



Sensitivity Analysis Techniques Applied to a System of Hyperbolic Conservation Laws, Part I

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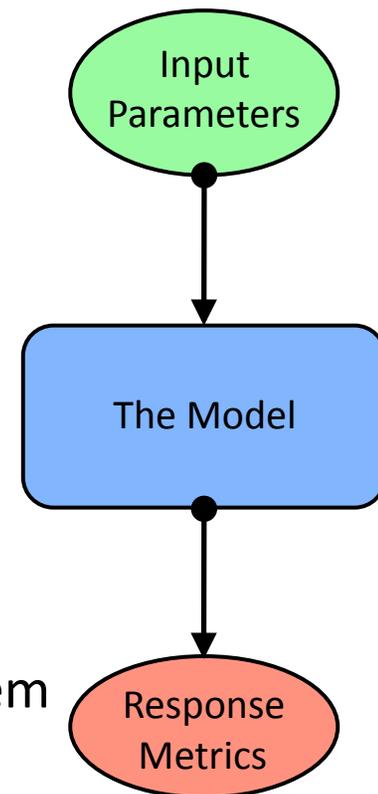
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The Sensitivity Analysis Story

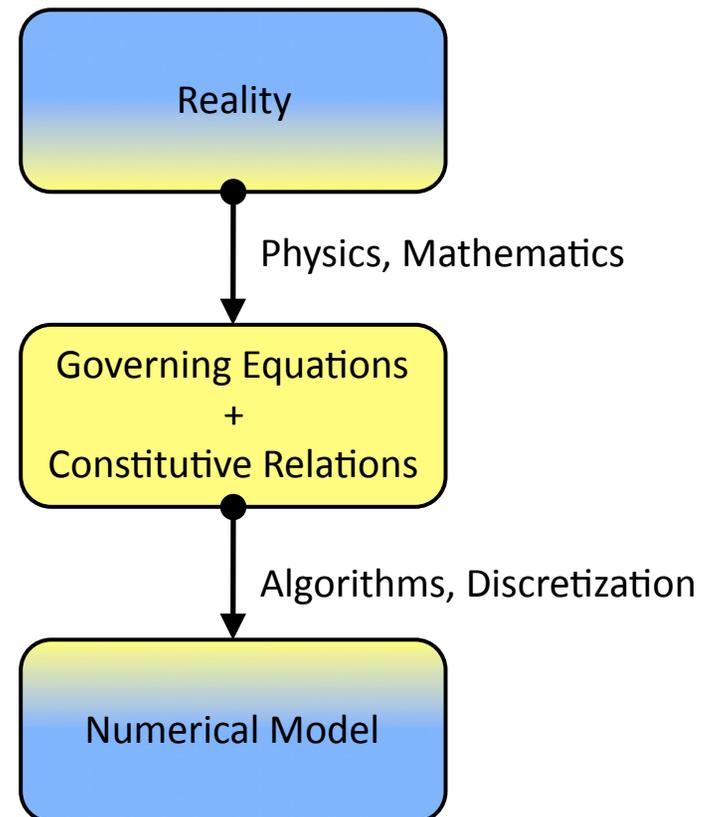
- Our problem of interest has 4 inputs and 8 outputs
- Outputs (responses) have different properties:
 - monotonic vs. non-monotonic
 - smooth vs. discontinuous
 - noisy vs. clean
- We examine different SA techniques:
 - LHS, LP-Tau } sampling
 - PCE } stochastic expansion
 - SDP, ACOSSO, DACE } surrogates
- We compute sensitivity indices and compare them to exact values; in particular, we examine performance with respect to sampling resolution





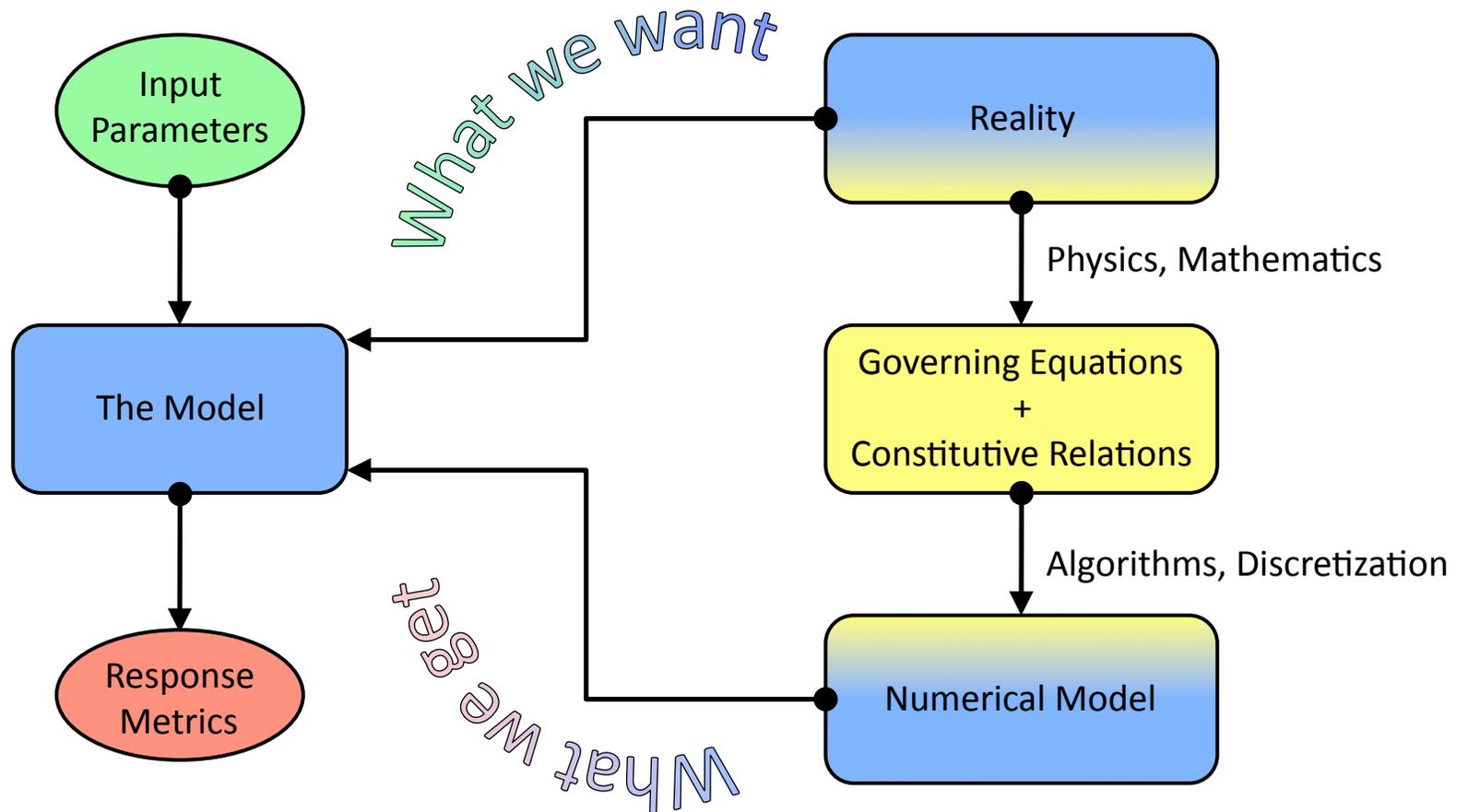
The Application Space Story

- Hyperbolic Conservation Laws are PDEs that describe the conservation of mass, momentum, and energy.
 - Constitutive relations describing specific materials are also required.
 - This combination is a mathematical model of reality.
- We use algorithms to obtain discrete equations from the mathematical model, and solve the discrete equations using a computer.
 - Such simulations provide approximate numerical solutions to the mathematical model.



