PRISM
NNSA Center for Prediction
of Reliability, Integrity and
Survivability of Microsystems

ME 597/AAE 590 : Introduction to Uncertainty Quantification

Lecture 1: Introduction to V&V, UQ

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ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

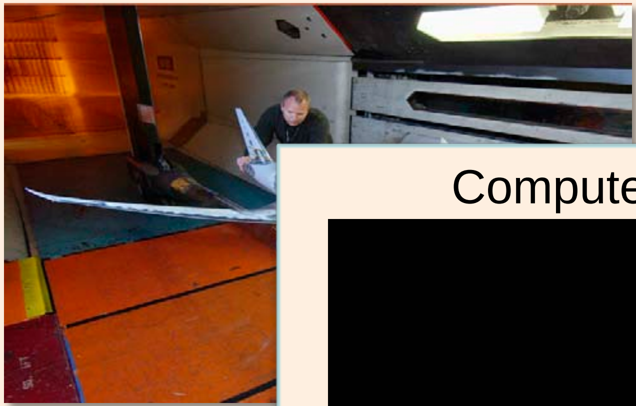
PURDUE
UNIVERSITY

THE UNIVERSITY of
NEW MEXICO

Making of 787 Dreamliner

Assembly: 3 days

Wind tunnel tests: 15,000 hrs

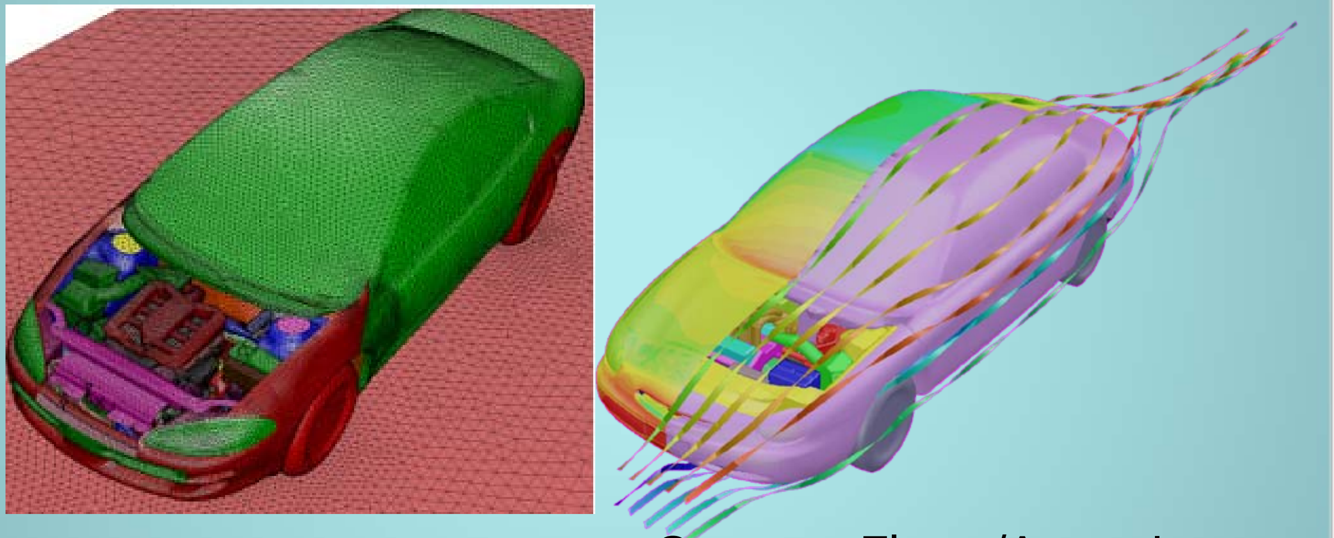


Computer simulations: ~ 1,000,000 hrs

Source: Boeing Commercial Airplanes

Motivation

- Simulati
  enginee
- Simulat
  - Mesh
  - Inapp
  - Inade
  - Unce
  - Unce
  - Toler



Courtesy Fluent/Ansys Inc.

