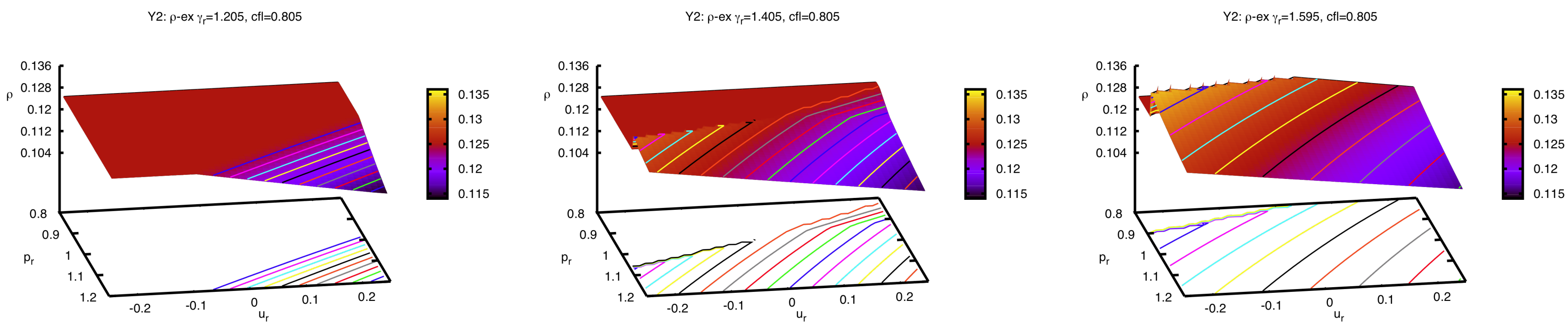
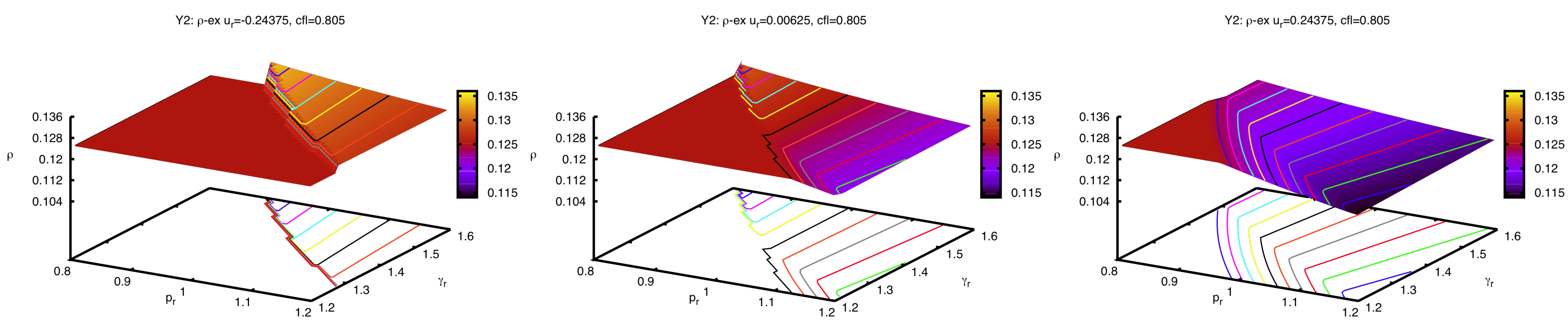
Y2: ρ at x = 1.16
Output surface slices for the Exact Model



X3 increasing

X1, X2 varying
X3 fixed



X2 increasing

X1, X3 varying
X2 fixed

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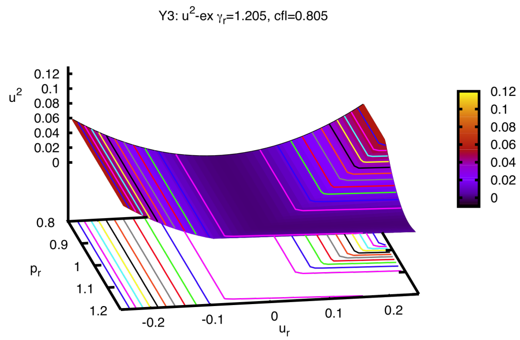
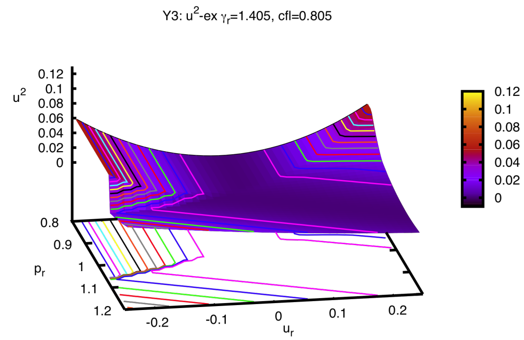
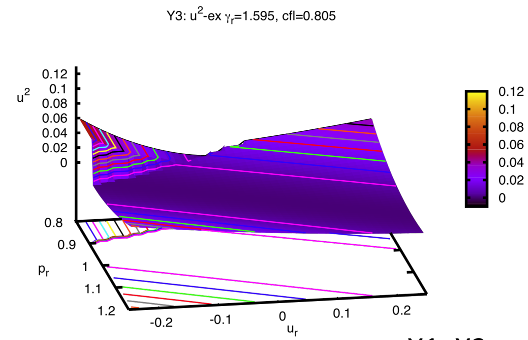
Y3: u^2 at x = 1.16
Output surface slices for the Exact Model



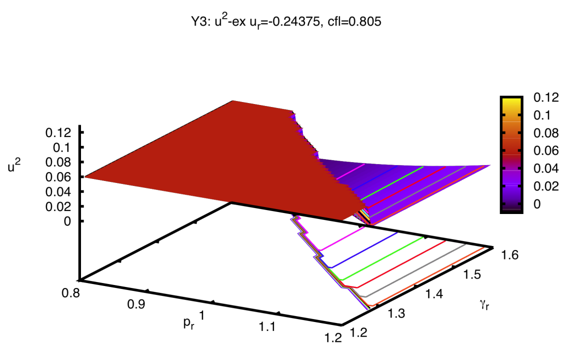


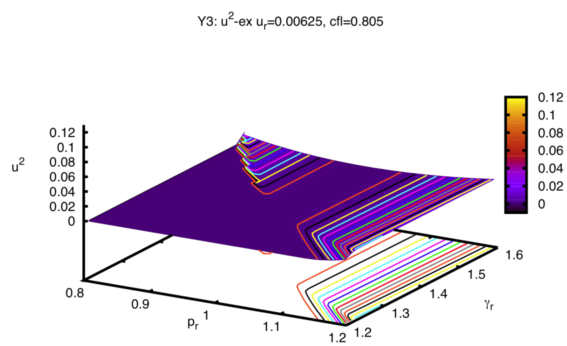


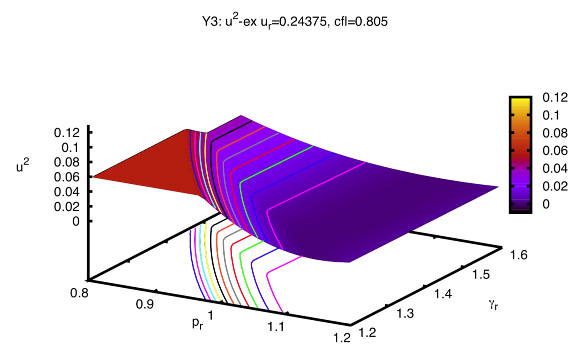
X3 increasing

X1, X2 varying

X3 fixed







X2 increasing

X1, X3 varying

X2 fixed

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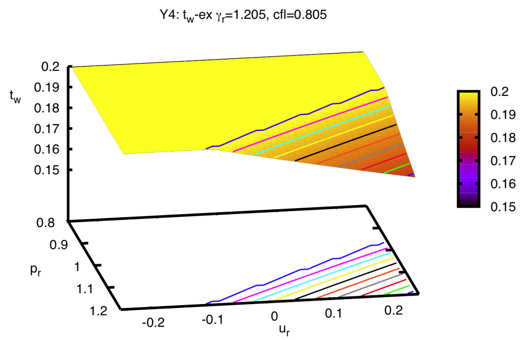
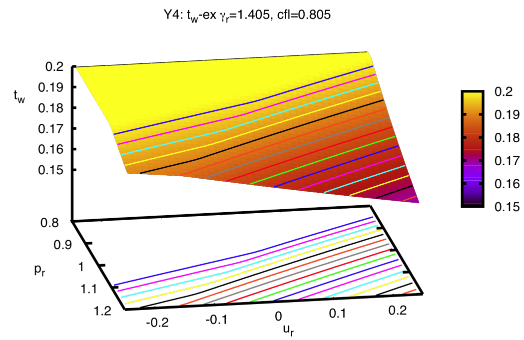
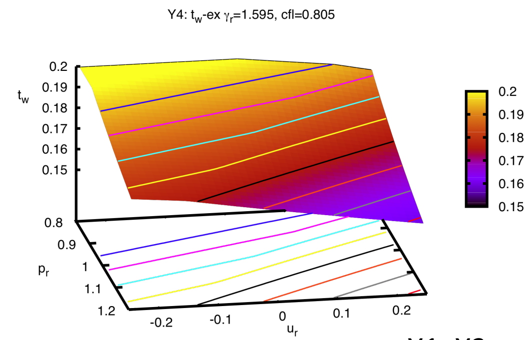
Y4: t_w at x = 1.16
Output surface slices for the Exact Model





