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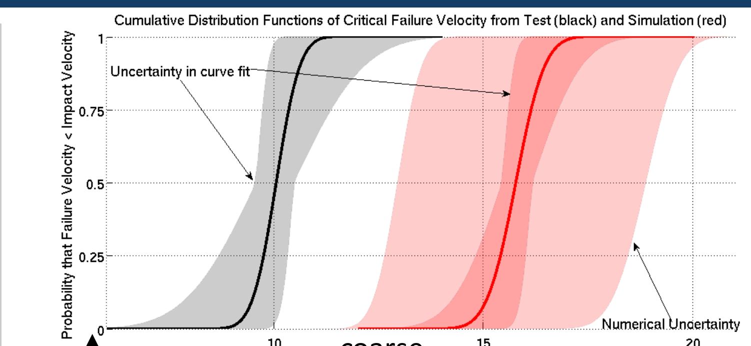

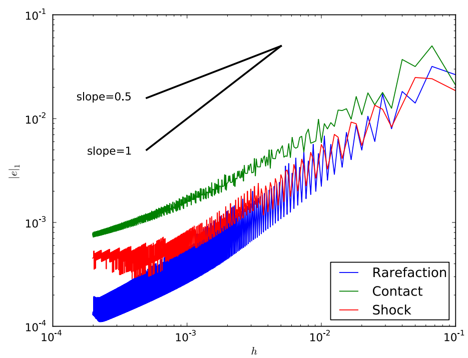

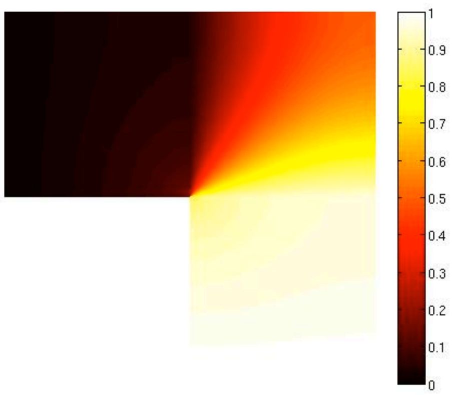

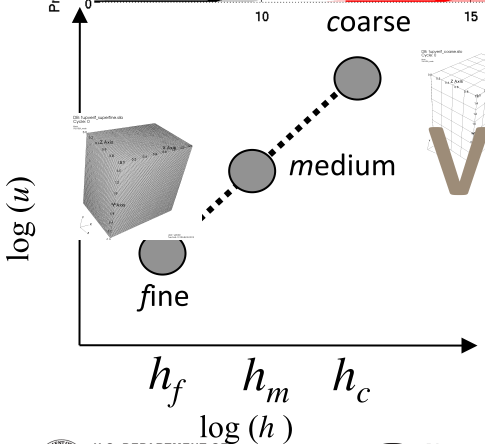

Verification and Model Selection

Bill Rider, WCCM, Barcelona July 21, 2014

U.S. DEPARTMENT OF ENERGY
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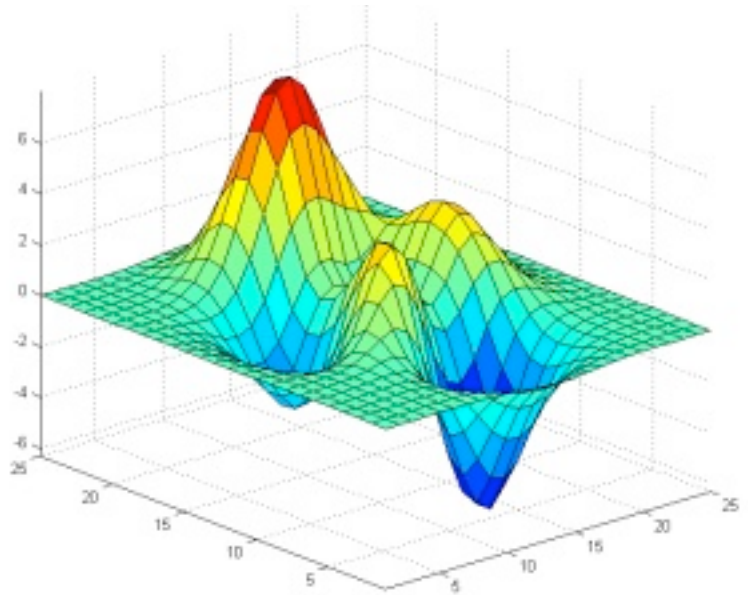
What verification means in numerical analysis!