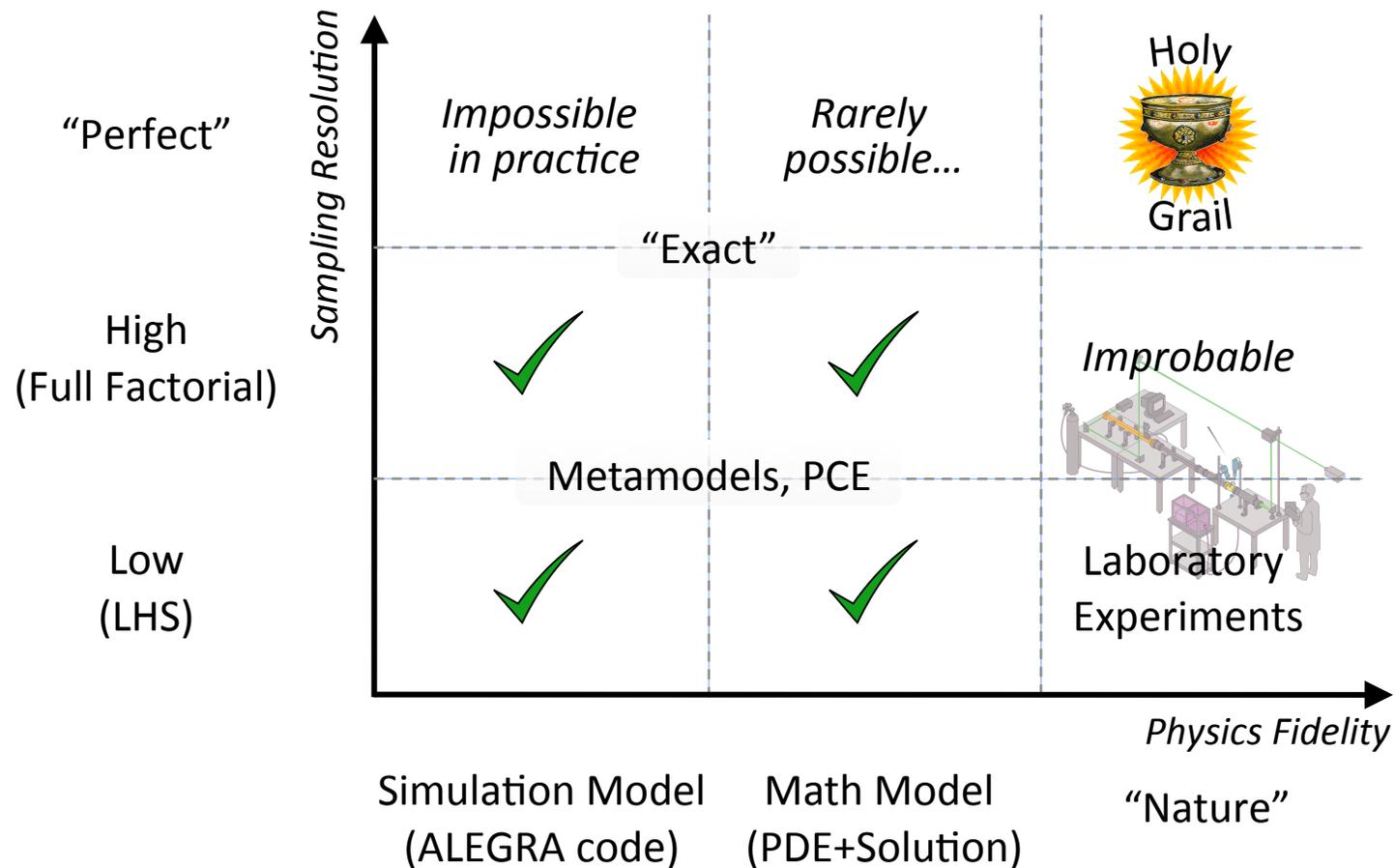


What we get from Sensitivity Analysis of Computer Simulations





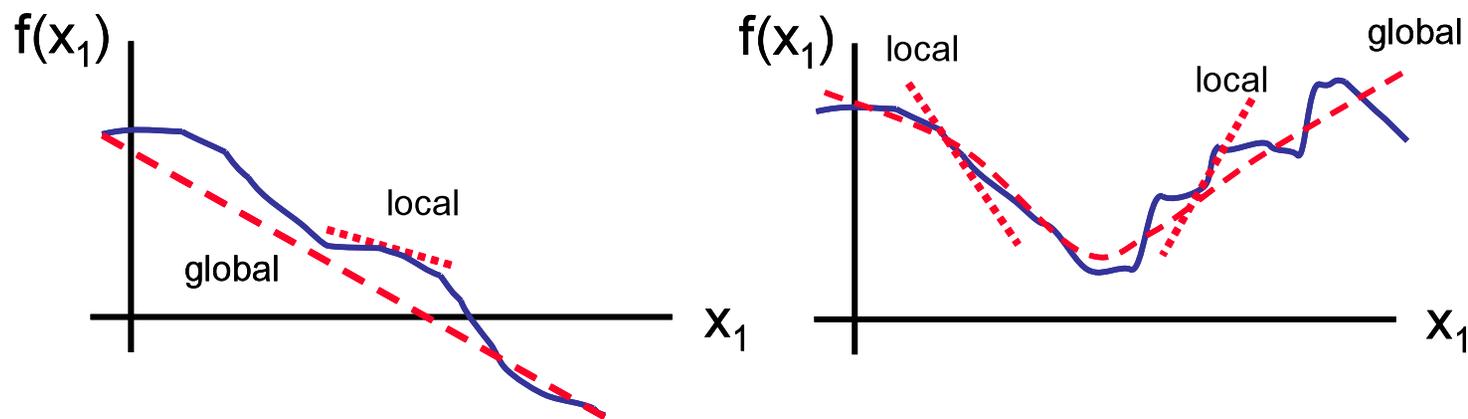
These models and analyses are an attempt to quantify variability of a physical system.





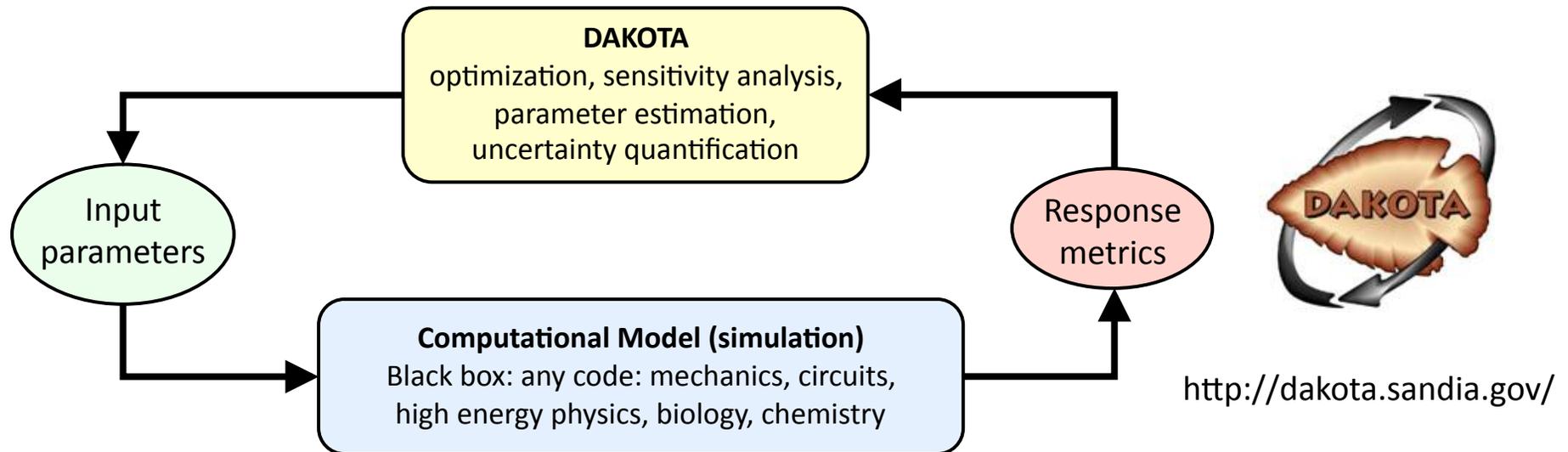
Why Sensitivity Analysis?

- 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.





We conduct sensitivity analyses with DAKOTA.



- 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



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*

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

– 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*

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



I.M. Sobol' developed these ideas

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

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

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



How sensitivity indices are calculated

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

- 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. $E(Y | X_i = x_{ik})$
 - Calculate the variance of this expectation (variance over n values) $\text{Var}(E(Y | X_i))$
- 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 i^{th} column of A and substituting it into B.
 - Y_A , Y_B , and Y_{C_i} 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

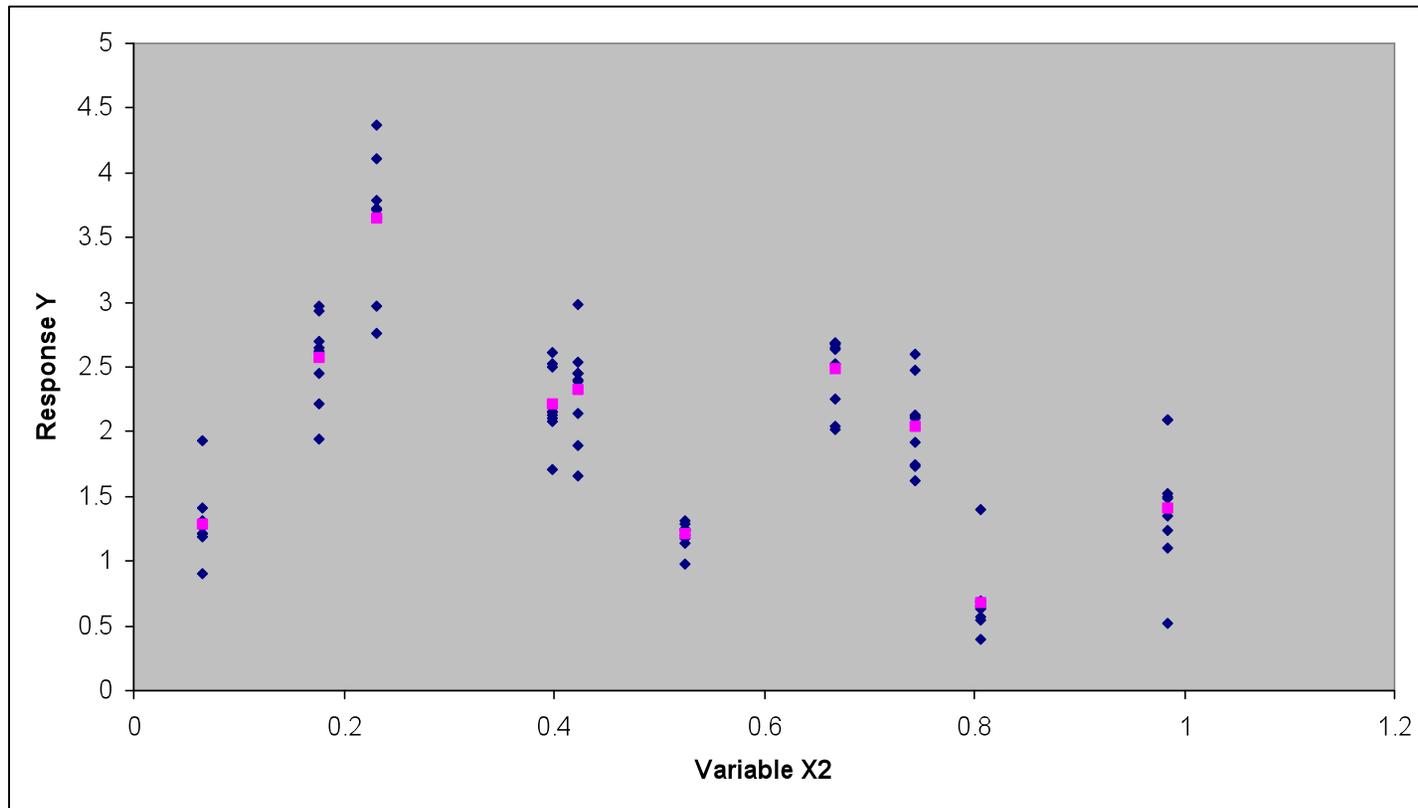
$$f = \frac{Y_A \cdot Y_B}{N}$$
$$\text{estimated var}(Y) = \left(\frac{1}{N-1} Y_A \cdot Y_A \right) - f^2$$

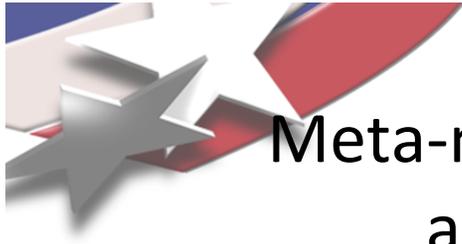
$$S_i = \frac{\left(\frac{1}{N-1} Y_A \cdot Y_{C_i} \right) - f^2}{\text{estimated var}(Y)}$$



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





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)



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 indices 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.