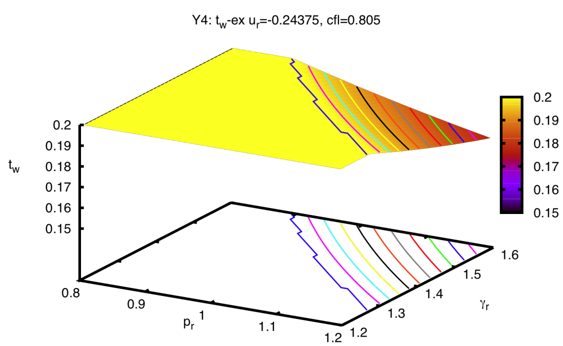


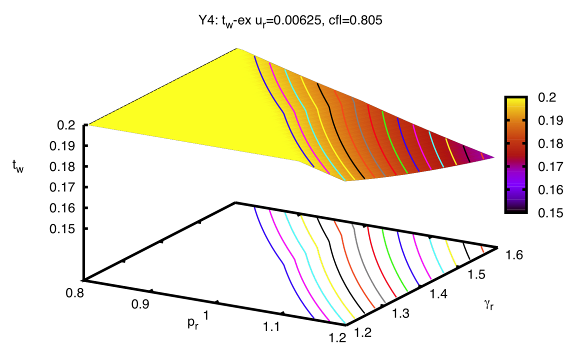
X3 increasing

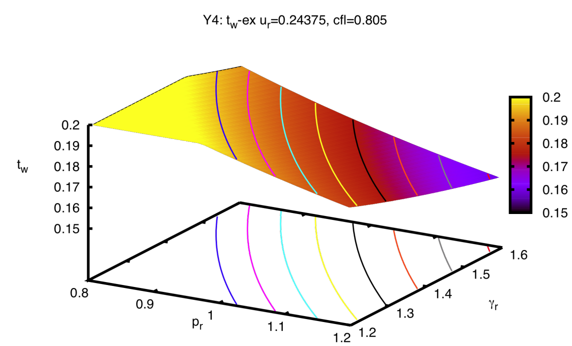
X1, X2 varying

X3 fixed

Plateaus:
Simulations end
at t=0.2.







X2 increasing

X1, X3 varying

X2 fixed

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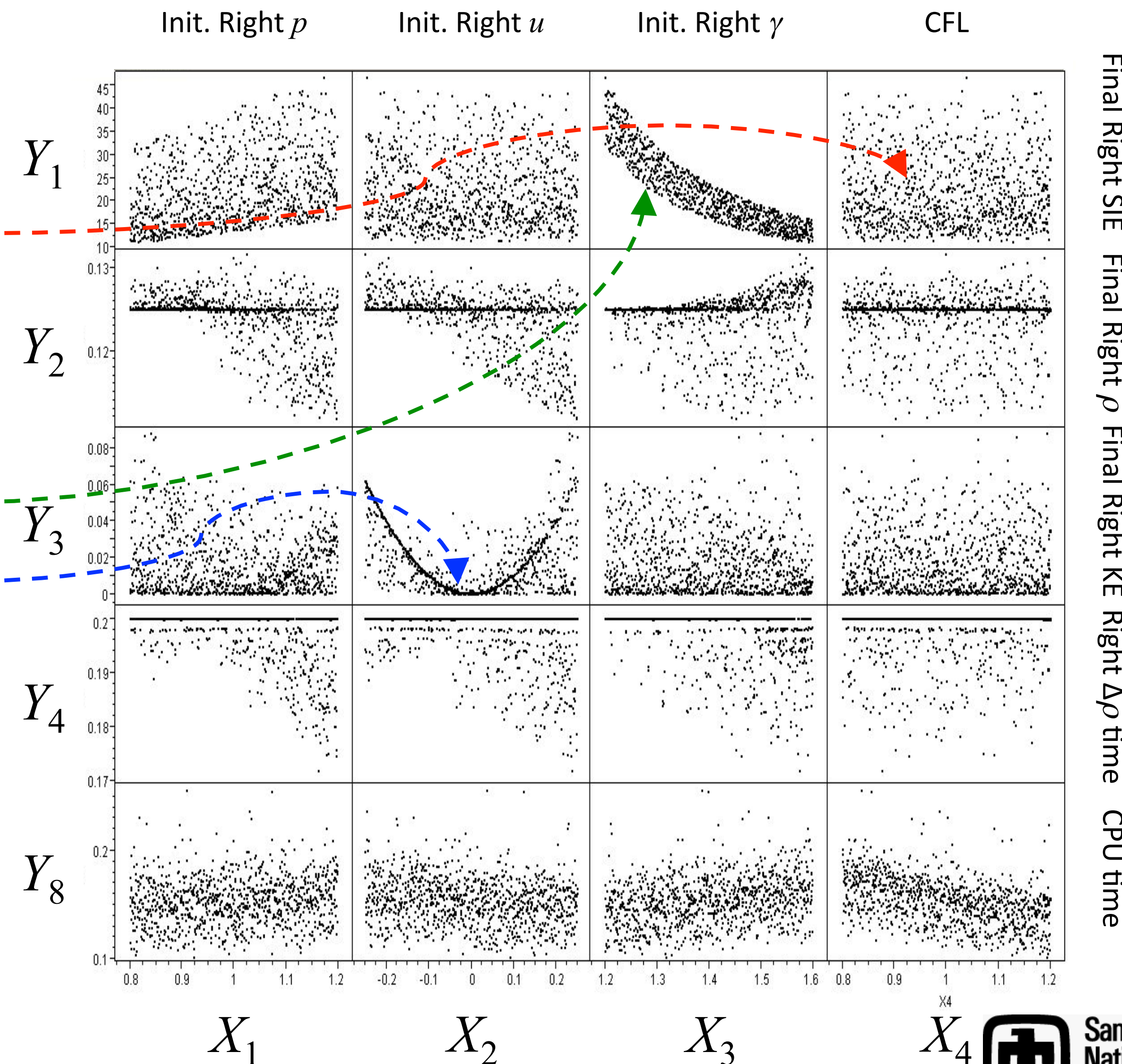
Scatterplots of model outputs give some insights into the distributions.

- Some outputs appear insensitive:
  - Y_1 variation with X_4
- Some trends in the data are clear:
  - Y_1 variation with X_3
  - Y_3 variation with X_2
- VBD sensitivity indices quantify this behavior…



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We show results for estimators of the main and total sensitivity indices S and T for several methods.

Meta-models

- DACE 256 Gaussian process approach, 256 samples
- ACOSSO 256 adaptive smoothing spline, 256 samples
- SDP 256 non-parametric smoothing, 256 samples

Analytic VBD

- PCE6 1296 analytic VBD, 6th-order, uniform distr., 1296 samples
- JRC 196k 196k sample, Sobol´/Saltelli estimates *The usual "gold standard"*
- PCE4 256 analytic VBD, 4th-order, uniform distr., 256 samples

LHS Sampling

- LHS 60000 6.e+4 samples, LHS sampling-based VBD
- LHS 6000 6.e+3 samples, LHS sampling-based VBD

Full Factorial

- A-EXACT 160k 1.60e+5 (=20^4) ALEGRA samples, F.F. VBD
- A-EXACT 2.56M 2.56e+6 (=40^4) ALEGRA samples, F.F. VBD
- R-EXACT 160k 1.60e+5 Riemann (exact) samples, F.F. VBD
- R-EXACT-2.56M 2.56e+6 Riemann (exact) samples, F.F. VBD

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These analyses present several questions.