"For the numerical analyst there are two kinds of truth; the truth you can prove *and the truth you see when you compute*." – Ami Harten



Code Verification vs. *Solution* Verification

Code Verification:

- You have an exact solution, so you compute exact errors
- You are testing your code (implementation, algorithm)
- Hard estimates of convergence properties
- Metrics are defined by numerical analysis

Solution Verification:

- You don't have an exact solution, you estimate numerical errors
- You test your solution(s)
- Soft estimates of numerical error
- **Metrics are defined by the analyst** – integrated quantities, point values, functionals of the solution

The Standard Setting For Calculation Verification: Richardson extrapolation for error estimation

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- We begin with the standard error form,

$$\tilde{u} = u_h + A h^p$$

- **Mesh converged solution, i.e., h→0** ($\tilde{u}$)
- Computed solution on mesh of char'c size h (u_h)
- **Prefactor** (A)
- Characteristic length scale of mesh cell, "Δx" (h)
- **Convergence rate** (p)

- The standard safety factor gives an uncertainty estimate (the *GCI**):

$$\delta = \tilde{u} - u_f \qquad U_{num} = F_s \left|\delta\right| ; F_s = 1.25$$

- This safety factor gives an ostensible 95% confidence interval,
  - ~2 std. dev. from CFD "experience" and computational experiments.
- Other forms will provide different estimates of F_s.
- For two grids, no estimate for δ is possible, and the uncertainty is intentionally "generous": $U_{num} = F_s \left|u_f - u_c\right| ; F_s = 3$

* GCI: Grid Convergence Index, i.e., Roache's approach

Error bars are subject to interpretation

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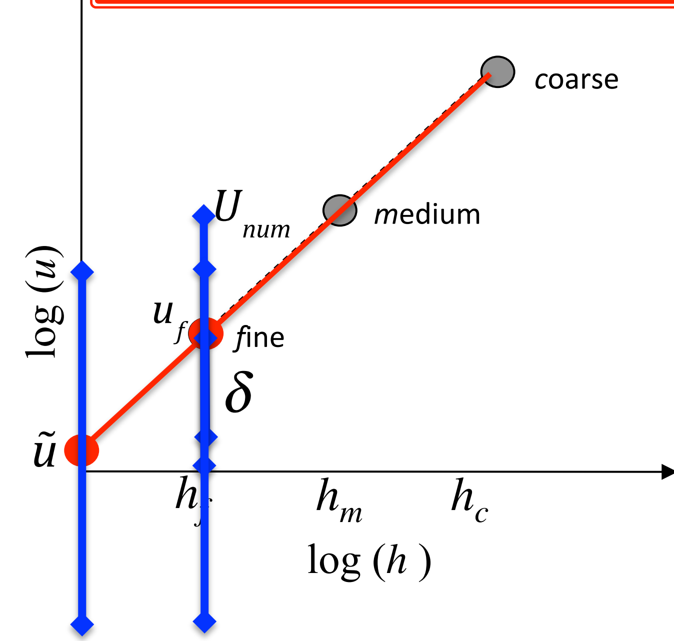
$$\delta = \tilde{u} - u_f \qquad\qquad U_{num} = F_s\left|\delta\right|; F_s = 1.25$$

Where should the error bar be placed (i.e., centered)?

- We have choices (two examined here):
  - Around the finest grid solution
  - Around the mesh converged solution
  - **The mesh converged solution is a best estimate and should define error.**
  - Error on the fine grid "should" be asymmetric.
  - The difference is significant

$$u_{best} = \tilde{u} \pm U_{num}$$

$$Error = \delta \pm U_{num} \rightarrow u_f + \delta \pm U_{num}$$



There are some potential dangers to conscientiously avoid.

Prefactor — **Convergence rate**

Mesh converged solution, i.e., $h \rightarrow 0$

$$\tilde{u} = u_h + A h^p$$

Characteristic length scale of mesh cell, "Δx"

Computed solution on grid of mesh size h

- This ansatz is valid for data in the asymptotic range of convergence.
  - Usually, we <u>assume</u> that the calculations are in the asymptotic range of convergence.
  - With two calculations, we have an under-determined fit through the results ( ).
  - With many calculations, the error ansatz is fully determined or over-determined; one can perform a **regression** fit.