- What is the effect of these uncertainties on predictions?
- What is the sensitivity of outputs to inputs?
  - What inputs are the most important?
  - What should we spend money/time quantifying better? What experiments would have the most payoff?

Motivation (Cont’d)

- What if my simulations don’t match experiments?
  - Does the fault lie in inadequate physical models?
  - Bad experiments? Bad models of the experiments?
- Experiments have uncertainties too
  - How should I compare experiments to simulations?
- Ultimately, as a decision maker, what confidence can I place on the predictions my engineers give me?

We seek to provide answers to these questions through uncertainty quantification

Course Overview

- Focus is on quantifying uncertainty in engineering simulations
- Will introduce concepts of verification, validation, sensitivity analysis, uncertainty propagation and uncertainty quantification (UQ)
- Give a broad overview of available techniques, with examples
- Small homework projects to help solidify ideas
- Would like each student to indentify a UQ component to their research

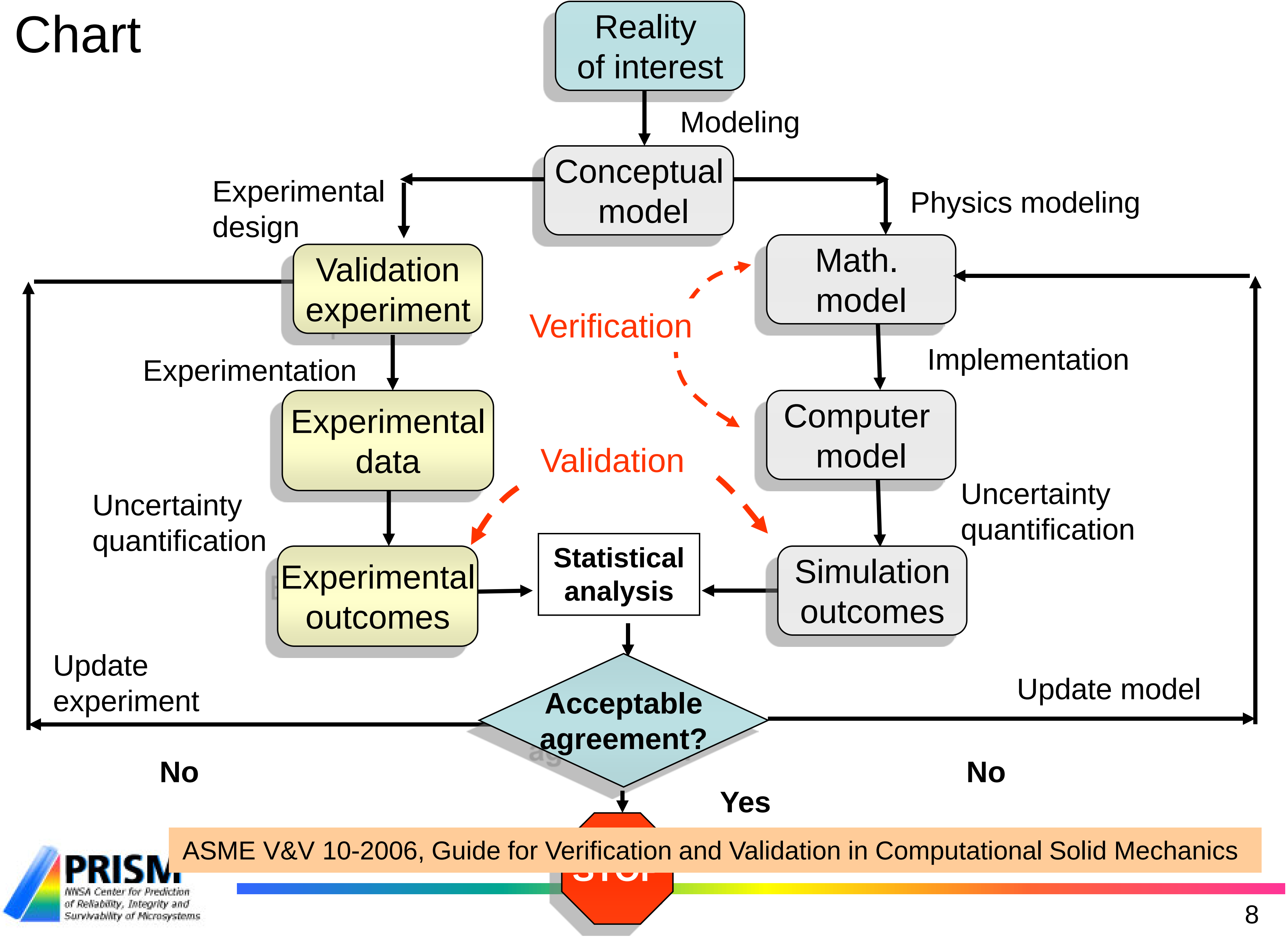
Course Content

Week	Topic	Lecturer
27-Aug	Intro to Verification & Validation, Uncertainty Quantification	Alexeenko
3-Sep	Linear sensitivity analysis; finite difference, code differentiation	Mathur
10-Sep	Uncertainty propagation - sensitivity equation, variance propagation eqn, non-deterministic sampling (Monte Carlo, LHS)	Sun
17-Sep	Polynomial chaos - Galerkin and collocation	Xiu/Narayan