- *Do these approaches give consistent results, e.g., for rankings?*
- *Do these results vary for the different outputs, Y_1–Y_4, Y_8?*
- *How do these results depend on the different inputs, X_1–X_4?*
- *Do these results "converge"?*
- *How do sampling and meta-model results compare?*
- *Can we distinguish among different meta-models?*
- *How do exact solution results compare to ALEGRA results?*

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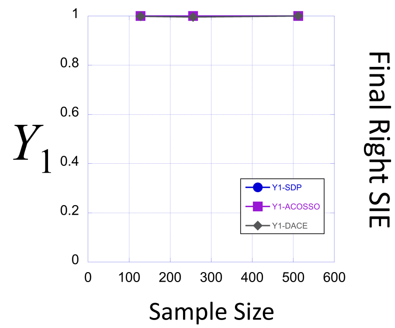
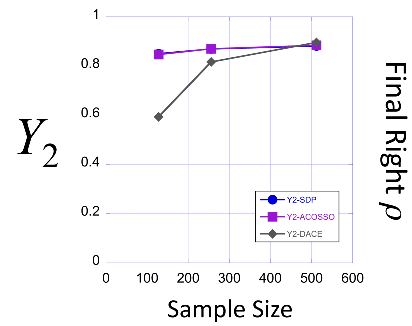
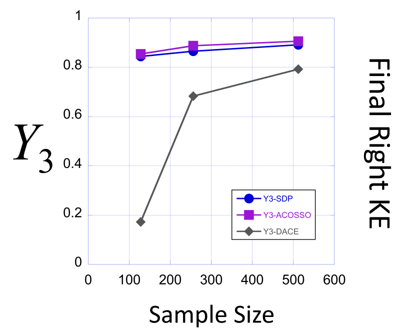
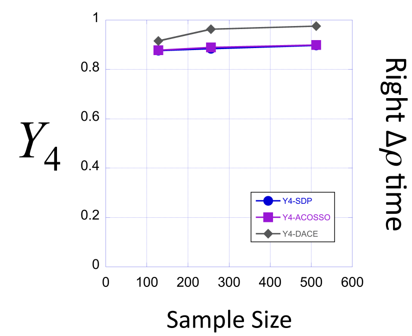
Comparison of R^2 for different meta-models under sample size gives a measure of the goodness-of-fit.

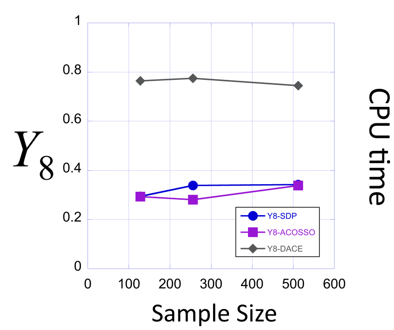
- The R^2 statistic is plotted for SDP, ACOSSO, and DACE (GP) emulators built with sample sizes: N=128, 256, 512.
- The goodness-of-fit clearly varies with the output:
  - Y_1 is very well fit
  - Y_2, Y_4 are reasonably well fit
  - Y_3 is reasonable with SDP, ACOSSO, but not so well with DACE (GP)
  - Y_8 is fit consistently better with DACE than the consistently poor fit with SDP and ACOSSO











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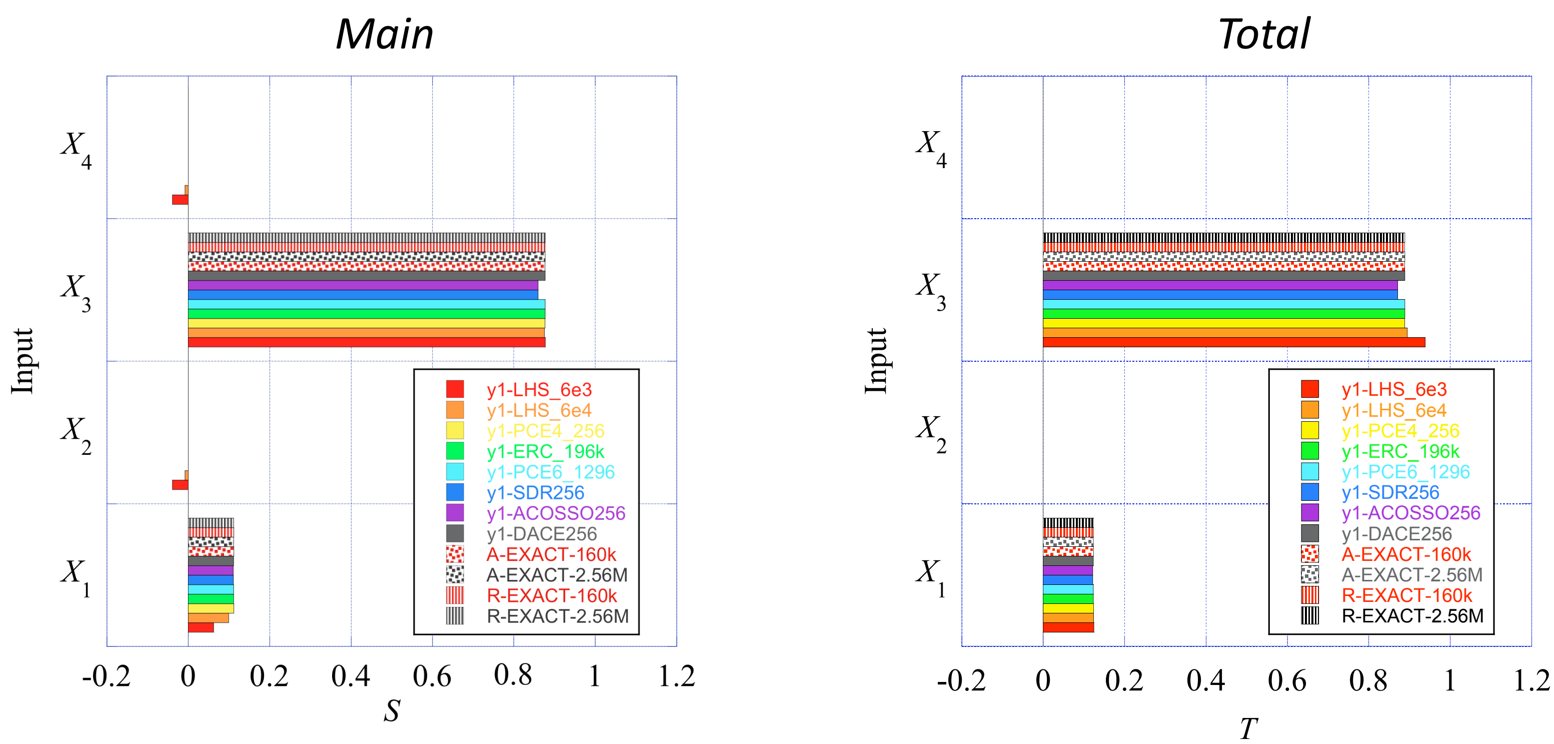
The sensitivity indices S and T for Y_1 perform similarly for all approaches.

- As anticipated, Y_1 (SIE) depends strongly on X_1 (p_R) and X_3 (γ_R)
- Sampling, meta-model, and "exact" results are all consistent.