An example of how verification can go "off the rails"

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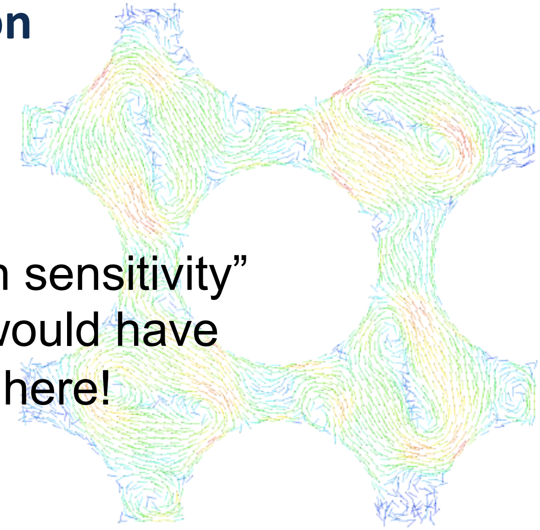
Preliminary Verification Results for CFD* for a CASL challenge problem (GTRF) with Fuego and Drekar (Δp), just spatial resolution

# ele.	Mesh	Fuego	Drekar
664K	Coarse	31.8 kPa	26.7 kPa
1224K	Medium	24.6 kPa	23.8 kPa
1934K	Fine	24.4 kPa	22.0 kPa

A "mesh sensitivity" study would have us stop here!



Fuego

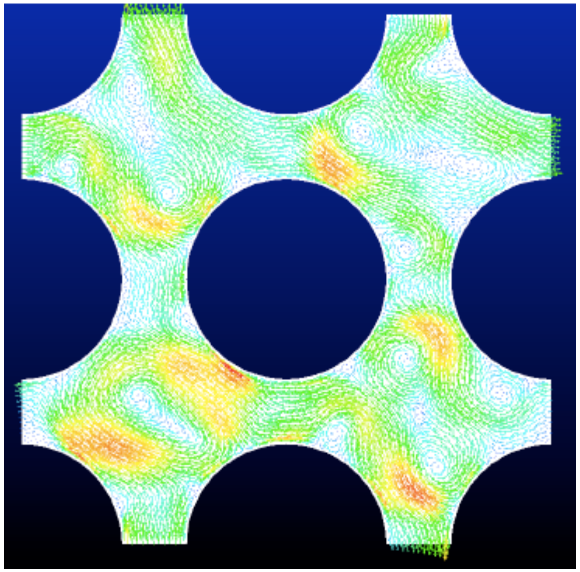
$$\Delta p(h) = 24340 + 26.6h$$

15.85!!

95 % Error Bound 80Pa (Roache, GCI) to 18.6kPa (Stern)

Drekar

$$\Delta p(h) = 17420 + 16370h^{1.234}$$



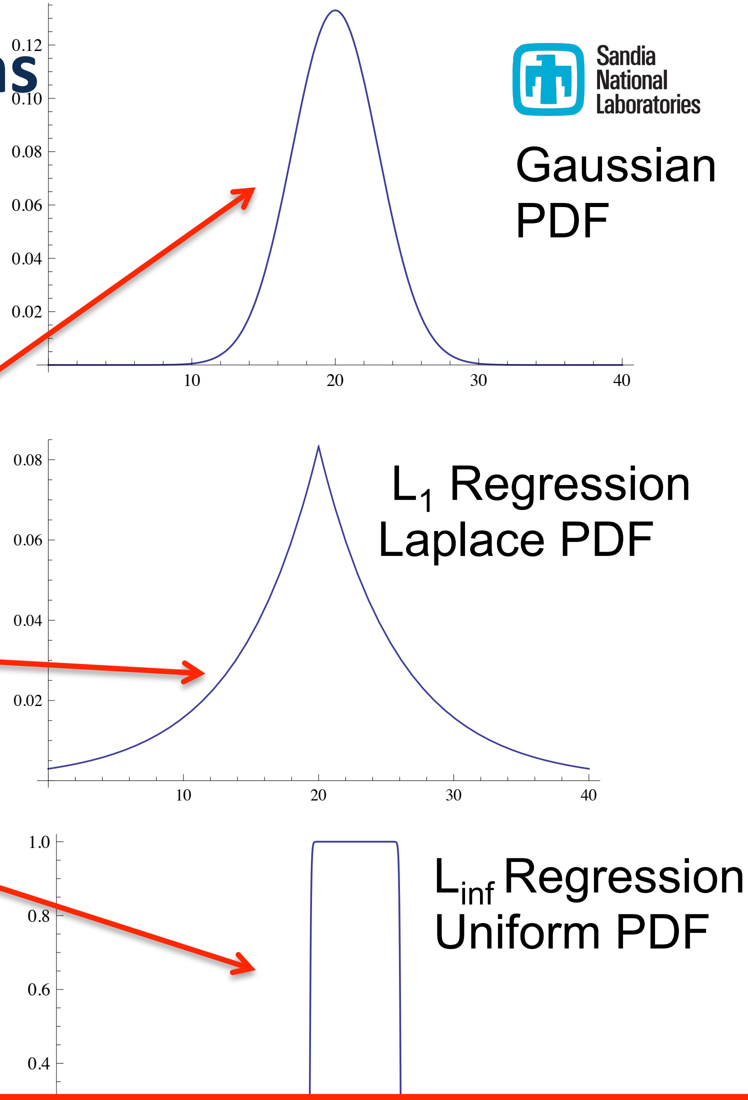
The Fuego result exemplifies one of the problems with the standard setting, 16th order convergence is absurd!