24-Sep	Polynomial chaos - Galerkin and collocation	Xiu/Narayan
1-Oct	Verification and validation of computational models	Alexeenko
8-Oct	Uncertainty quantification in experiments	Raman
15-Oct	Using MEMOSA UQ software	Hunt
22-Oct	Introduction to DAKOTA	Pax
29-Oct	No lecture	
5-Nov	Introduction to Bayesian methods and Bayesian calibration	Mahadevan
19-Nov	Uncertainty quantification for PRISM MEMS device	Alexeenko
26-Nov	No lecture (Thanksgiving)	
3-Dec	Uncertainty quantification across scales	Koslowski
10-Dec	Epistemic error in molecular dynamics; Closure	Strachan

Course Policies

- Grading based on
  - Attendance: 50%
  - Homework: 25%
  - Short project: 25%
- Project: VV & UQ plan for your thesis
  - How you will use verification, validation and uncertainty quantification in your thesis research
  - Identify main uncertainties
  - 2-page write up for review by instructors and peers

V&V and UQ Flow Chart



Reality of interest

Modeling

Conceptual model

Experimental design

Physics modeling

Validation experiment

Math. model

Verification

Experimentation

Implementation

Experimental data

Computer model

Validation

Uncertainty quantification

Uncertainty quantification

Experimental outcomes

Statistical analysis

Simulation outcomes

Update experiment

Update model

Acceptable agreement?

No

No

Yes

ASME V&V 10-2006, Guide for Verification and Validation in Computational Solid Mechanics

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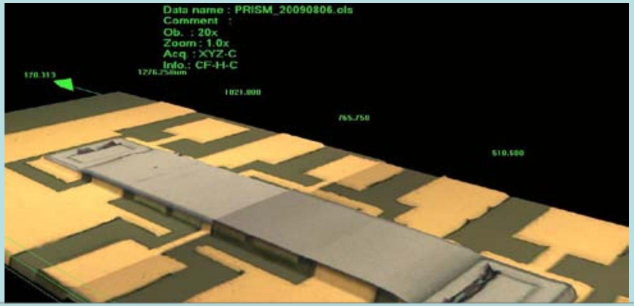
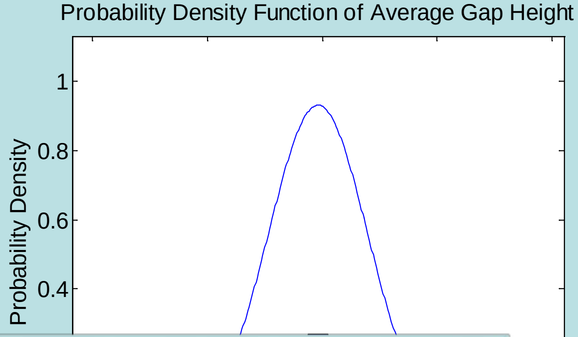
Definitions