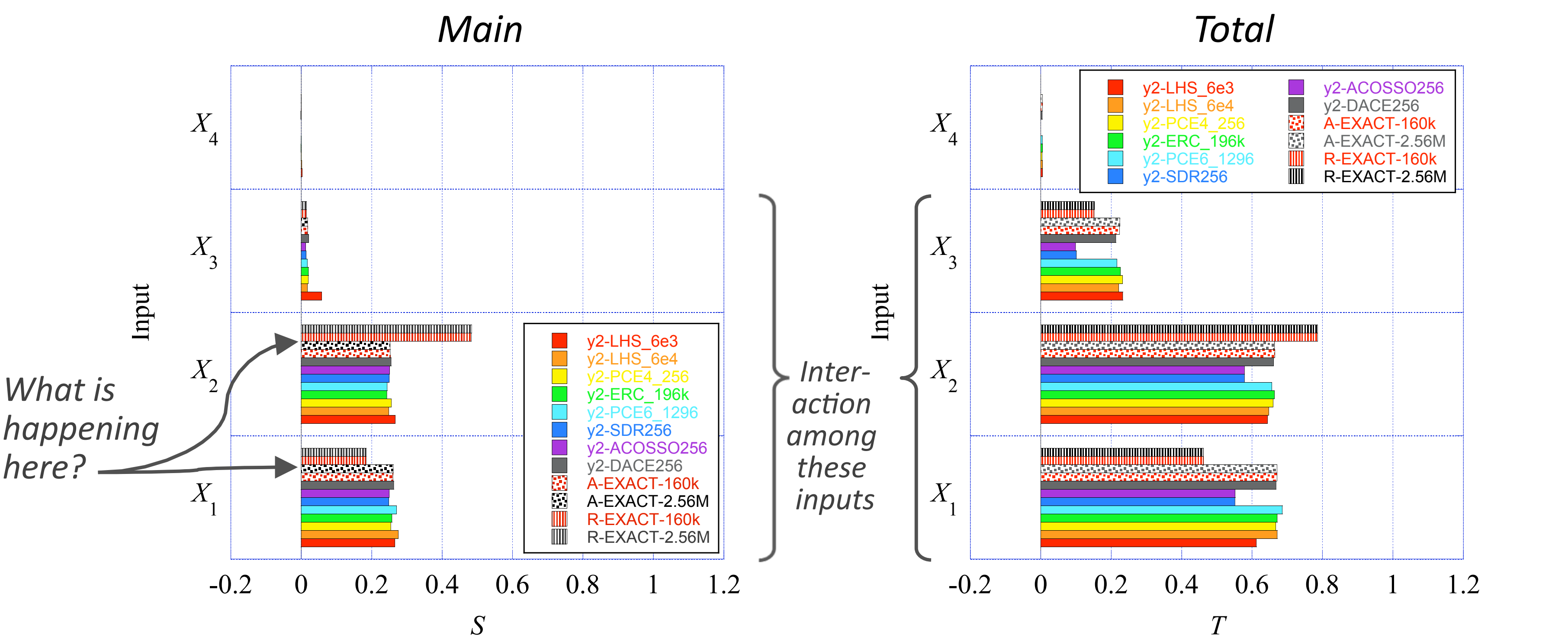


LHS 6000 PCE4 256 PCE6 1296 ACOSSO 256 A-EXACT 160k R-EXACT 160k

LHS 60000 JRC 196k SDP 256 DACE 256 A-EXACT-2.56M R-EXACT-2.56M

The sensitivity indices for Y_2 have some interesting features.

- For Y_2 (final right ρ), main and total indices have different values, indicating those inputs interact with others.

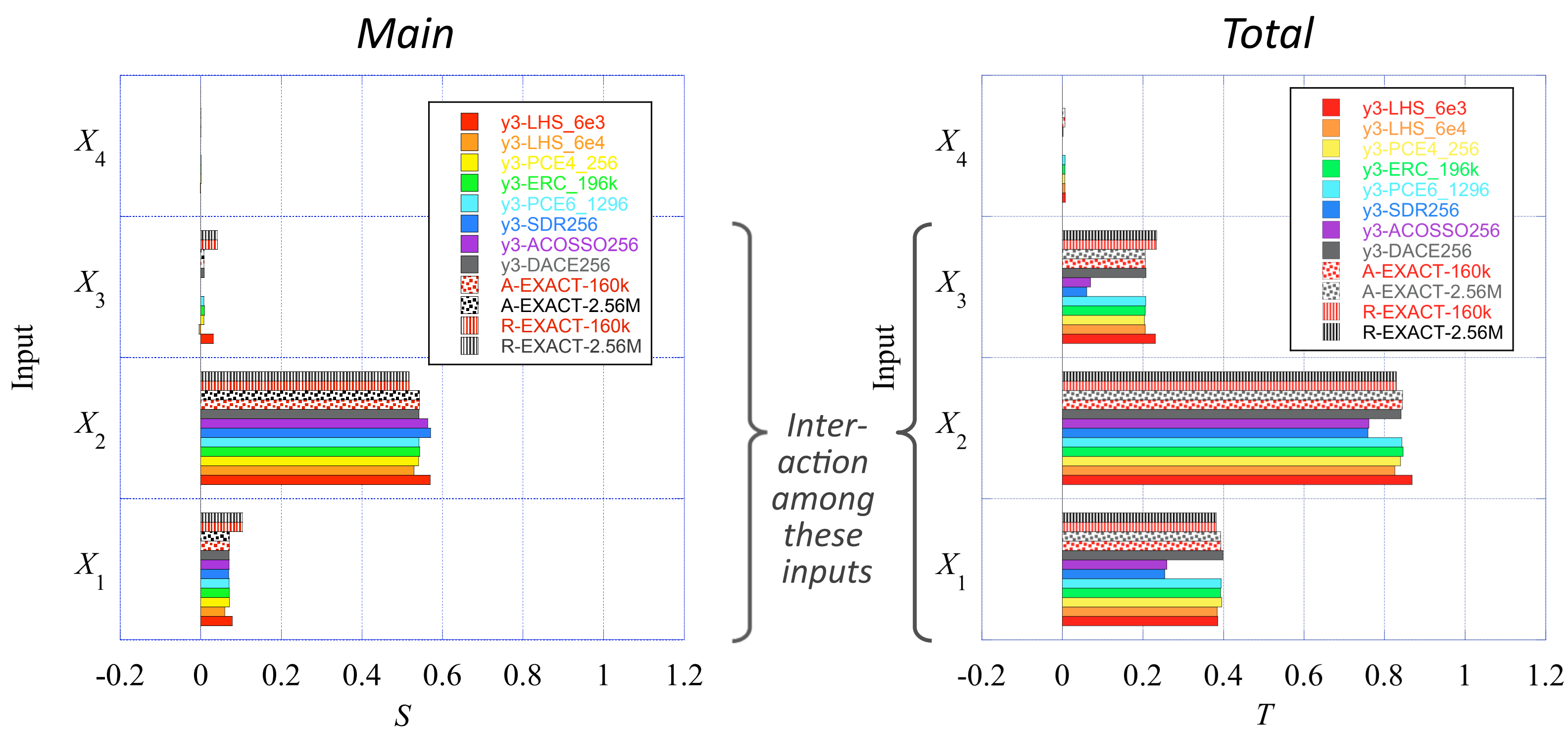


LHS 6000 PCE4 256 PCE6 1296 ACOSSO 256 A-EXACT 160k R-EXACT 160k

LHS 60000 JRC 196k SDP 256 DACE 256 A-EXACT-2.56M R-EXACT-2.56M

The sensitivity indices for Y_3 perform similarly for all approaches.

- As anticipated, Y_3 (final right KE) depends strongly on X_2 (u_R).
  - Sensitivity on X_3 (γ_R) is less than heuristically expected.



LHS 6000 | PCE4 256 | PCE6 1296 | ACOSSO 256 | A-EXACT 160k | R-EXACT 160k

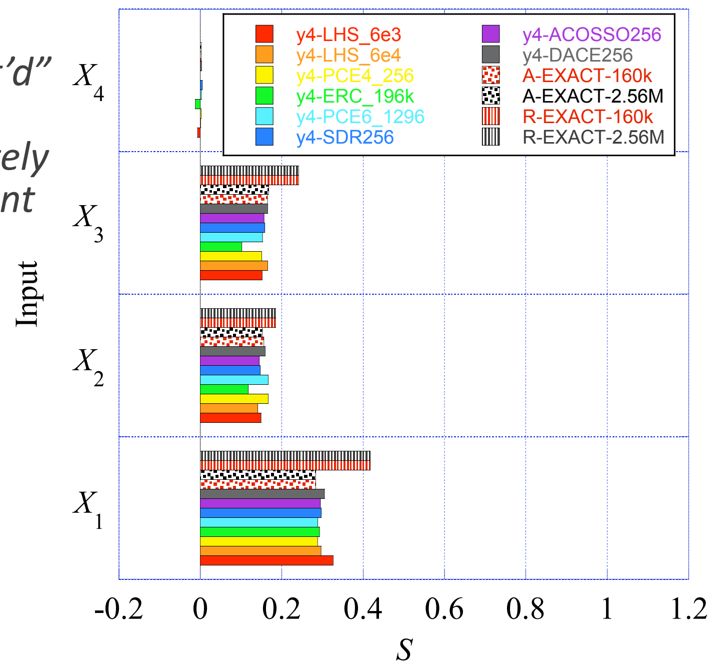
LHS 60000 | JRC 196k | SDP 256 | DACE 256 | A-EXACT-2.56M | R-EXACT-2.56M

The sensitivity indices for Y_4 also show some unusual features.