Preview: Our procedure gives *a Δp=16.1kPa ±13.5kPa.*

***CASL: Consortium for the Advanced Simulation of Light Water Reactors,** CFD: computational fluid dynamics
GTRF: Grid-to-rod-fretting

Brief Digression: Regression, norms and probability distributions

- Minimization of the residual for regression carries implications about optimality. The fit is optimal if the errors are distributed:
  - Gaussian implies L_2, *the standard approach* (unweighted)
  - Laplace (double exponential) implies L_1 (absolute value)
  - Uniform implies $L_{infinity}$ (maximum)
- *Regression can be done in any norm if the data is either under- or over-determined and can include constraints as well.*



Use robust statistics not standard statistics

We define a robust multi-regression (RMR) method to encode expert information, with robust statistics.

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- **The standard method is fragile and includes implicit assumptions regarding statistics, error and convergence, which are not included in the analysis.**
- We apply the following algorithm to the data (2 or more grids):

1. **A structured principled way to introduce specific expert knowledge.** Bounds on extrapolated solution could be entered too (such as positivity).
2.
3. **Produce a set of estimates with defined explicit assumptions regarding statistics of the error, and free of the fragility of a single estimate.**
4. **Apply robust statistical techniques to produce results with confidence. Run over subsets of data (jack-knife).**
5. **Produce a bounding estimate using the same approach. Useful when the data is non-monotonic.**

We can demonstrate our method by solving a linear ODE.

- The equation is trivially solvable. We use a forward Euler method here.

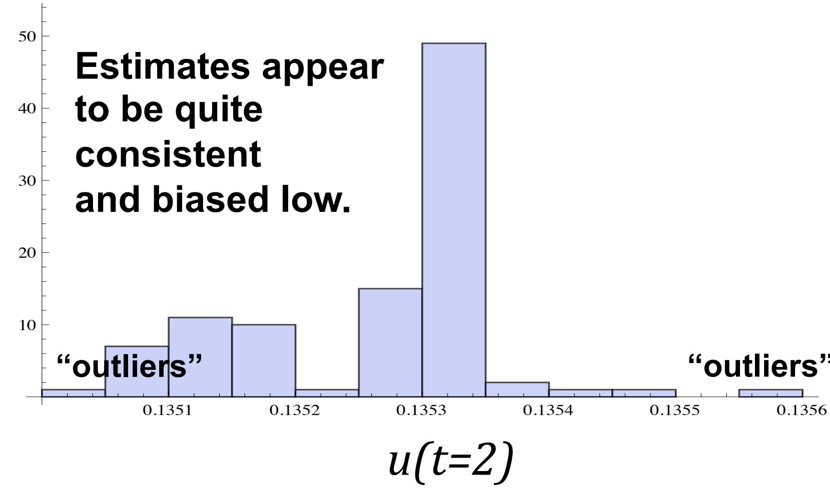
$$\dot{u} = -u \rightarrow u^{n+1} = u^n - \Delta t u^n$$