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 :

$$R = \sum_{n=0}^N \alpha_n \psi_n(\xi) \quad \text{such that}$$

$$\begin{aligned} \Psi_0(\xi) &= \psi_0(\xi_1) \psi_0(\xi_2) = 1 \\ \Psi_1(\xi) &= \psi_1(\xi_1) \psi_0(\xi_2) = \xi_1 \\ \Psi_2(\xi) &= \psi_0(\xi_1) \psi_1(\xi_2) = \xi_2 \\ \Psi_3(\xi) &= \psi_2(\xi_1) \psi_0(\xi_2) = \xi_1^2 - 1 \\ \Psi_4(\xi) &= \psi_1(\xi_1) \psi_1(\xi_2) = \xi_1 \xi_2 \\ \Psi_5(\xi) &= \psi_0(\xi_1) \psi_2(\xi_2) = \xi_2^2 - 1 \quad \text{etc.} \end{aligned}$$

- 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



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 flexible 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:

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

- 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 spline analysis of variance models," *Ann. Stat.*, **34**, pp. 2272–2297 (2006).



Hyperbolic conservation laws form the basis of many computational physics investigations.

- Hyperbolic conservation laws are the PDE form of balance laws.
 - For example, the conservation of mass, momentum and energy
- The general form of these equations is given by:

$$\frac{\partial U}{\partial t} + \operatorname{div} f(U) = 0 \quad x \in \Omega \subset \mathbb{R}^d, \quad t \geq 0$$

State → U $f(U)$ → *Flux function*

- The state $U(x,t): \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^n$ is the array of conserved quantities
 - There may be additional constraints or source terms on the RHS
 - Appropriate initial and boundary conditions must also be given
- These equations admit complicated solutions with discontinuities.
 - For example, shock waves are governed by equations of this form
- Here, we consider the conservation laws that govern the 1-D equations for compressible fluid flow.



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

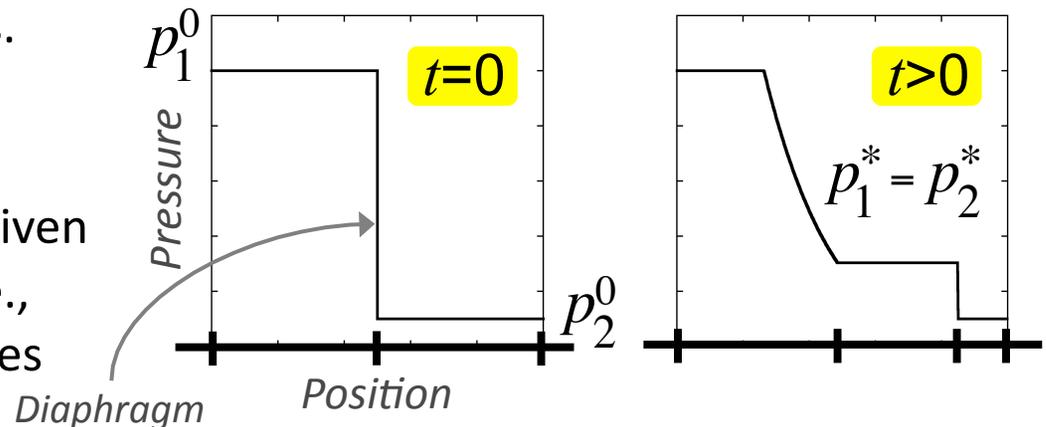
- For 1-D compressible, inviscid, non-heat-conducting flow, the state U and flux f are given by

$$U = [\rho, \rho u, \rho E]^T \quad f = [\rho u, \rho u^2 + p, \rho E u + p u]^T$$

where $E = e + \frac{1}{2}u^2$ 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.



What is the “Riemann Problem”?

- 1D gas dynamics equations: $U_t + f_x(U) = 0$

$$U = [\rho, \rho u, \rho E]^T \quad f = [\rho u, \rho u^2 + p, \rho E u + p u]^T$$

with a an ideal gas EOS:

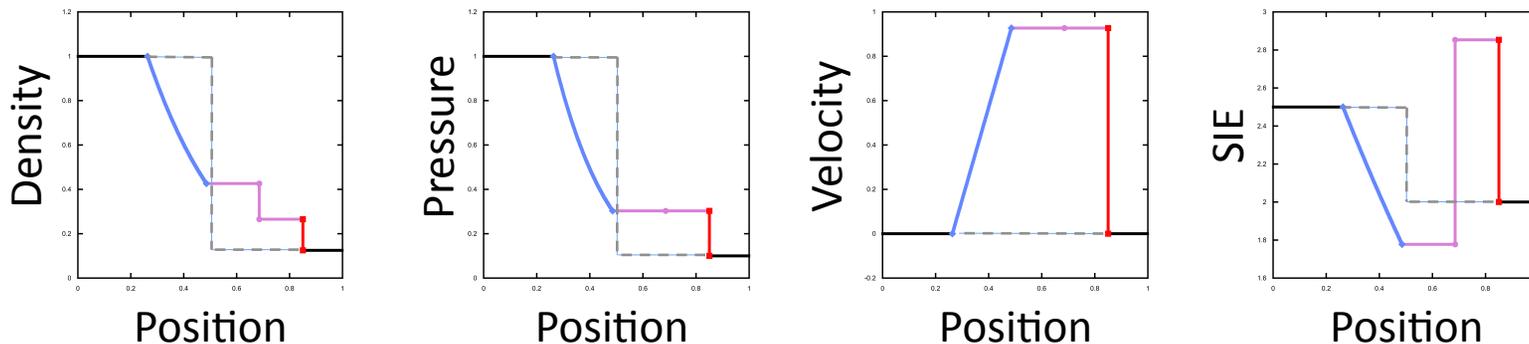
Constitutive model $\rightarrow p = p(\rho, \varepsilon) = (\gamma - 1) \rho \varepsilon$



G.F. Bernhard Riemann
(1826-1866)

- RPs* are the canonical IVP, with two constant initial states, leading to standard solutions:

“the greatest mathematician” — Peter Lax



– Canonical wave structures: **Rarefaction**, **Contact**, **Shock**

*This is a generalization of the concepts introduced by Riemann in “Über die Fortpflanzung ebener Luftwellen von endlicher Schwingungsweite”, *Abh. Königl. Gesell. Wiss. Göttingen, Math.-phys. Klasse*, **8**, pp. 43–65 (1860).

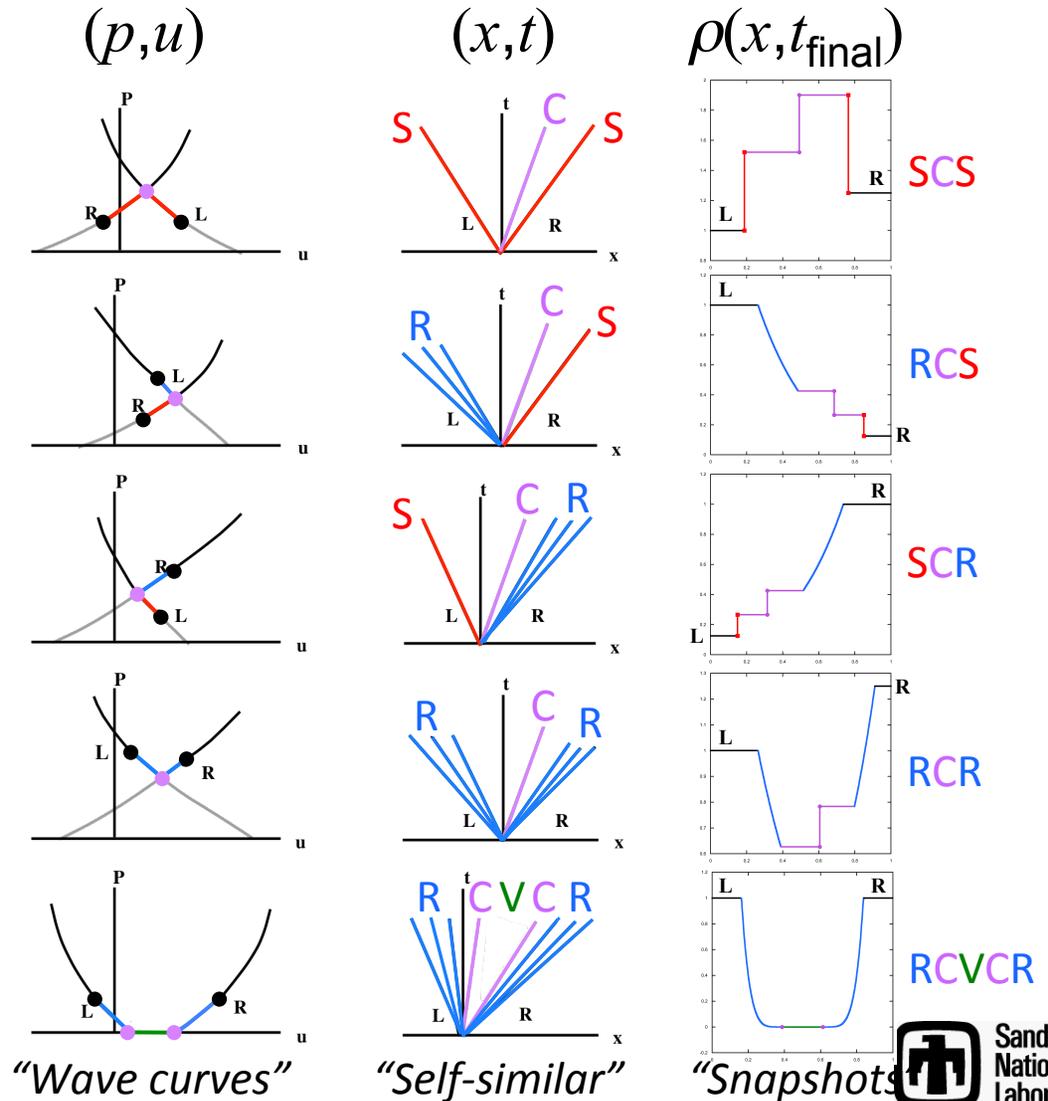


The Riemann problem can have *very different* solutions, depending on the initial conditions.