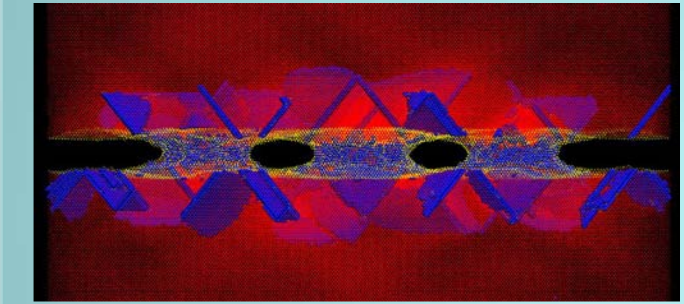
- Verification: "*The process of determining that the equa*
- Valid *equa*
- Quar *quan*
- Aleat *input*
  - Ty
- Episte *proces*
  - Unk
  - Mod

Aleatoric Uncertainty





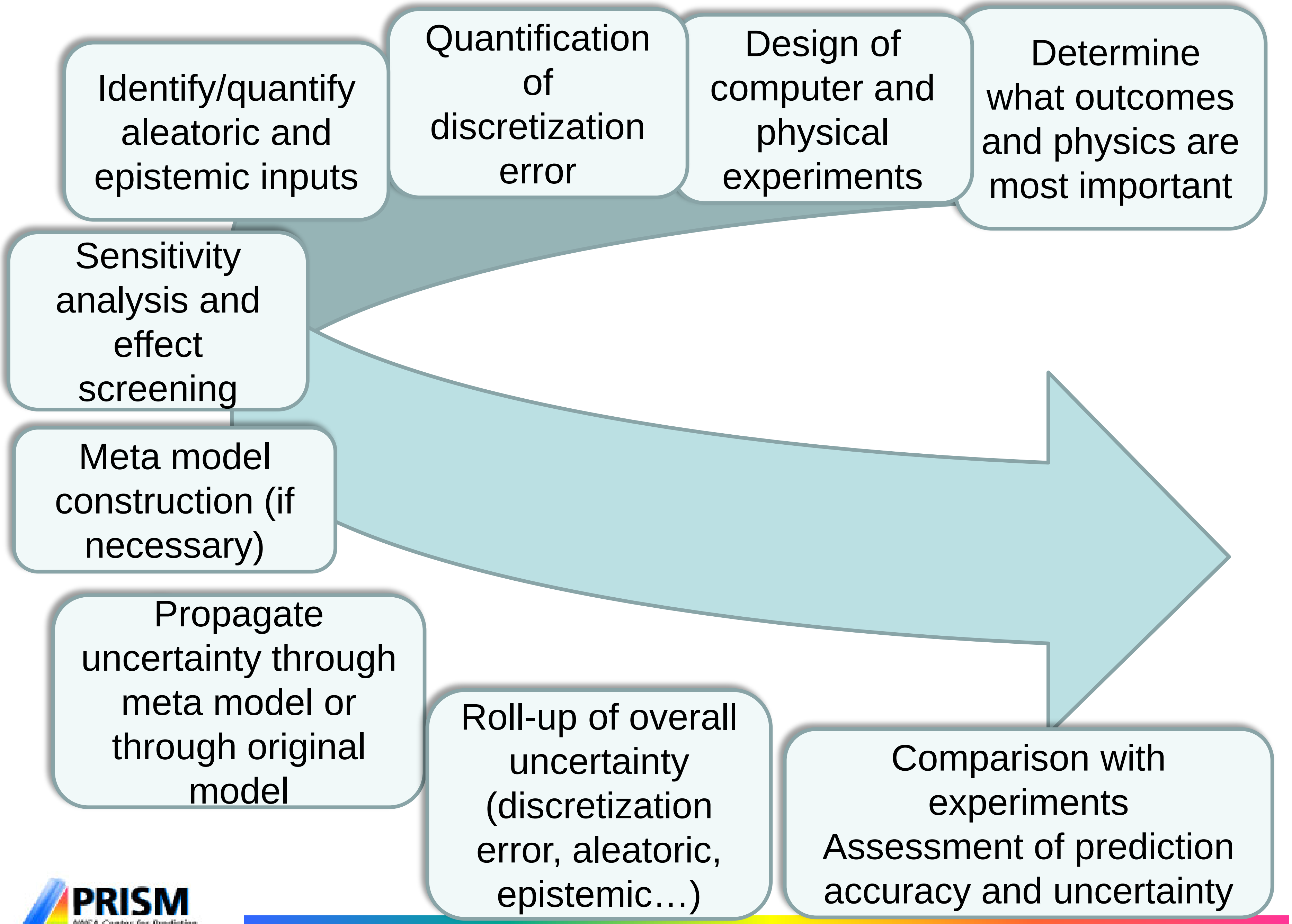
Epistemic Uncertainty



Molecular dynamics simulations of contact

- Form of the interatomic potential?
- Constants in the interatomic potential?

Courtesy Strachan group



Determine what outcomes and physics are most important

Design of computer and physical experiments

Quantification of discretization error

Identify/quantify aleatoric and epistemic inputs

Sensitivity analysis and effect screening

Meta model construction (if necessary)

Propagate uncertainty through meta model or through original model

Roll-up of overall uncertainty (discretization error, aleatoric, epistemic…)

Comparison with experiments