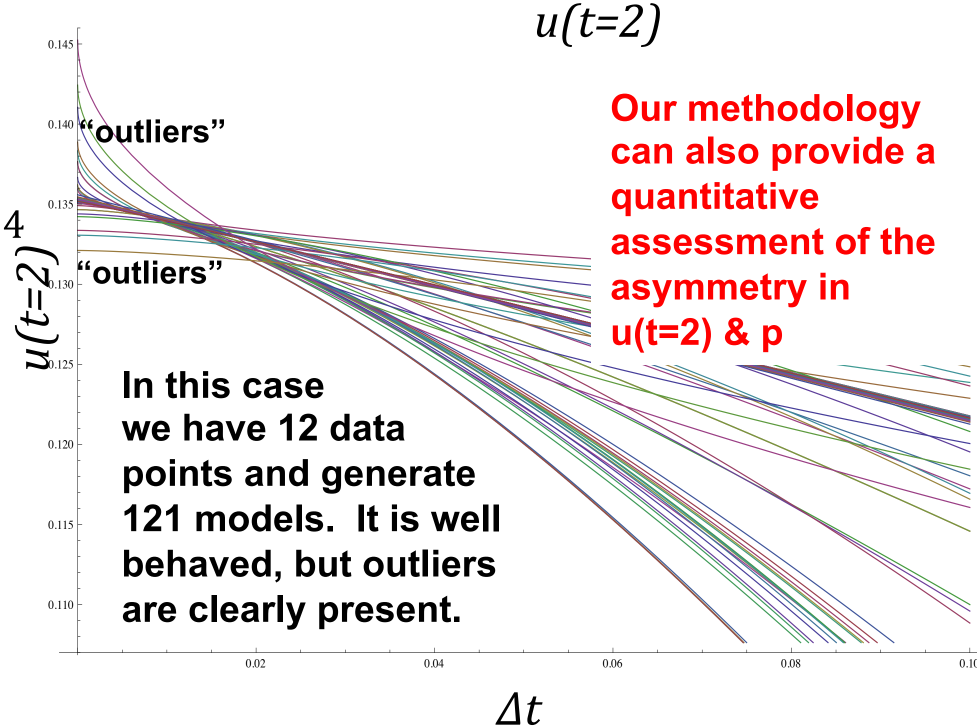
- The estimate and uncertainty strongly coincide with the analytical result.

$$u(t=2) = 0.135316 \pm 0.000138247, p = 1.0219 \pm 0.0154$$

  - The uncertainty "fans out" for Δt smaller than the finest time step used for computed results.
  - Roache's GCI approach does not capture the analytical solution!

$$u(t=2) = 0.134794 \pm 0.000517851, p = 1.03878$$





Solution Verification for Drekar gives estimates are very close to the three grid estimates given earlier!

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Mesh	Δp (pa)
671K	23400
1049K	26781
2664K	23804
5832K	22040
12522K	20745

RMR (all)

$$\Delta p = 16500 \pm 5435 + Ah^{0.53 \pm 0.09} Pa$$

RMR (drop coarse grid)

$$\Delta p = 16280 \pm 7060 + Ah^{1.08 \pm 0.27} Pa$$

GCI (all)

$$\Delta p = 23250 \pm 1635 + Ah^{0.5} Pa$$

GCI (drop coarse grid)

$$\Delta p = 16450 \pm 6960 + Ah^{1.05} Pa$$

- The results are convergent, but at a rate comparable with expectations for "rough" flows like turbulence, that is 1st order accurate.
- Uncertainties are large.
- RMR gives reliable results with or without dropping the non-convergent data point (671K)
  - The CGI is extremely unreliable without screening the data.

The estimated solution is frighteningly close to the estimates from the earlier Fuego calculations!

*RMR:Robust multi-regression, CGI: Grid Convergence Index

Next: Investigate Model Selection Procedures

- Verification is usually done with an assumed error ansatz
  - Almost always a power law form
- It would be beneficial to assume less, and define a better error model more supported by the data.
- Statistical estimation procedures exist for examining the form of the model that best fits the data
- Examples: AIC, BIC, **LASSO**
- Note, that these methods are well-defined for linear models, and verification has been shown to generally require nonlinear models

We decided to explore the LASSO Method in this context

- LASSO has already been applied to verification as one of the fits used in the robust verification work
- In its linear form it is a simple regularized least squares method

$$\min \left\| A\mathbf{x} - \mathbf{b} \right\|_2 + \lambda \left\| \mathbf{x} \right\|_1$$

  - As the Lagrange multiplier is increased in size the solution becomes increasingly "sparse".
  - Closely related to $\min \left\| \mathbf{x} \right\|_1$ constrained by $A\mathbf{x} = \mathbf{b}$
- **Our greatest leap is applying it to the nonlinear model selection**

$$\min \left\| f\left(\mathbf{x}\right) - \mathbf{b} \right\|_2 + \lambda \left\| \mathbf{x} \right\|_1$$

Variants of LASSO that may be better

- One does not have to do a regularized least squares.
- The L1 norm might be useful

$$\min \left\| f\left(\mathbf{x}\right) - \mathbf{b} \right\|_1 + \lambda \left\| \mathbf{x} \right\|_1$$

- …or the Danzig estimator using the infinity norm.

$$\min \left\| f\left(\mathbf{x}\right) - \mathbf{b} \right\|_\infty + \lambda \left\| \mathbf{x} \right\|_1$$

- All work the same way, as the Lagrange multiplier becomes large most of the coefficients go to zero.