- 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)

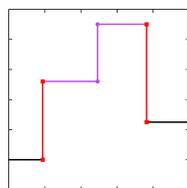
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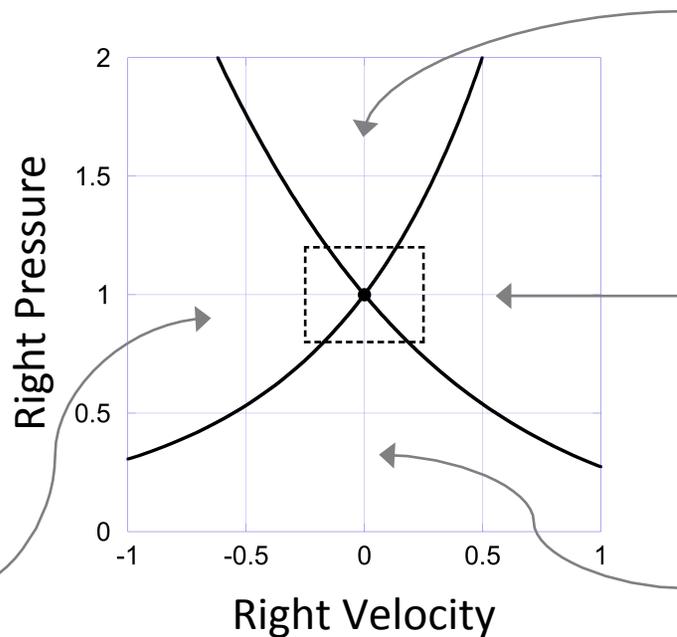


We focus on sensitivity analysis for a single problem, related to the well-known Sod shock tube.

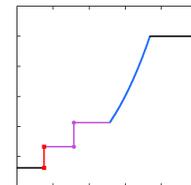
- Initial state: $(\rho, p, u, \gamma) = \begin{cases} (1.0, 1.0, 0.0, 1.4), & 0 \leq x < 0.5 \text{ "Left"} \\ (0.125, 1.0, 0.0, 1.4), & 0.5 < x \leq 1.0 \text{ "Right"} \end{cases}$
- Fix the left state; vary the right state; consider fixed $t_{\text{final}} = 0.2$
- The solution structure varies significantly near the initial point (\bullet).
- Evaluate the sensitivity near that point.



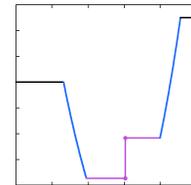
Shock
Contact
Shock



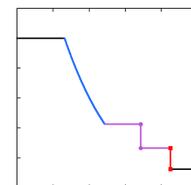
Shock
Contact
Rarefaction



Rarefaction
Contact
Rarefaction



Rarefaction
Contact
Shock



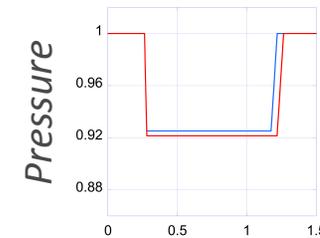
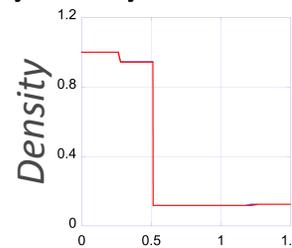
Sod G., : "A Survey of Several Finite Difference Methods for Systems of Nonlinear Hyperbolic Conservation Laws", *J. Comput. Phys.*, **27**, pp. 1–31 (1978).



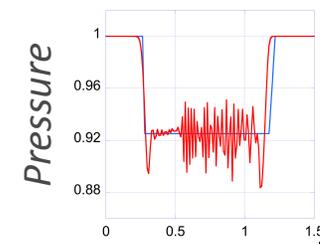
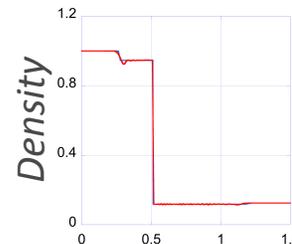
We fix the final time and the left state, but vary both the right state and a numerical parameter.

	<i>Input</i>	<i>Why?</i>
} <i>Right</i>	X_1 Initial pressure on right	Uncertainty in initial condition
	X_2 Initial velocity on right	Uncertainty in initial condition
	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 $\gamma \rightarrow$ higher sound speeds and faster wave propagation
- $0 < CFL < 1 \rightarrow$ stable
 $CFL > 1 \rightarrow$ unstable



Nominal
High γ



Nominal
High CFL



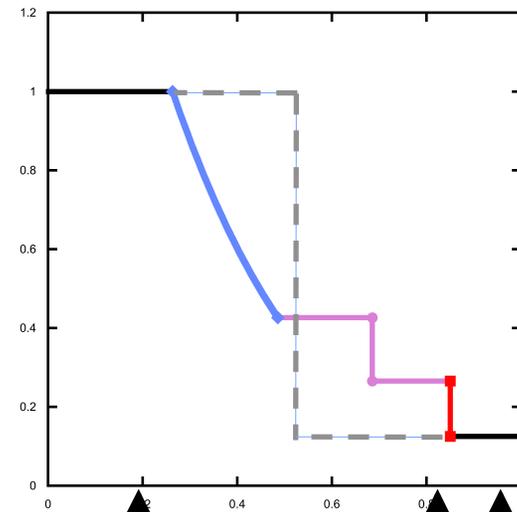
Most of our responses are from probes

- 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





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

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

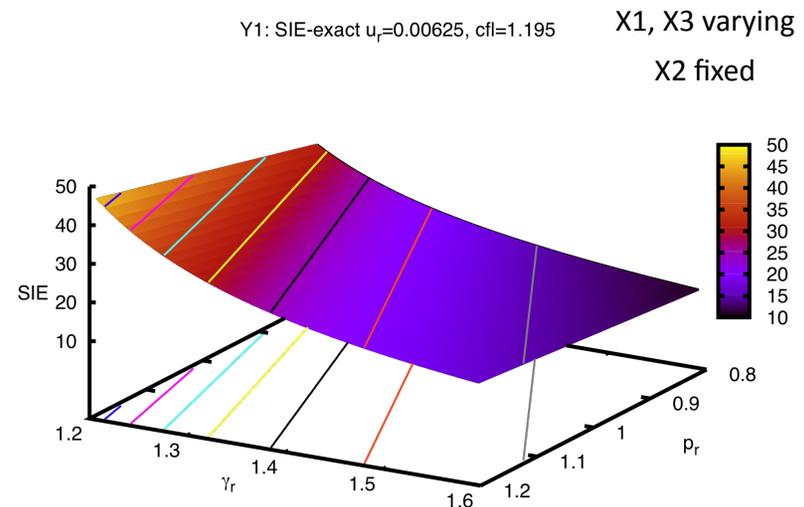
- Shock-Physics analysts think of the problem in these terms