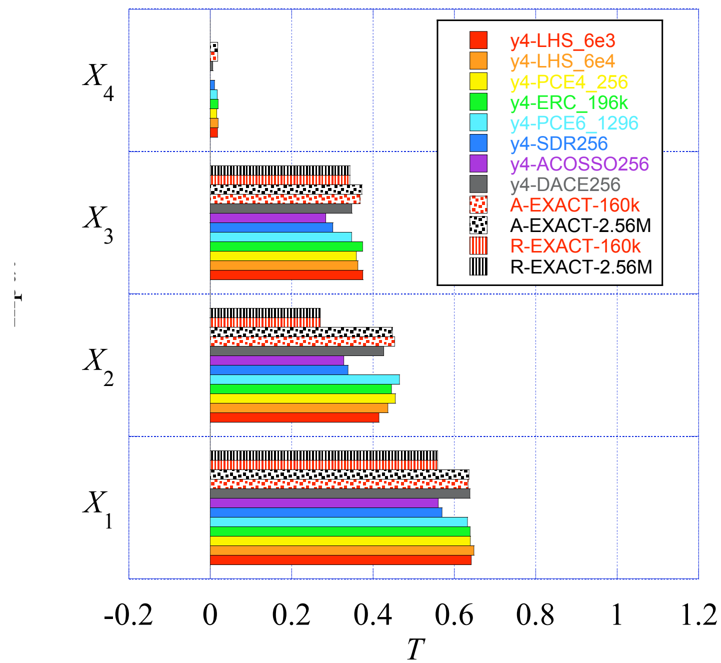
- As expected, Y_4 (right $\Delta\rho$ time) depends strongly on X_1 (p_R).

"Gold St'd" is not completely consistent

Main



Total



LHS 6000	PCE4 256	PCE6 1296	ACOSSO 256	A-EXACT 160k	R-EXACT 160k
LHS 60000	JRC 196k	SDP 256	DACE 256	A-EXACT-2.56M	R-EXACT-2.56M

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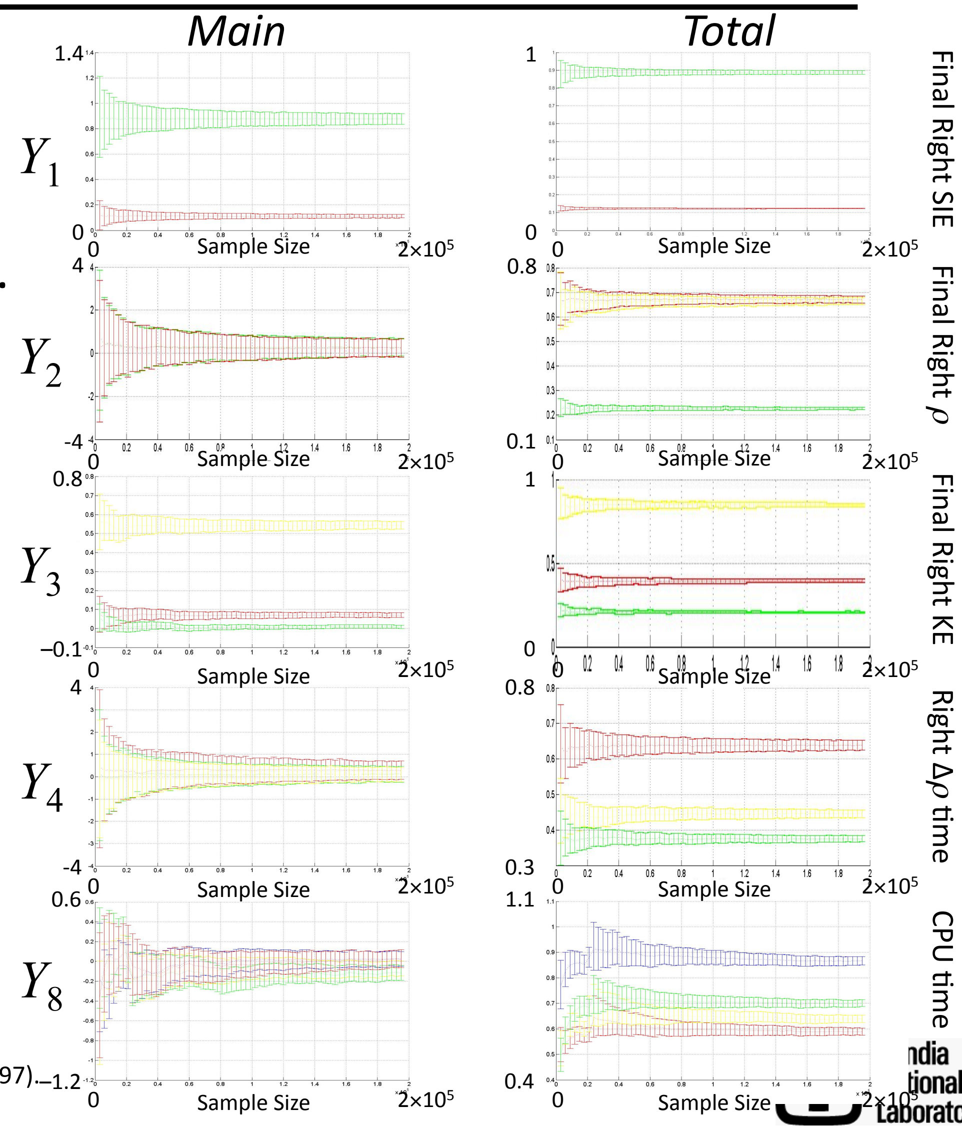
Estimators of the main and total sensitivity indices§ converge under quasi-random sampling.

- Confidence intervals obtained with bootstrap technique.*
- Confidence intervals decrease with increasing # of model runs.
- The lower/upper bounds of the main indices are wider than those of the total indices.
- The estimator of the main indices appears to have a larger variance than the estimator of the total indices.

X_1 Init. Right p	X_3 Init. Right γ
X_2 Init. Right u	X_4 CFL parameter



§ Saltelli, A., P. Annoni, I. Azzini, F. Campolongo, M. Ratto, S. Tarantola, "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index," *Comp. Physics Comm.*, **181**, 259–270 (2010).

* G.E.B. Archer, A. Saltelli, I.M. Sobol′, "Sensitivity Measures, ANOVA-Like Techniques and the Use of Bootstrap," *J. Statist. Comput. Simul.*, **58**, pp. 99–120 (1997).

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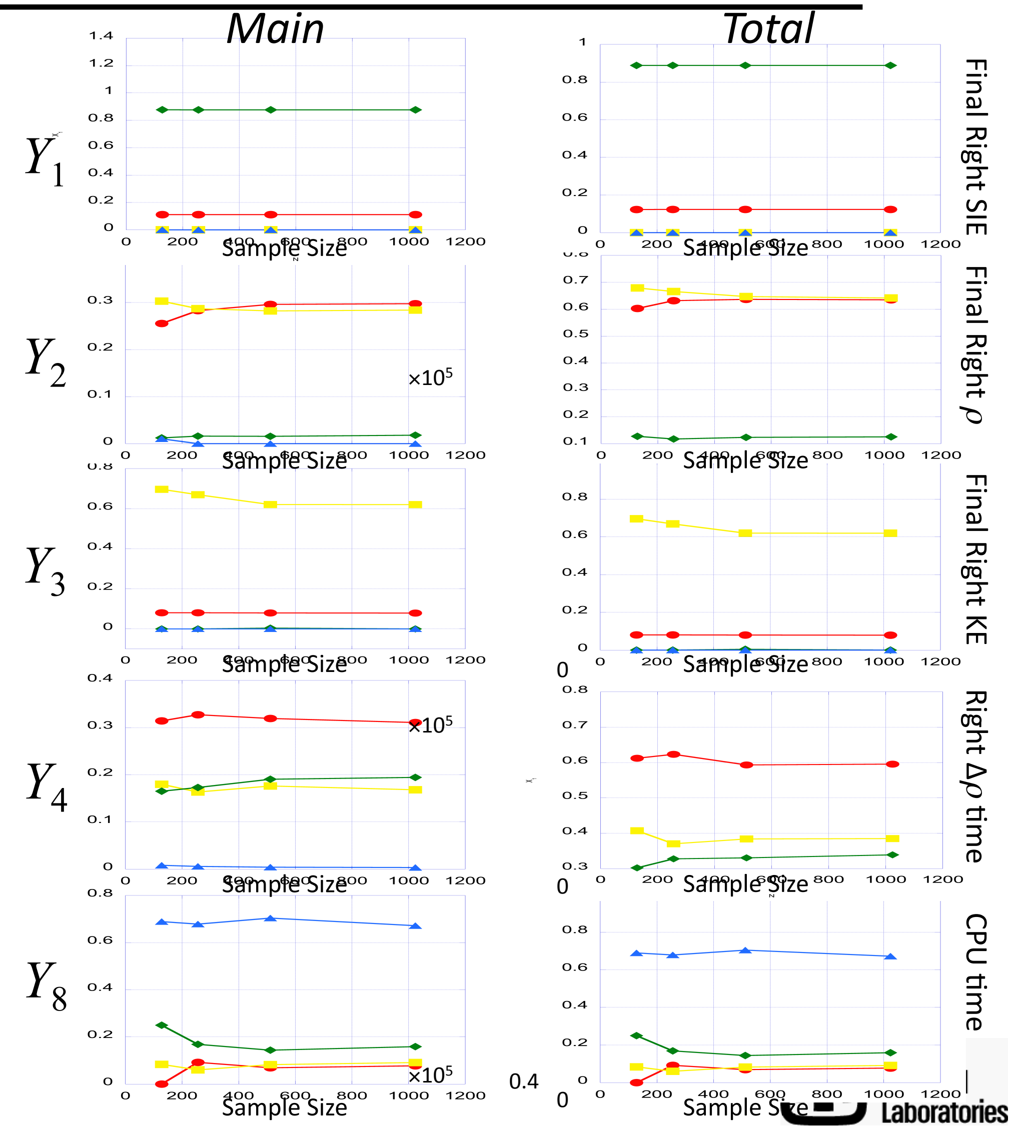
Variation of SDP + Sobol´ results with sample size…

- Meta-model results are for SDP + Sobol´ esimators built with sample sizes: N=128, 256, 512, 1024.
- Sobol´ indices are are obtained executing the meta-model at a set of untried points.
- Both main and total indices are well-behaved from the perspective of convergence.
- Again, the indices from N=256 are already quite robust to further refinement.