The L1 Norm has some remarkable properties useful for model selection

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- *Some have said that L1 is "magic"*
- Specifically, the L1 norm promotes sparsity under the minimization framework
- This is used in compressed sensing (and basis pursuit)

$$\min \|\mathbf{x}\|_1 \text{ constrained by } A\mathbf{x} = \mathbf{b}$$

$$\min \|\mathbf{x}\|_1 \text{ constrained by } \|A\mathbf{x} - \mathbf{b}\|_2 < \varepsilon$$

- The approach allows us to rank the portions of the model form piece-by-piece by examining the terms that remain nonzero for a changing Lagrange multiplier.

“Any sufficiently advanced technology is indistinguishable from magic.”

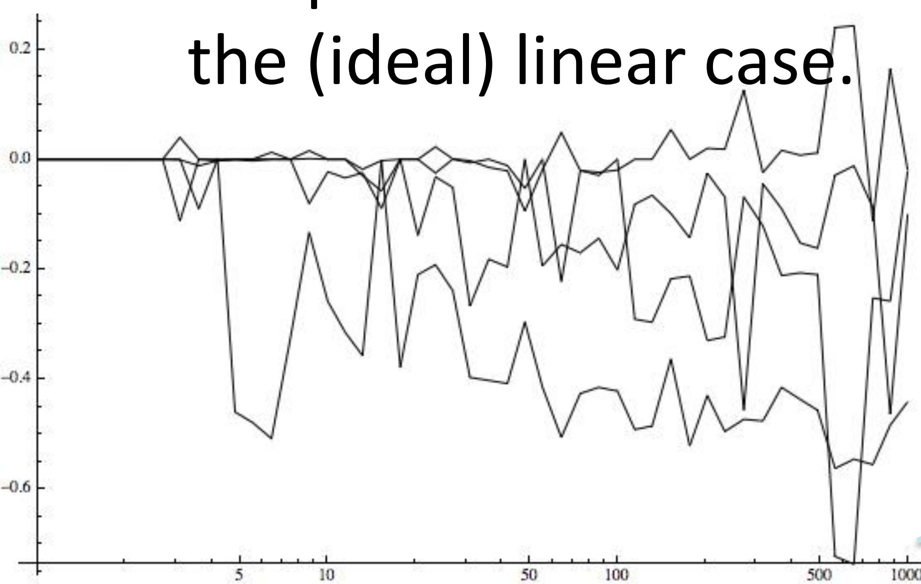
– Arthur C. Clarke

Simple example with model selection

- I will use the simple ODE problem as the first test.
- Broaden the potential terms in the model to include other possible terms: $\tilde{u} = u_h + A h^p$

$$\tilde{u} = u_h + A_p h^p + A_1 h + A_2 h^2 + A_e\left[1 - \exp(b_e h)\right] + A_L \log(1 + b_L h)$$

- The results are unexpected. The trends are clear, but the plots of the coefficients are not nearly as clean as the (ideal) linear case.



$$\min \left\| \tilde{u}(\mathbf{A}) - u_h \right\|_\infty + \lambda \left\| \mathbf{A} \right\|_1$$

$$\tilde{u} = u_h + A_1 h + A_2 h^2$$

Let's look at the performance as error estimators term-by-term

- We use a L1 estimator for each (if you do one fit, I'd recommend L1 instead of L2!)

$$u_{\text{true}} = \exp(-2) = 0.135335$$

- The linear plus quadratic was chosen (polynomial)

$$u_{1,2} = 0.135337 - 0.135337h - 0.0211486h^2; r = 0.0000609$$

- Exponential

$$u_{\text{exp}} = 0.135337 - 0.454392\left[1 - \exp(0.298264h)\right]; r = 0.000146$$

- Logarithmic

$$u_{\log} = 0.135470 - 2.130270\log(1 + 0.298264h); r = 0.002867$$

- Power Law $u_{\text{power}} = 0.135235 - 0.148584h^{1.03656}; r = 0.000640$

Example with picking out cross terms

- We are testing a model with two-dimensional transient heat conduction and chemistry for solute deposition in nuclear reactor cores. The code is poorly documented and it is not clear how coupled it actually is.
- We are going to use the LASSO to investigate what the error model should look like

$$\tilde{u} = u_h + A_x \Delta x^{p_x} + A_y \Delta y^{p_y} + A_t \Delta t^{p_t} + A_{xy} (\Delta x \Delta y)^{p_{xy}} + A_{xt} (\Delta x \Delta t)^{p_{xt}} + A_{yt} (\Delta y \Delta t)^{p_{yt}} + A_{xyt} (\Delta x \Delta y \Delta t)^{p_{xyt}}$$

  - If we just use every term over-fitting is a distinct possibility
- We find that the model that stands out is rather different than we would have chosen a priori. This model does well,