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

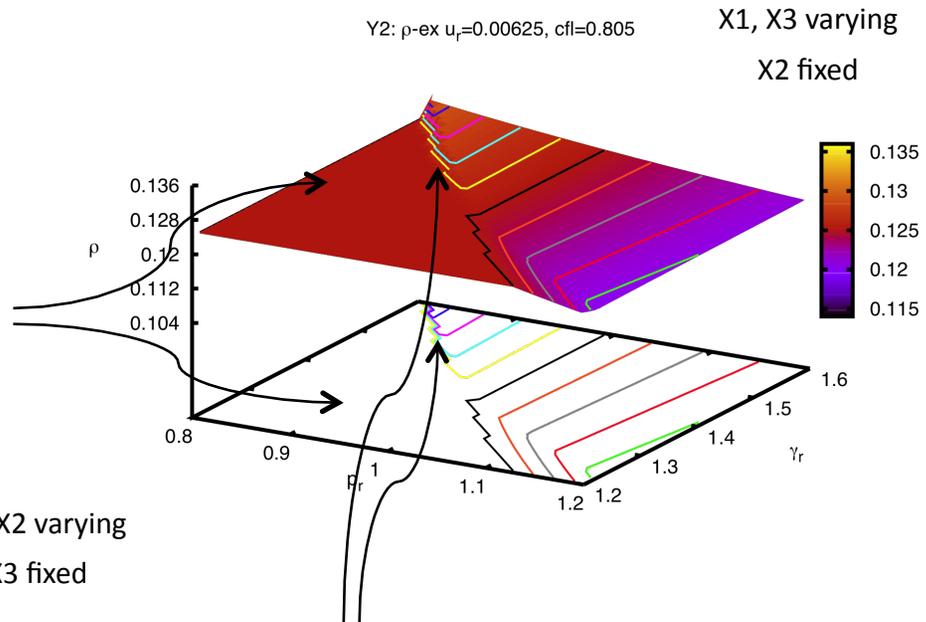




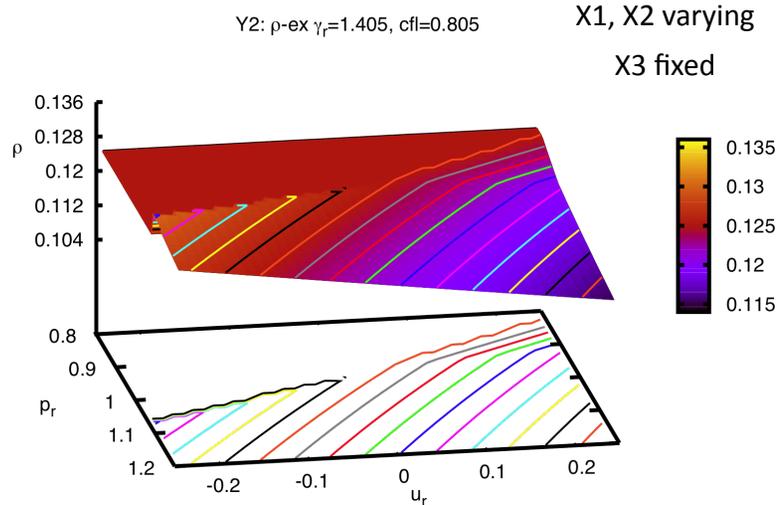
Y2: ρ at $x = 1.16$

Output surface slices for the Exact Model

Flat plateaus indicate no waves have reached this location



Sharp jumps indicate shocks

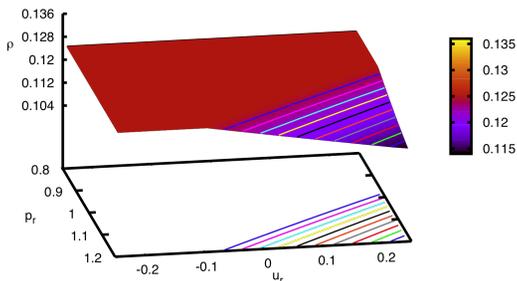




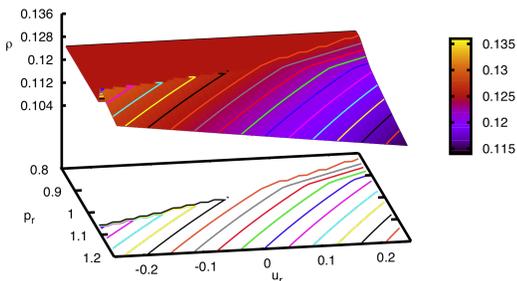
Y2: ρ at $x = 1.16$

Output surface slices for the Exact Model

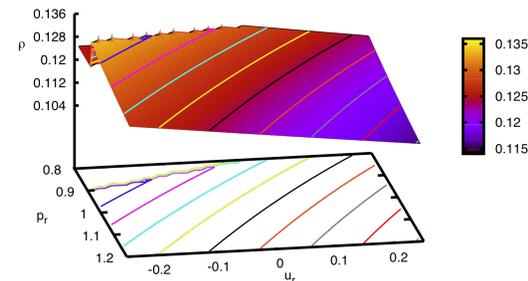
Y2: ρ -ex $\gamma_r=1.205$, cfl=0.805



Y2: ρ -ex $\gamma_r=1.405$, cfl=0.805



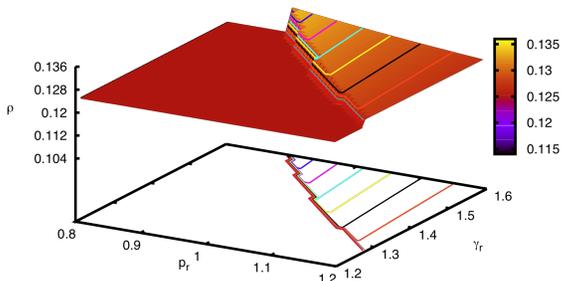
Y2: ρ -ex $\gamma_r=1.595$, cfl=0.805



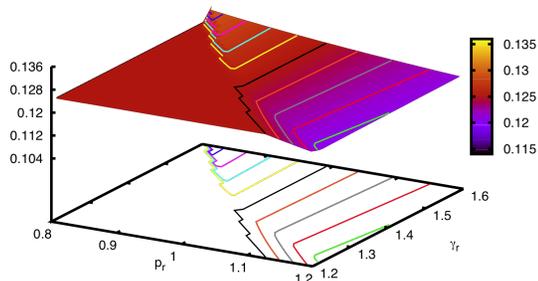
X3 increasing

X1, X2 varying
X3 fixed

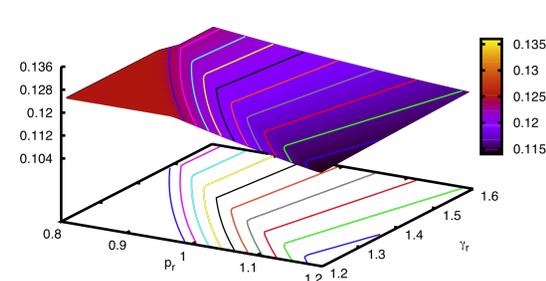
Y2: ρ -ex $u_r=-0.24375$, cfl=0.805



Y2: ρ -ex $u_r=0.00625$, cfl=0.805



Y2: ρ -ex $u_r=0.24375$, cfl=0.805



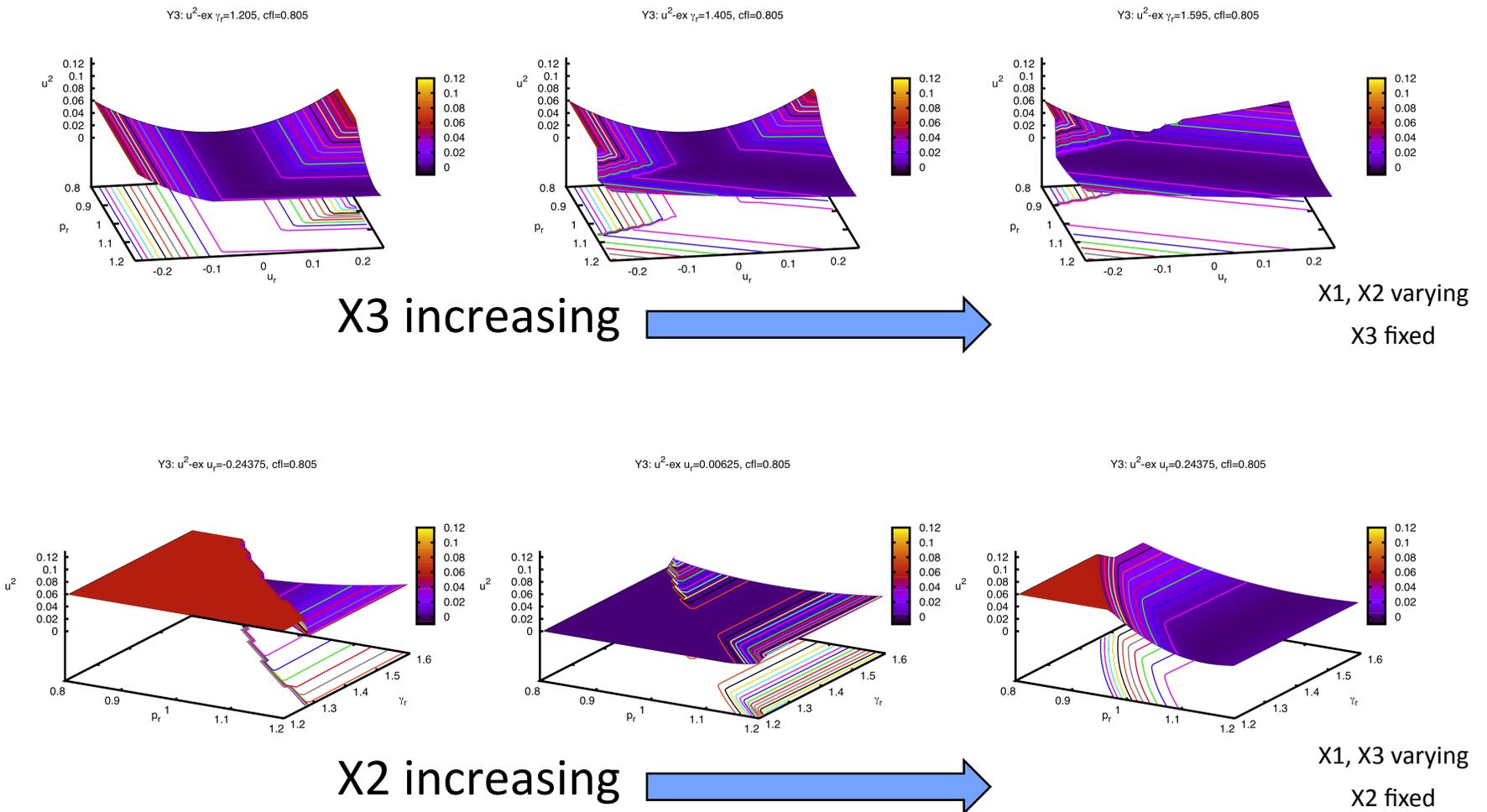
X2 increasing

X1, X3 varying
X2 fixed



Y3: u^2 at $x = 1.16$

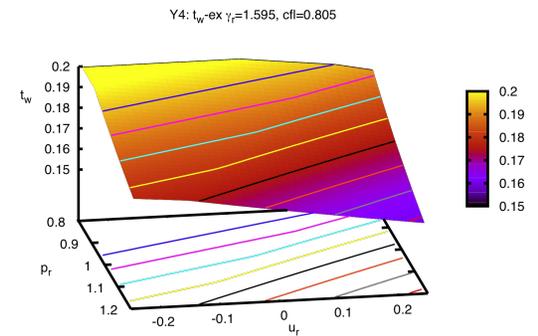
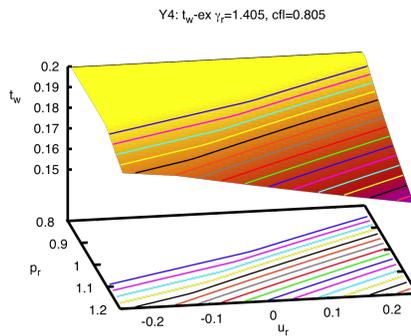
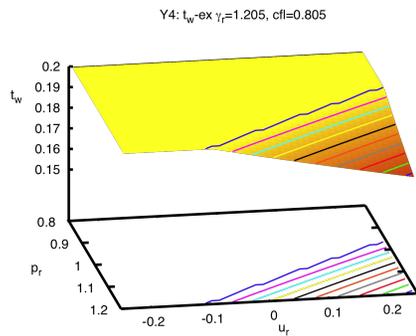
Output surface slices for the Exact Model





Y4: t_w at $x = 1.16$

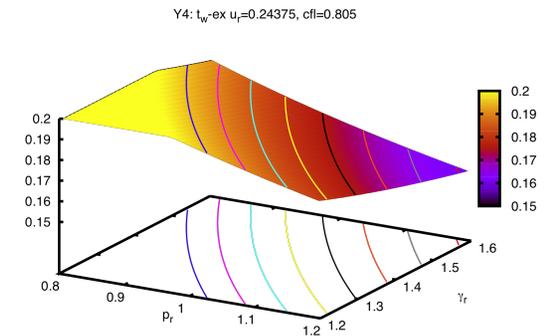
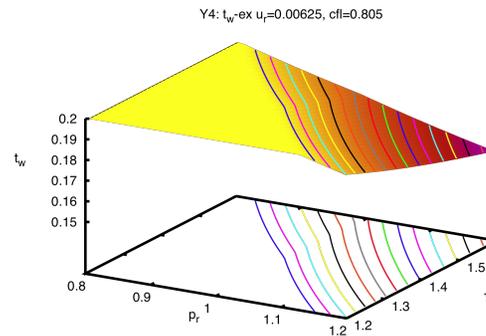
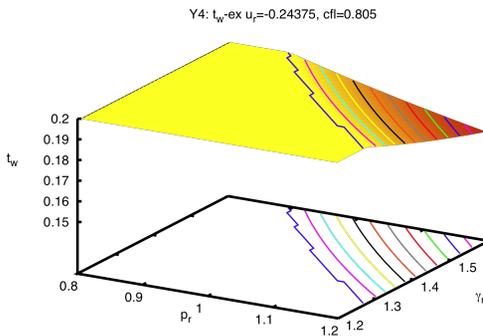
Output surface slices for the Exact Model



X3 increasing

X1, X2 varying
X3 fixed

Plateaus:
Simulations end
at $t=0.2$.