- X_1 Init. Right p
- X_2 Init. Right u
- X_3 Init. Right γ
- X_4 CFL parameter

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We have some answers to our questions…

- *Do these approaches give consistent results, e.g., for rankings?*
  - In general, the different meta-models are consistent, both in ranking and magnitude, particularly for main effects (less so for total effects).
- *Do these results vary for the different outputs?*
  - “Well-behaved” outputs (e.g., Y_1 and Y_3) are quite consistent.
  - “Less-well-behaved” output (Y_8) shows much greater variability.
- *How do these results depend on the different inputs?*
  - “Well-behaved” inputs (e.g., X_1, X_2) follow the above pattern.
  - Other inputs (X_3, X_4) show more variation for SDP and ACOSSO.
  - Correct index values can be more challenging to properly calculate when there are significant interactions among the inputs (e.g., Y_2)

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We have some answers to our questions…

- *Do these results "converge"?*
  - Yes (empirically): more samples → the results "settle down"
  - Yes and No: the "converged" value might differ from the exact value.
- *How do sampling and meta-model results compare?*
  - Generally very well, at least under adequate resolution.
- *Can we distinguish among different meta-models?*
  - The actual numbers varied slightly, but the rankings are robust.
- *How do exact solution results compare to ALEGRA results?*
  - "Well-behaved" inputs (e.g., X_1, X_2) follow the above pattern.

- LHS 6000
- LHS 60000
- PCE4 256
- JRC 196k
- PCE6 1296
- SDP 256
- ACOSSO 256
- DACE 256

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Conclusions: What we determined

- We considered real-physics test problem, with an exact sol'n.
- We also generated an exact (full factorial) solution for the sensitivity analysis problem.
- For this well resolved (many samples) problem, all sampling approaches and meta-models gave consistent main effects index values:
  - Comparable values
  - Comparable rankings
  - Converged
- We found that small details about how the sensitivity indices were estimated had an effect on the results.
- Differences between the computational model and the exact model were observed.

Backup Slides

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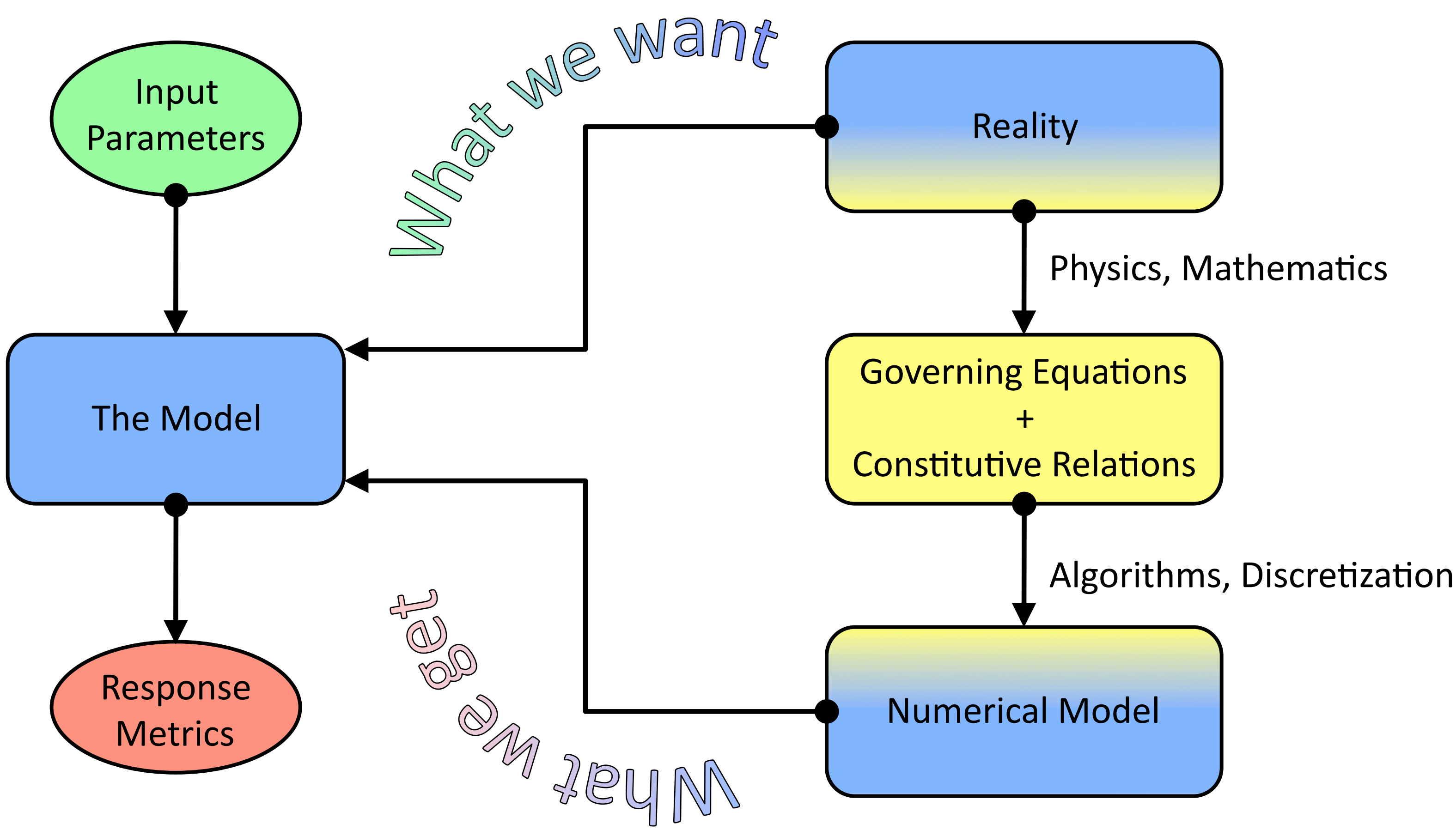
What we get from Sensitivity Analysis of Computer Simulations