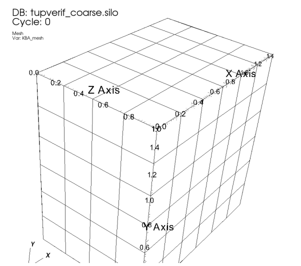
$$\tilde{u} = u_h + A_x \Delta x^{p_x} + A_y \Delta y^{p_y} + A_t \Delta t^{p_t} + A_{xy} (\Delta x \Delta y)^{p_{xy}} + A_{xyt} (\Delta x \Delta y \Delta t)^{p_{xyt}}$$

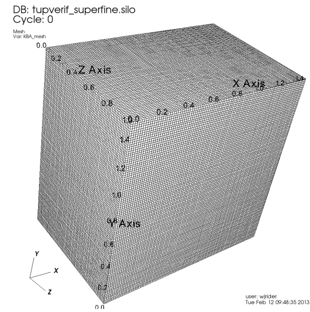
Applying this to Sn Neutronics

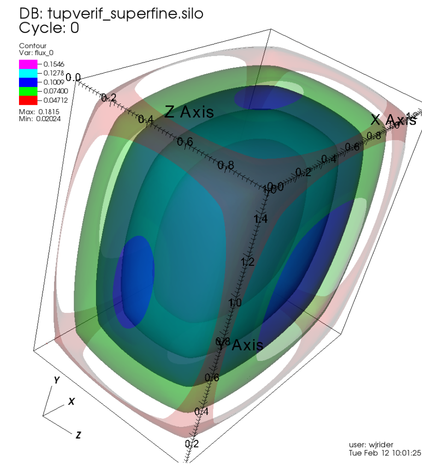
- We apply the verification techniques to the ORNL neutronics code Denovo, which solves the transport equation using discrete ordinates.

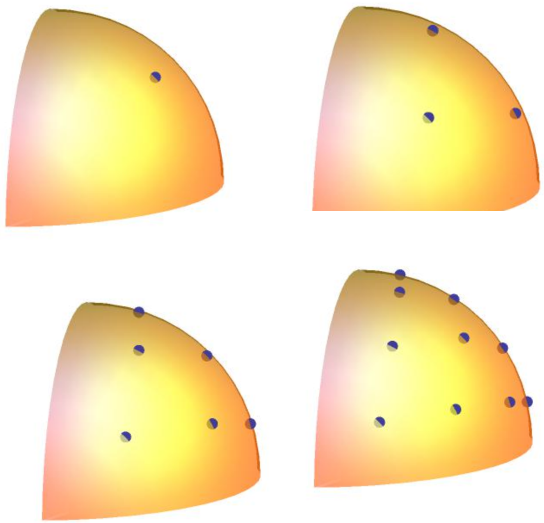
$$\Omega\cdot\nabla\psi(x,\Omega,E)+\sigma(x,E)\psi(x,\Omega,E)=\int dE'\int_{4\pi}d\Omega'\sigma_s(x,\Omega'\cdot\Omega,E'\to E)\psi(x,\Omega',E')$$

- The solution depends on six “coordinates” three space, two angular, and energy.
- We reduce this to space and angle while examining their distinct discretization.
- At this point only very simple problems have been examined.