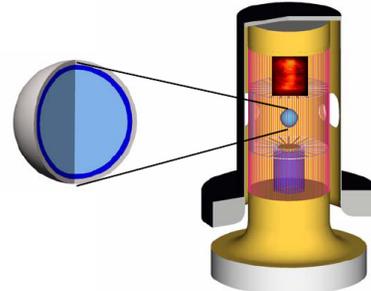
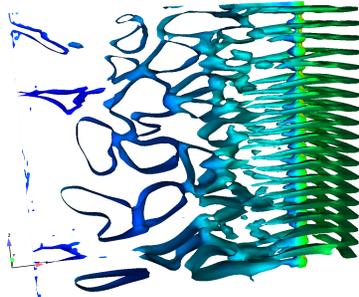
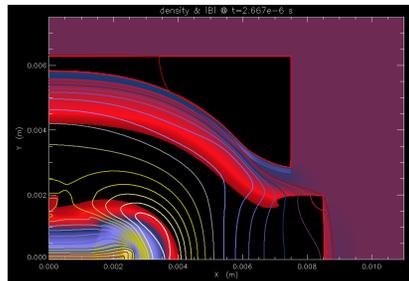
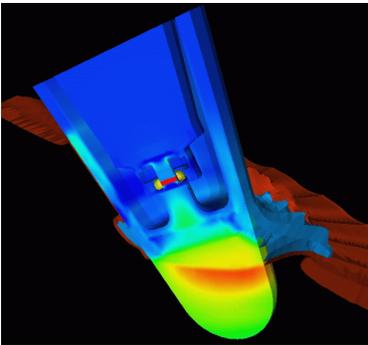
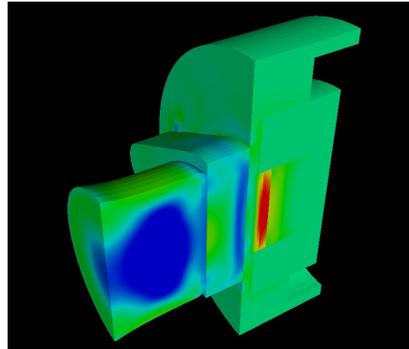
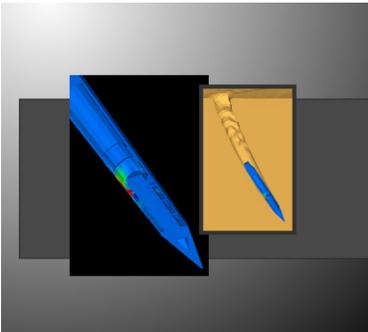
X2 increasing

X1, X3 varying
X2 fixed



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

Shock and Multi-physics HEDP Theory and ICF Target Design

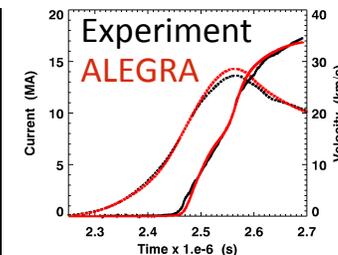
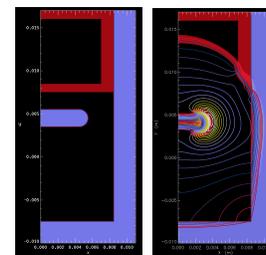


Overview

- 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



SAND2010-4561C

Isentropic Compression: Magnetic Flyer Prediction vs. Experiment





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

- The fundamental equations are statements of conservation laws:

$$\frac{\partial U}{\partial t} + \operatorname{div} f(U) = S(U) \quad x \in \Omega \subset \mathbb{R}^3, \quad t \geq 0$$

State → U $f(U)$ → *Flux function* $S(U)$ → *Source term*

- 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.

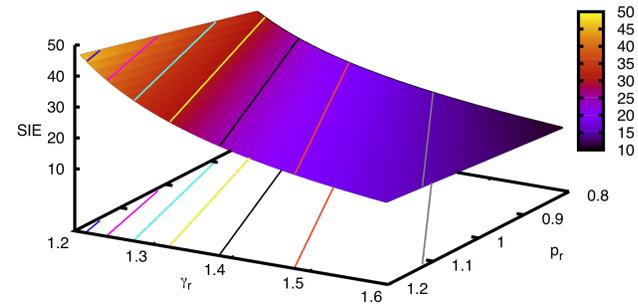


Y1: SIE at $x = 1.4$

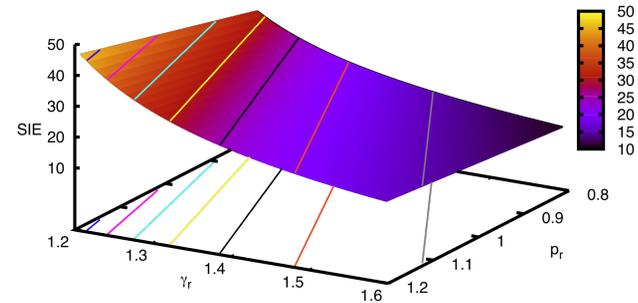
Output surfaces for the Simulation Model

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

Exact Model
Y1: SIE-exact $u_r=0.00625$, $cfl=1.195$
X1, X3 varying
X2 fixed



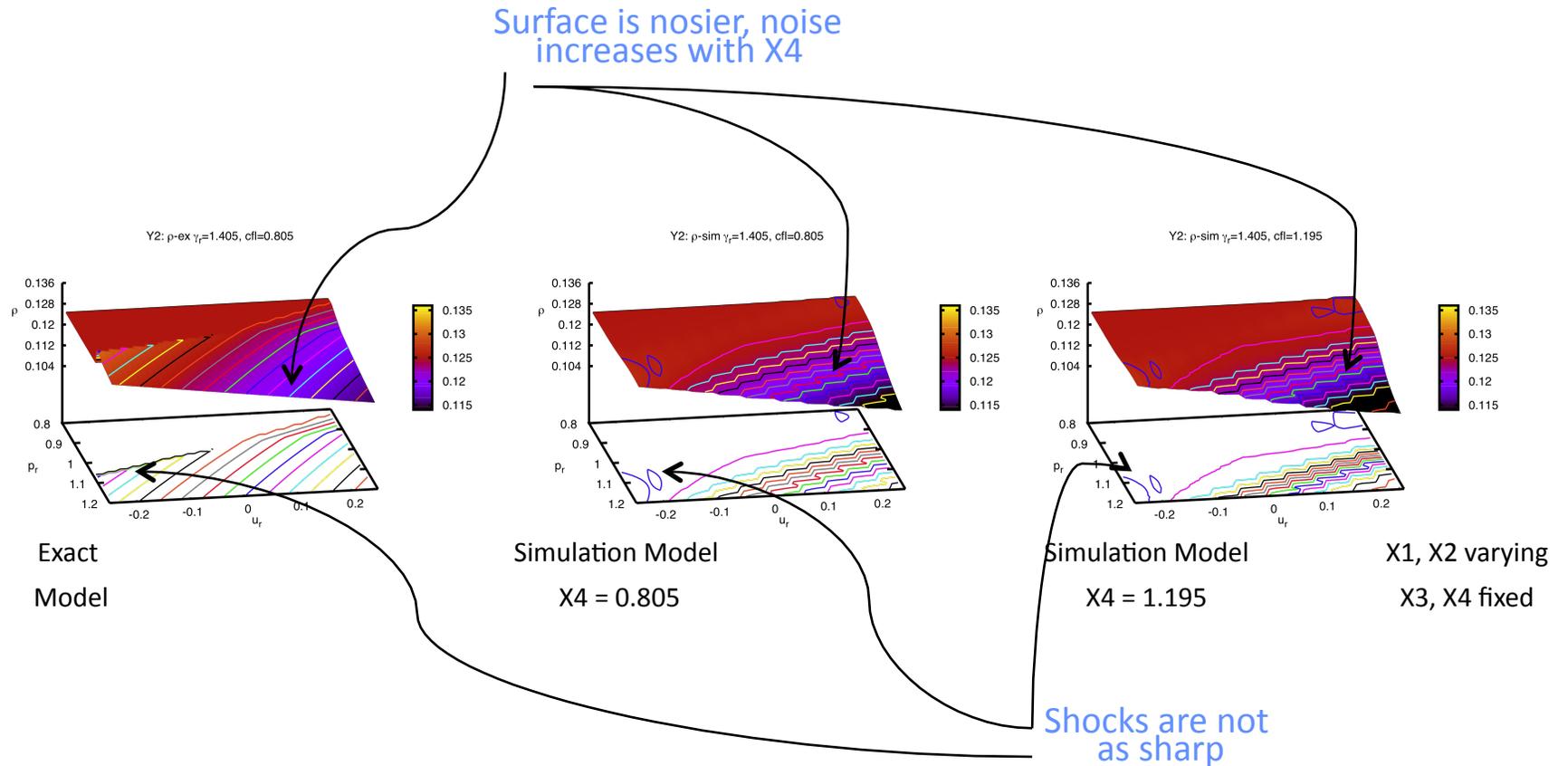
Simulation Model
Y1: SIE-sim $u_r=0.00625$, $cfl=1.195$
X1, X3 varying
X2, X4 fixed





Y2: ρ at $x = 1.16$

Output surface slices for the Simulation Model

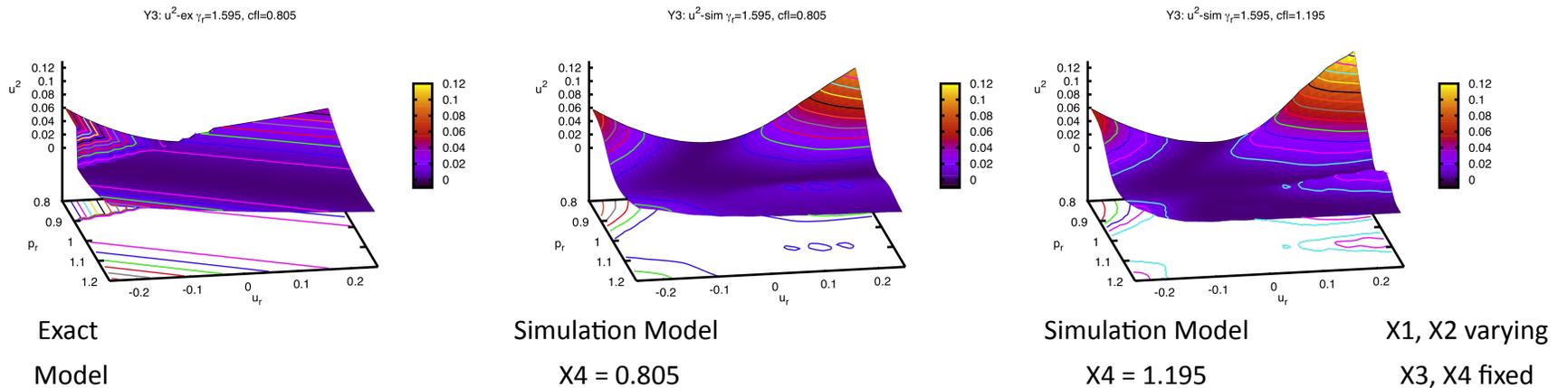


- Compared to the Exact Model, most simulation Model response surfaces show only mild differences