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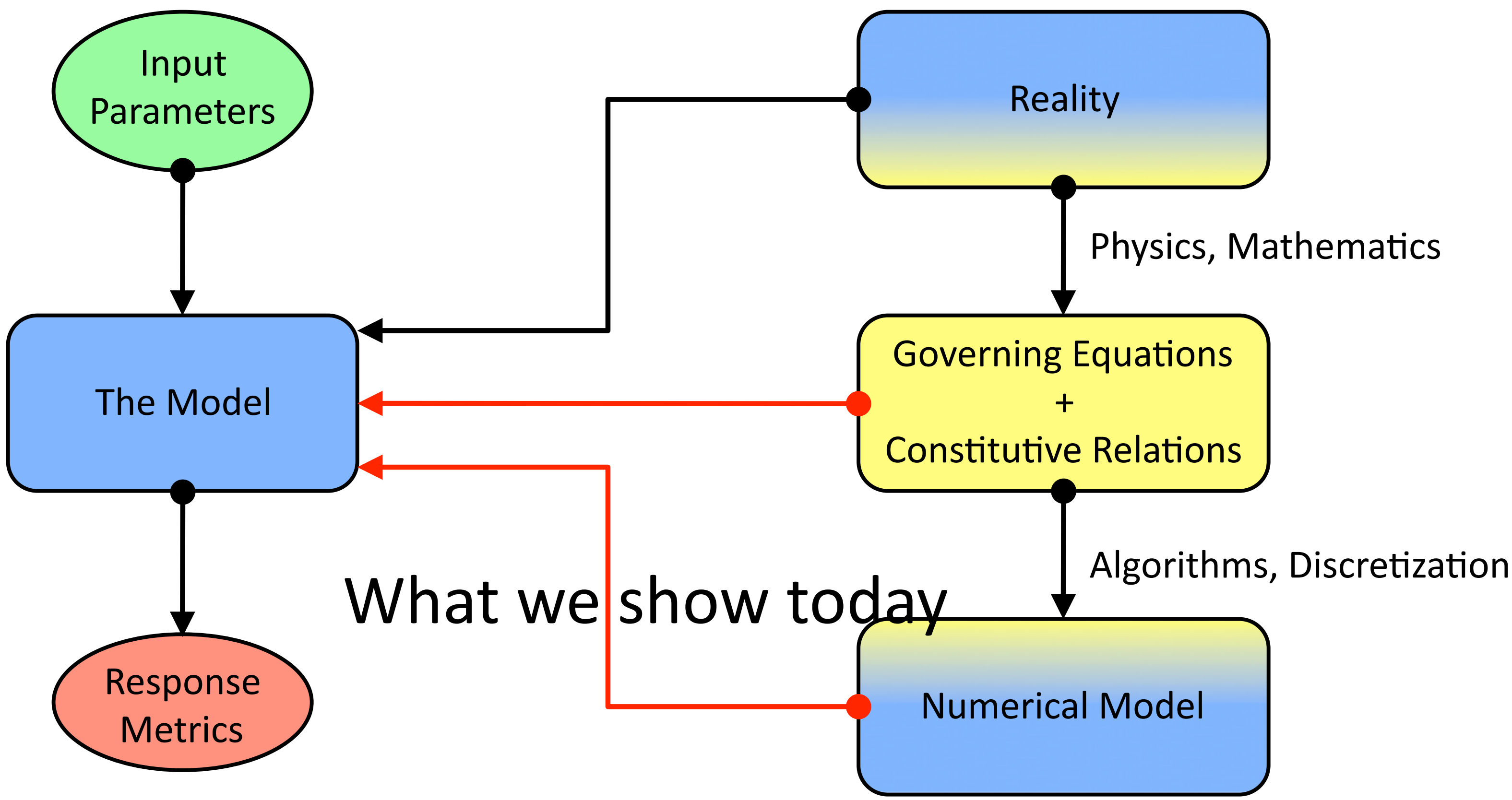
What we get from Sensitivity Analysis of Computer Simulations



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Y8: CPU time

- Y8 (CPU time) has no analog in the Exact Model
- Expectations:
  - Linear dependence on X4 (cfl number)
  - Weak, indirect dependence on the other inputs through wave speeds
  - *Dominated by strong random noise*
  - Not clear that results for different SA techniques *should* match

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The sampling implementation of VBD can be computationally demanding.

- Requires $N \times (D + 2)$ function evaluations, where D is the number of input variables and N is the number of samples.
  - Common practice: N should be *at least* a few hundred to obtain reasonably accurate variance estimates.

$$\begin{pmatrix} X_{11} & \dots & X_{D1} \\ X_{12} & \dots & X_{D2} \\ X_{13} & \dots & X_{D3} \\ & & \\ X_{1N} & \dots & X_{DN} \end{pmatrix} \quad \dots \quad \begin{pmatrix} X_{11} & \dots & X_{D1} \\ X_{12} & \dots & X_{D2} \\ X_{13} & \dots & X_{D3} \\ & & \\ X_{1N} & \dots & X_{DN} \end{pmatrix} \quad \dots \quad \xrightarrow{\text{Column Swap}} \quad \begin{pmatrix} X_{11} \dots X_{i1} \dots X_{D1} \\ X_{12} \dots X_{i2} \dots X_{D2} \\ X_{13} \dots X_{i3} \dots X_{D3} \\ \\ X_{1N} \dots X_{iN} \dots X_{DN} \end{pmatrix}$$

Sample 1   Sample 2   Sample i

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Generalized Polynomial Chaos Expansions approximate the response with a spectral projection using orthogonal polynomial basis functions.

- Expand the response R in terms of prescribed basis functions ψ_j:

$$R = \sum_{n=0}^{N} \alpha_n \psi_n(\xi) \qquad \text{such that} \qquad \begin{array}{rclcl} \Psi_0(\xi) & = & \psi_0(\xi_1)\,\psi_0(\xi_2) & = & 1 \\ \Psi_1(\xi) & = & \psi_1(\xi_1)\,\psi_0(\xi_2) & = & \xi_1 \\ \Psi_2(\xi) & = & \psi_0(\xi_1)\,\psi_1(\xi_2) & = & \xi_2 \\ \Psi_3(\xi) & = & \psi_2(\xi_1)\,\psi_0(\xi_2) & = & \xi_1^2 - 1 \\ \Psi_4(\xi) & = & \psi_1(\xi_1)\,\psi_1(\xi_2) & = & \xi_1\xi_2 \\ \Psi_5(\xi) & = & \psi_0(\xi_1)\,\psi_2(\xi_2) & = & \xi_2^2 - 1 \end{array} \quad \text{etc.}$$

  - The basis functions are orthogonal wrt some weight function
  - The coefficients α_n are fit to the data
- This approach is *nonintrusive* by estimating the coefficients α_n using:
  - Sampling (expectation)
  - Point collocation (regression)
  - Tensor-product quadrature
  - Smolyak sparse grid quadrature
- Wiener-Askey Generalized PCE is an "optimal" form of this method.
  - *Key idea*: use a set of basis functions $\psi_n(\xi)$ that are related to the assumed underlying distribution, leading to exponential convergence
  - E.g., the set of Legendre polynomials $P_n(\xi)$, orthogonal on [-1,1] with weight function unity, are the optimal basis for a uniform distribution

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Stochastic Collocation with Lagrange interpolation uses interpolants for the basis functions.

- Instead of estimating coefficients for known basis functions, form interpolants for known coefficients

$$L_i = \prod_{\substack{j=1 \\ j \neq i}}^{m} \frac{x - x_j}{x_i - x_j}$$

$$R = \sum_{j=1}^{N_p} r_j \boldsymbol{L}_j(\boldsymbol{\xi})$$

$$\boldsymbol{L} = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r\left(\xi_{j_1}^{i_1}, \ldots, \xi_{j_n}^{i_n}\right) \left(L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n}\right)$$

- Form sparse interpolant using sum of tensor products

Same as forming the sparse grid

- Key concept: use the same Gauss points/weights from the orthogonal polynomials for specified input PDFs

Gives the same exponential convergence rates!

- *Advantages relative to PCE:*
  - Simpler (no expansion order)
  - Adapts to integration approach/collocation pts
- *Disadvantages relative to PCE:*
  - Needs structured data sets: quadrature/sparse grid, no random sampling sets (as in PCE)

$$\mu_R = \sum_{j=1}^{N_p} r_j w_j$$

$$\sigma_R^2 = \sum_{j=1}^{N_p} r_j^2 w_j - \mu_R^2$$

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The underlying equations in ALEGRA are related to hyperbolic conservation laws.

- The fundamental equations are statements of conservation laws:

$$\frac{\partial \underbrace{\boxed{U}}_{\text{State}}}{\partial t} + \operatorname{div} \underbrace{\boxed{f(U)}}_{\text{Flux function}} = \underbrace{\boxed{S(U)}}_{\text{Source term}} \quad x \in \Omega \subset \Re^3, \; t \geq 0$$

  - Depending on the physics modeled, the state U may include, e.g.:
    - Internal state variables from material strength models
    - Magnetic field quantities for MHD simulations
  - These are discretized on a hexahedral mesh in the Arbitrary Lagrangian-Eulerian framework, amenable to general meshing and remapping.
- The gas dynamics equations of this study are the simplest "nonlinear physics" equations that are an intrinsic part of the full suite of models in ALEGRA.
- This study is a prototype for the future analysis of more complicated, physics-rich problems.

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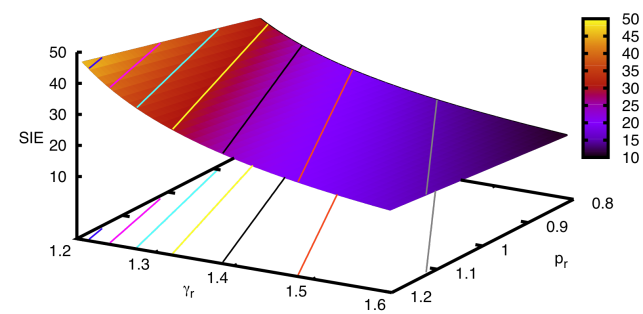
Y1: SIE at x = 1.4
Output surfaces for the Simulation Model

- Y1 is independent of X4.
- For Y1, the exact model and the simulation model are *identical*.