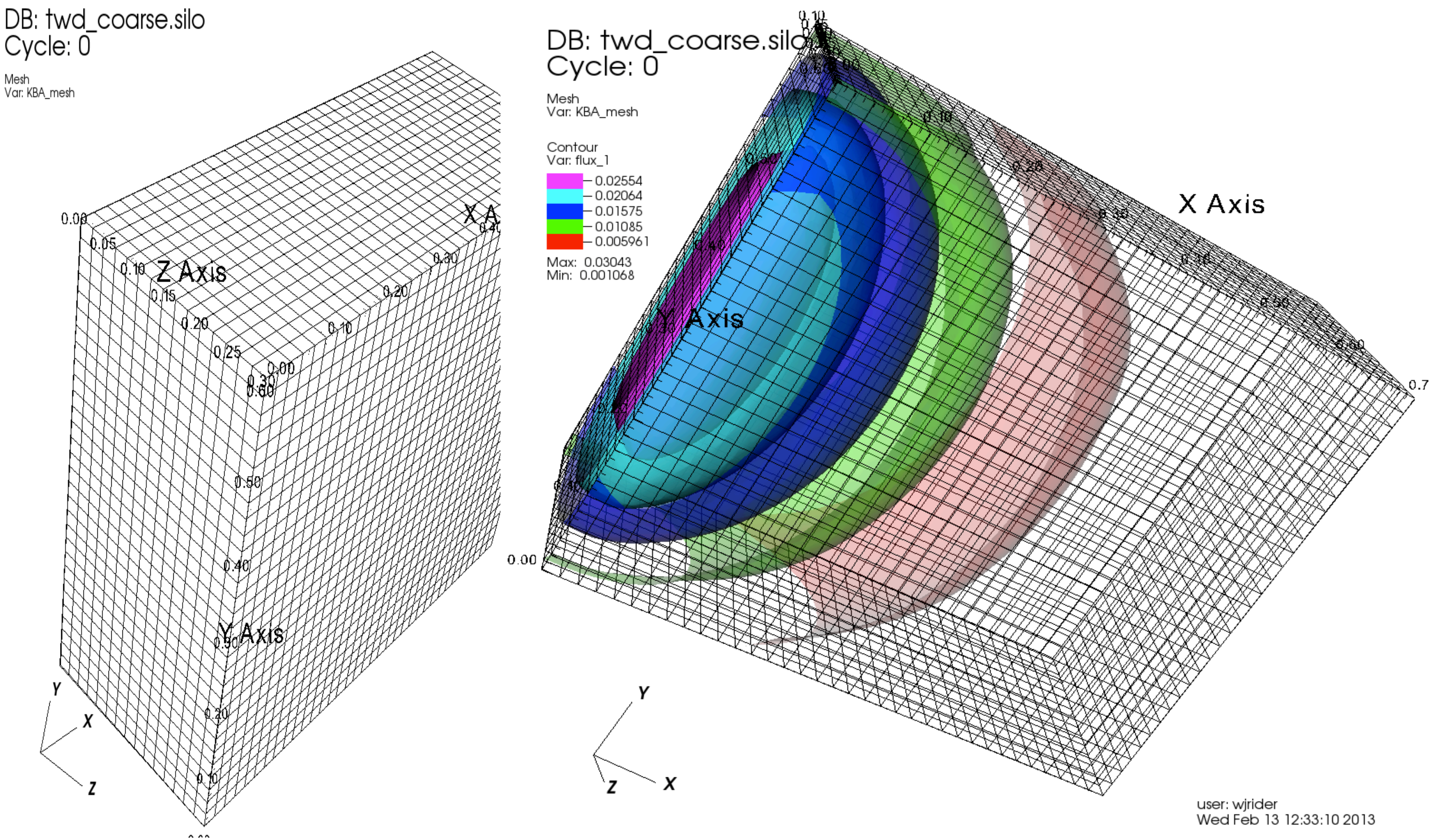
We need to modify the standard verification setting to accommodate the discrete ordinates method

- The basic approach remains, but we have two variables that convergence critically depends upon,

$$\tilde{u} = u_h + A h^p + B / n^q + C \left(h / n \right)^r$$

- A secondary issue is the theoretical expectations for the convergence with respect to the number of quadrature points where we have chosen a form like Jarrell (2010),
- We have examined four different spatial discretizations of the streaming term: Step characteristic, linear discontinuous, trilinear discontinous, and diamond differencing with negative flux fix-up
- We have examined four different quadratures: level symmetric, Gauss-Legendre, Quadruple Range, and LDFE.

The integrated scalar flux for the downscatter problem.



Neutronics Results

- We find little support for the h-p version of the error model
  - The third term in the error model drops out immediately as the size of the Lagrange multiplier is increased.
- We also examine the nature of the error model itself as before

$$\tilde{u} = u_h + \boxed{A h^p} + \alpha\left[1-\exp(\kappa h)\right] + B/n^q + \beta\left[1-\exp(\eta/n)\right] + \boxed{C(h/n)^r} + \gamma\left[1-\exp(\xi h/n)\right]$$

- We find the power law in space and the coupled space-angle power term dominate.

Summary and Future Work

- The basic idea appears to work well.
  - We have concerns about applying this to nonlinear models where theory is weaker.
- We can use it to determine the dominant terms in a proposed error model
- The exponential terms are repeatedly chosen by the procedure, this needs further examination
  - The exponential terms are a better basic error model
  - The LASSO procedure is somehow biased toward them
- We will continue the exploration.

Who Am I ?

- I'm a staff member at Sandia, and I've been there SNL for 7 1/2 years. Prior to that I was at LANL for 18 years. I've worked in computational physics since 1992.
- In addition, I have expertise in hydrodynamics (incompressible to shock), numerical analysis, interface tracking, turbulence modeling, nonlinear coupled physics modeling, nuclear engineering…
- I've written two books and lots of papers on these, and other topics.