Y3: u^2 at $x = 1.16$

Output surface slices for the Simulation Model

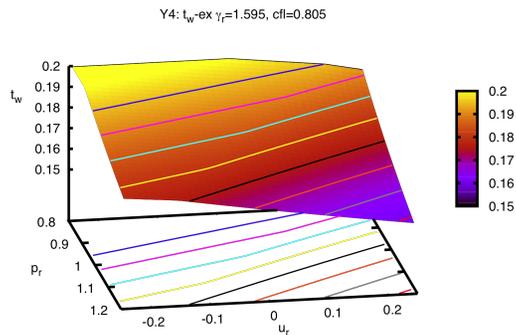


- Some simulation Model response surfaces show significant differences in values

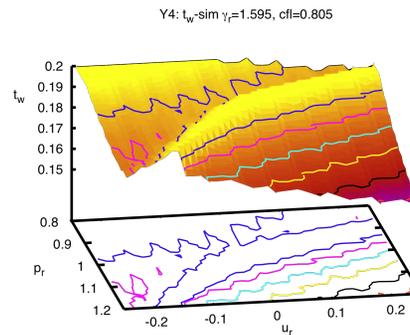


Y4: t_w at $x = 1.16$

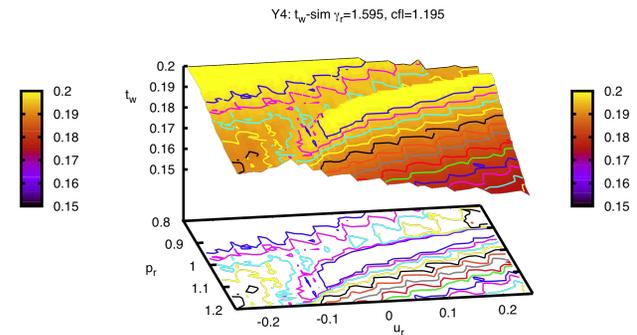
Output surface slices for the Simulation Model



Exact
Model

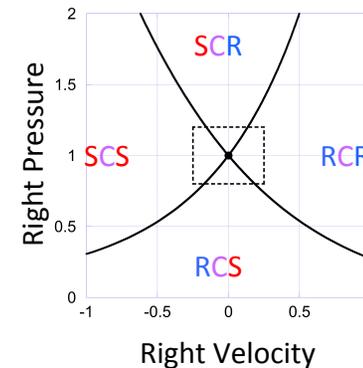


Simulation Model
 $X4 = 0.805$



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





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



These outputs have different characteristics.

		<i>Monotonicity</i>	<i>Continuity</i>	<i>“SNR”</i>	
<i>Outputs</i>	Y_1	Final Right SIE	Monotonic	<i>Continuous</i>	CLEAN
	Y_2	Final Right ρ	Non-monotonic	DISCONTINUOUS	NOISY
	Y_3	Final Right KE	Non-monotonic	DISCONTINUOUS	NOISY
	Y_4	Right $\Delta\rho$ time	Non-monotonic	DISCONTINUOUS	NOISY
	Y_5	Final Left ρ	Non-monotonic	DISCONTINUOUS	NOISY
	Y_6	Final Left KE	Non-monotonic	DISCONTINUOUS	NOISY
	Y_7	Left $\Delta\rho$ time	Non-monotonic	DISCONTINUOUS	NOISY
	Y_8	CPU time	Non-monotonic	DISCONTINUOUS	NOISY

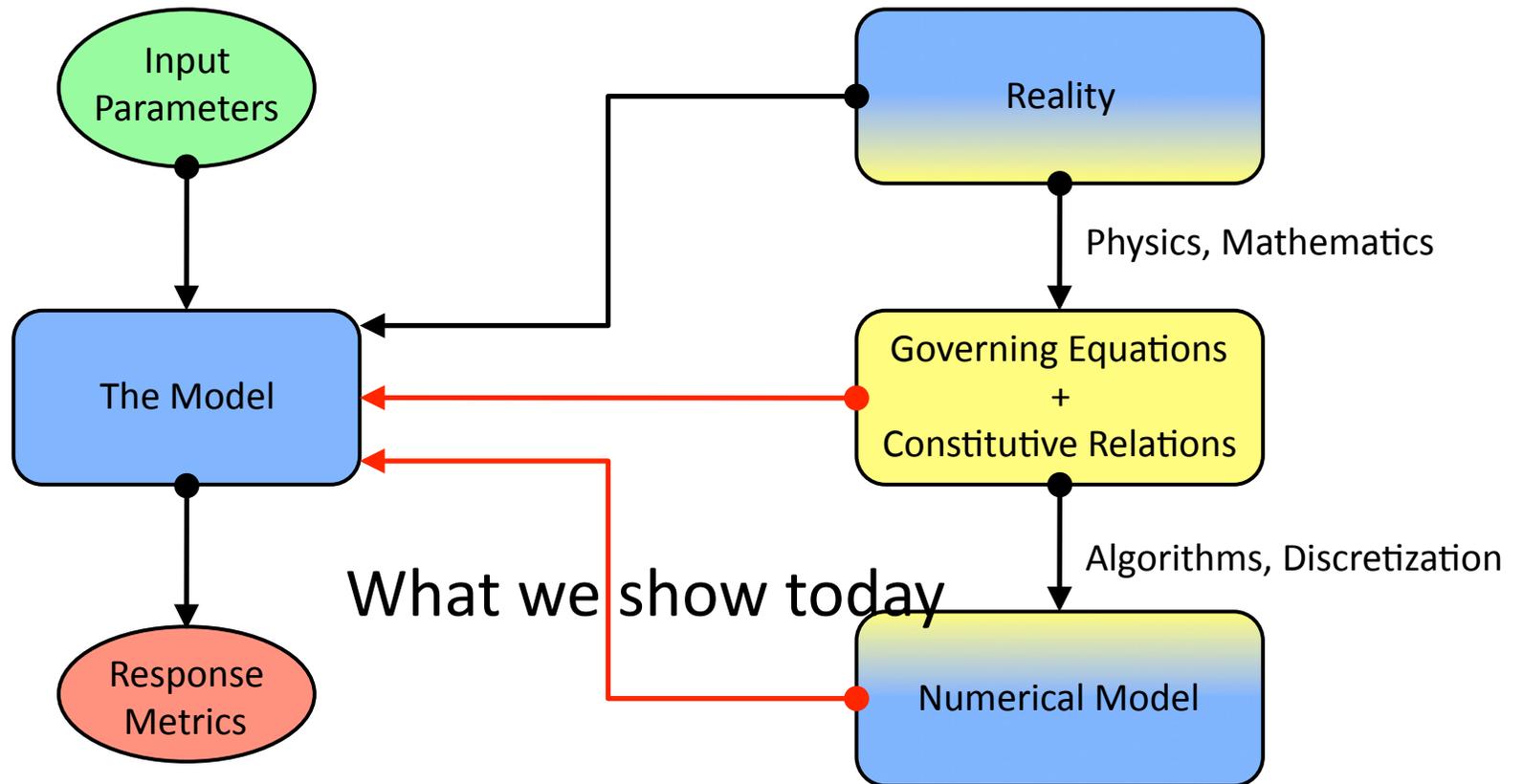


The physics suggests that certain outputs should be relatively sensitive to certain inputs.

		<i>Inputs</i> →	X_1	X_2	X_3	X_4
			Init. Right p	Init. Right u	Init. Right γ	CFL
Outputs	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



What we get from Sensitivity Analysis of Computer Simulations



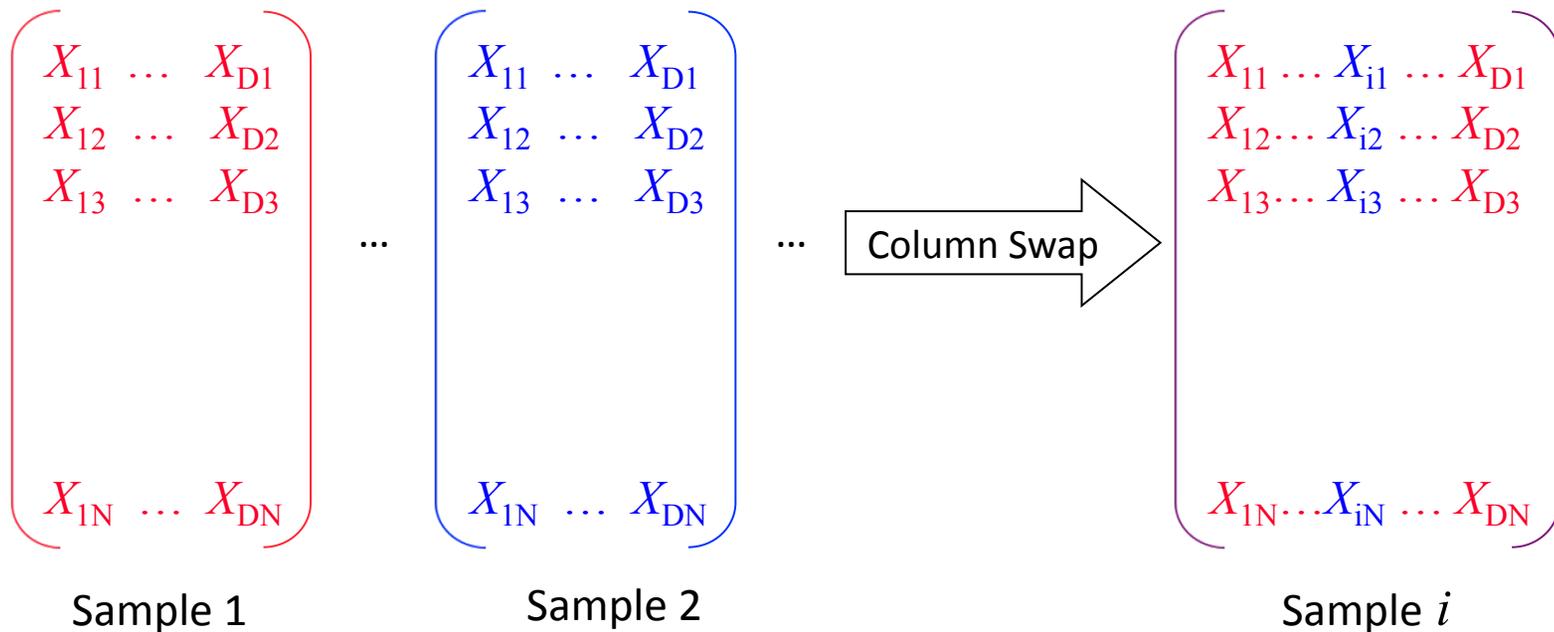


Backup Slides



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.