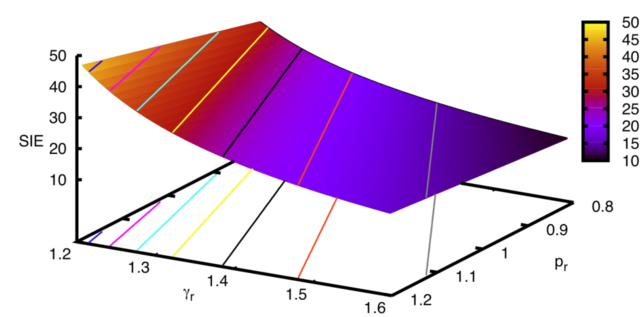
Exact Model

X1, X3 varying
X2 fixed



Simulation Model

X1, X3 varying
X2, X4 fixed



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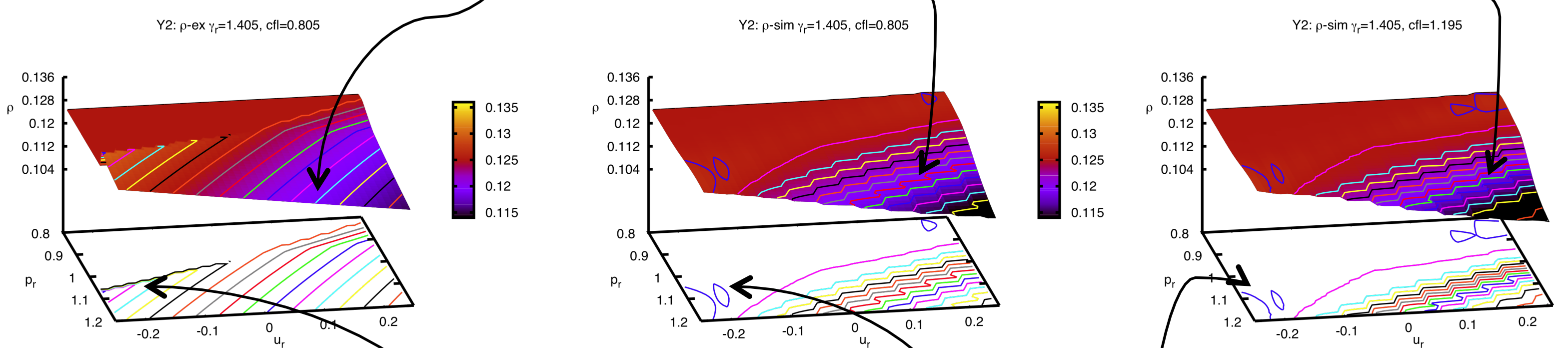
Y2: ρ at x = 1.16
Output surface slices for the Simulation Model

Surface is nosier, noise increases with X4



Exact Model

Simulation Model X4 = 0.805

Simulation Model X4 = 1.195

X1, X2 varying X3, X4 fixed

Shocks are not as sharp

- Compared to the Exact Model, most simulation Model response surfaces show only mild differences

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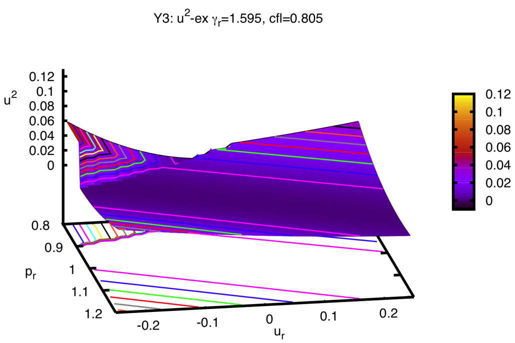
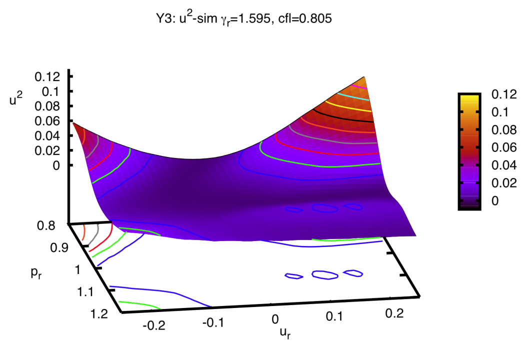
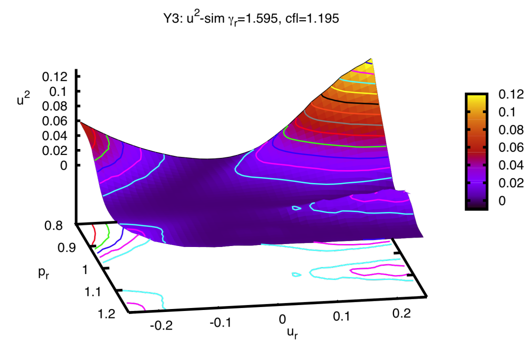
Y3: u^2 at x = 1.16
Output surface slices for the Simulation Model







Exact Model

Simulation Model X4 = 0.805

Simulation Model X4 = 1.195

X1, X2 varying X3, X4 fixed

- Some simulation Model response surfaces show significant differences in values

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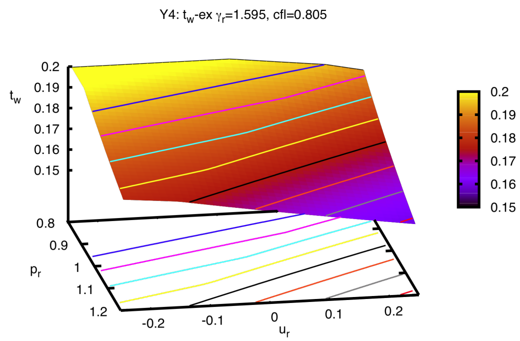
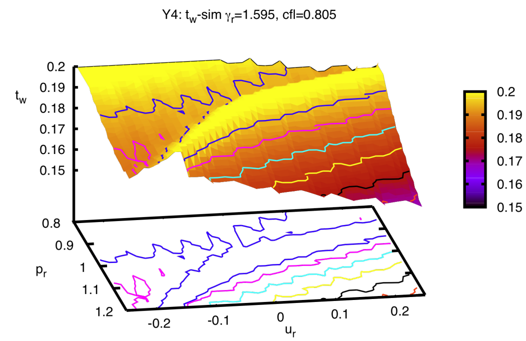
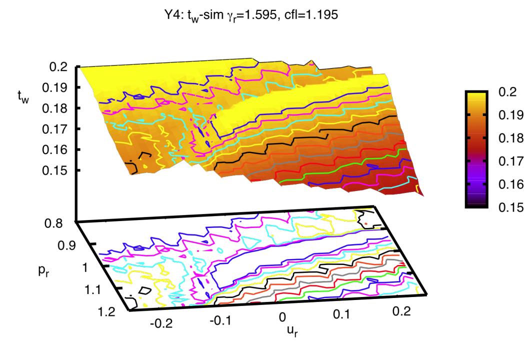
Y4: t_w at x = 1.16
Output surface slices for the Simulation Model



Exact Model



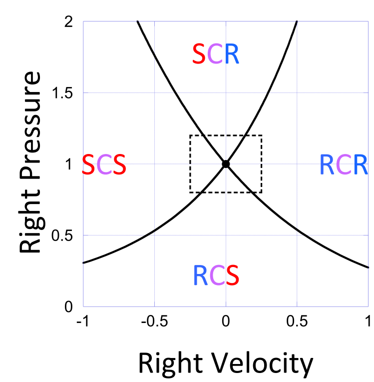
Simulation Model X4 = 0.805



Simulation Model X4 = 1.195

X1, X2 varying X3, X4 fixed

- In a few cases, Simulation Model response surfaces show a different topology than the Exact Model



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The physics suggests that certain outputs should be relatively sensitive to certain inputs.

	Inputs →	X_1	X_2	X_3	X_4
		Init. Right p	Init. Right u	Init. Right γ	CFL
Y_1	Final Right SIE	***STRONG***	NONE	***STRONG***	NONE
Y_2	Final Right ρ	SOME	***STRONG***	SOME	weak
Y_3	Final Right KE	SOME	***STRONG***	SOME	weak
Y_4	Right $\Delta\rho$ time	***STRONG***	SOME	***STRONG***	weak
Y_5	Final Left ρ	weak	SOME	weak	weak
Y_6	Final Left KE	weak	SOME	weak	weak
Y_7	Left $\Delta\rho$ time	SOME	weak	SOME	weak
Y_8	CPU time	NONE	NONE	NONE	SOME

Outputs

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