A simple example shows the effect of stochastic expansion versus sampling for VBD sensitivity indicators.

- We calculate the main effect sensitivity indices $S_i, i = 1, 2$, for the function:

$$f = x_1^2 - \frac{x_2}{2}$$

VBD Approach	Func Evals	S1	S2
LHS	400	0.811961	0.188291
LHS	4000	0.815006	0.195046
LHS	400000	0.809877	0.190123
PCE	4	0.8	0.2
PCE	16	0.810127	0.189873
PCE	64	0.810127	0.189873
SC	4	0.8	0.2
SC	16	0.810127	0.189873
SC	64	0.810127	0.189873
TRUE		0.810127	0.189873

Lots of evaluations } (points to LHS rows)

Very few evaluations } (points to PCE and SC rows)

Still not correct... (points to LHS rows)

Pretty good! (points to PCE and SC rows)

Exact value (points to TRUE row)

- Of course, there is overhead to set up the expansions.
 - The bigger the problem, the greater the advantage for SE...



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

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

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

$$\mathbf{L} = \sum_{j_1=1}^{m_{i_1}} \cdots \sum_{j_n=1}^{m_{i_n}} r(\xi_{j_1}^{i_1}, \dots, \xi_{j_n}^{i_n}) (L_{j_1}^{i_1} \otimes \cdots \otimes L_{j_n}^{i_n})$$

- 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)

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

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

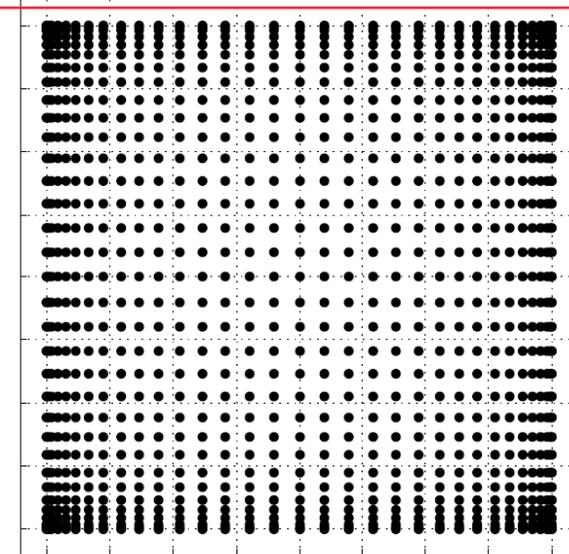


PCE/SC Expansions: Tensor Product Quadrature

- Numerical integration: tensor-product quadrature:

$$\mathcal{U}^i(f)(\xi) = \sum_{j=1}^{m_i} u(\xi_j^i) w_j^i$$

- Evaluate response at every combination of 1-D integration rules
- Weights for each point are product of 1-D weights
- Scales as m^n
- 1-D Gaussian rule of order m exactly integrates any polynomial up to order $2m - 1$
- Assuming RY_j of order $2p$, select $m = p + 1$



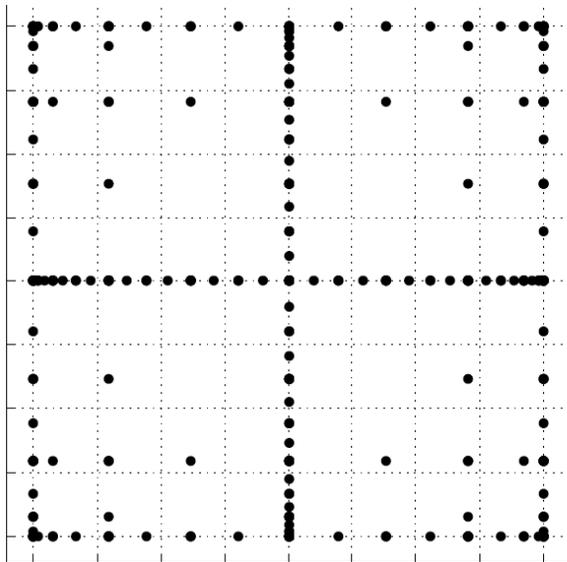
Clenshaw-Curtis tensor-product



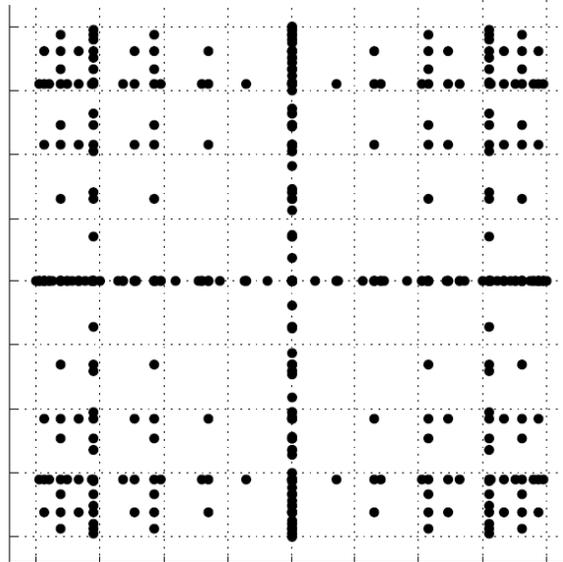


PCE/SC Expansions: Numerical Integration with Smolyak Sparse Grids

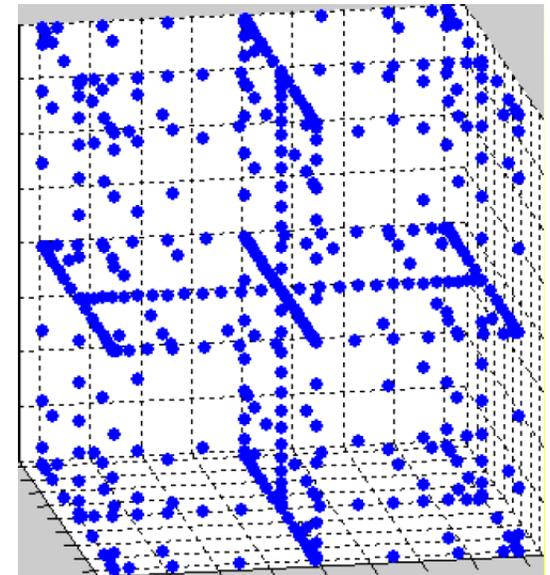
$$\mathcal{A}(w, n) = \sum_{|\mathbf{i}| \leq w+n} (\Delta^{i_1} \otimes \dots \otimes \Delta^{i_n}) \quad \text{for } \boxed{\phantom{\text{[]}}}$$



2D Clenshaw-Curtis sparse grid
(less optimal, more nesting)



2D Gauss-Legendre sparse grid
(more optimal, less nesting)



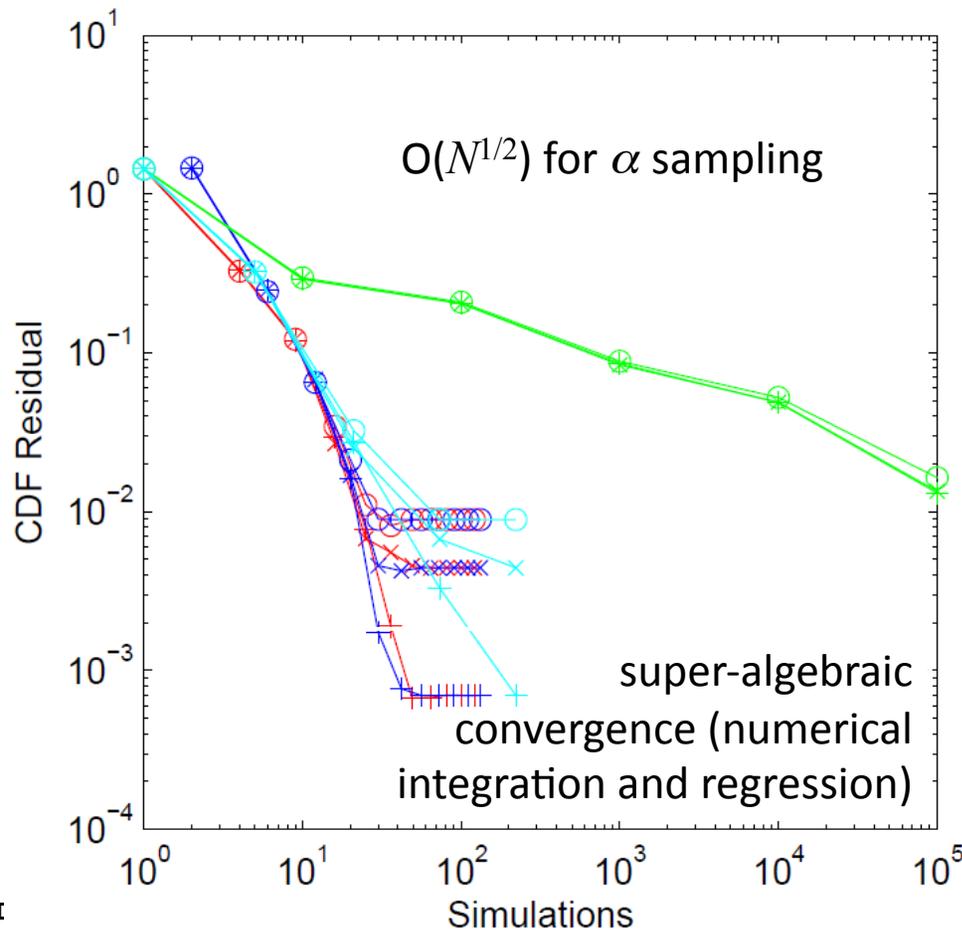
3D Clenshaw-Curtis sparse grid



Performance of traditional (total-order) PCE

$$g(\mathbf{x}) = \frac{x_1}{x_2}$$

x_1, x_2 are $\text{Log}N(1, 1/2)$ with $\rho_{1,2} = 0.3$



- quad $m = 1-11$, 10^4 CDF samples
- ×— quad $m = 1-11$, 10^5 CDF samples
- +— quad $m = 1-11$, 10^6 CDF samples
- pt colloc ratio = 2, 10^4 CDF samples
- ×— pt colloc ratio = 2, 10^5 CDF samples
- +— pt colloc ratio = 2, 10^6 CDF samples
- exp samples, $p = 10$, 10^4 CDF samples
- ×— exp samples, $p = 10$, 10^5 CDF samples
- +— exp samples, $p = 10$, 10^6 CDF samples
- sparse $w = 0-4$, 10^4 CDF samples
- ×— sparse $w = 0-4$, 10^5 CDF samples
- +— sparse $w = 0-4$, 10^6 CDF samples