Assessment of prediction accuracy and uncertainty

Code Verification

- Objective is to establish correct implementation of models and numerics
- This is done by
    - Using exact solutions where available
    - Method of manufactured solutions (MMS) to augment exact solutions
    - Establishing order of convergence of spatial and temporal operators

Example: Verification of Finite Volume Method for Stress Analysis

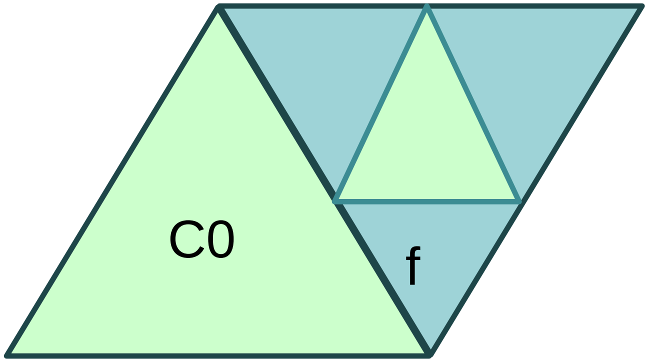
- Unstructured cell-centered formulation
  - Deformation vector stored at cell centroids
- Momentum balance written over cells
- Fully-implicit coupled formulation
- BiCGStab + algebraic multigrid linear solver
- Second-order spatial accuracy and first-order temporal accuracy

$$\frac{\partial^2(\rho\mathbf{w})}{\partial t^2} - \nabla\cdot\sigma = \rho\mathbf{f}$$

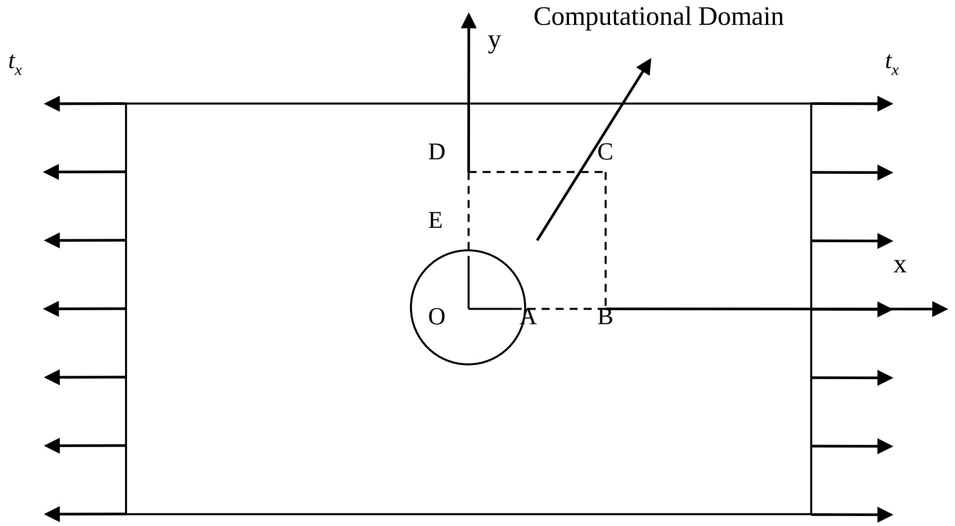
Hooke's Law:

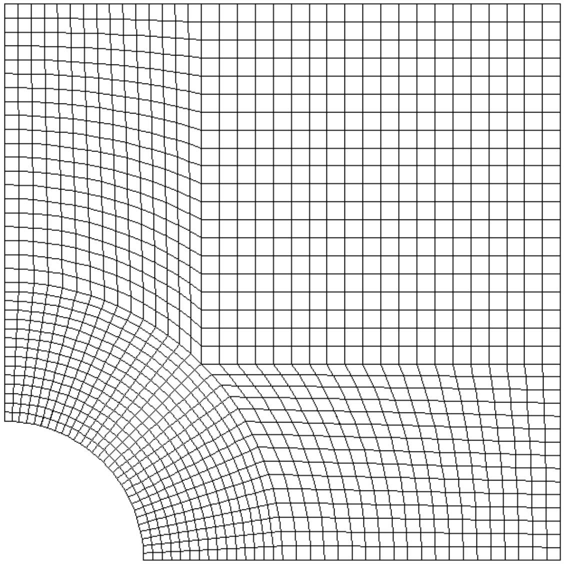
$$\sigma = 2\mu\varepsilon + \lambda\mathrm{tr}(\varepsilon)\mathbf{I}$$

$$\varepsilon = \frac{1}{2}\left[\nabla\mathbf{w} + (\nabla\mathbf{w})^{\mathrm{T}}\right]$$



Verification: Stress Around Circular Hole





Exact Stress Solution:

$$\sigma_{xx} = t_x \left[1 - \frac{a^2}{r^2}\left(\frac{3}{2}\cos 2\theta + \cos 4\theta\right) + \frac{3}{2}\frac{a^4}{r^4}\cos 4\theta \right]$$

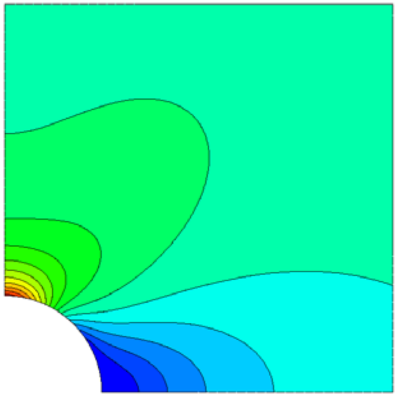
$$\sigma_{yy} = t_x \left[-\frac{a^2}{r^2}\left(\frac{1}{2}\cos 2\theta - \cos 4\theta\right) - \frac{3}{2}\frac{a^4}{r^4}\cos 4\theta \right]$$

$$\sigma_{xy} = t_x \left[-\frac{a^2}{r^2}\left(\frac{1}{2}\sin 2\theta + \sin 4\theta\right) + \frac{3}{2}\frac{a^4}{r^4}\sin 4\theta \right]$$

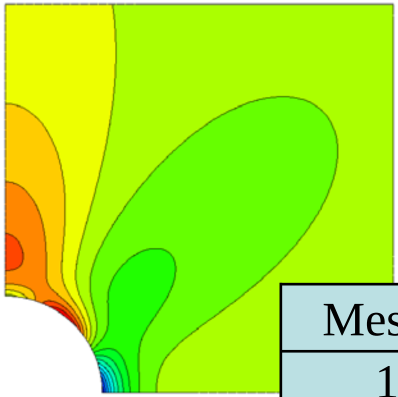
- Apply exact solution as boundary conditions
- Compute deformation vector and stress in interior

Stress Distribution

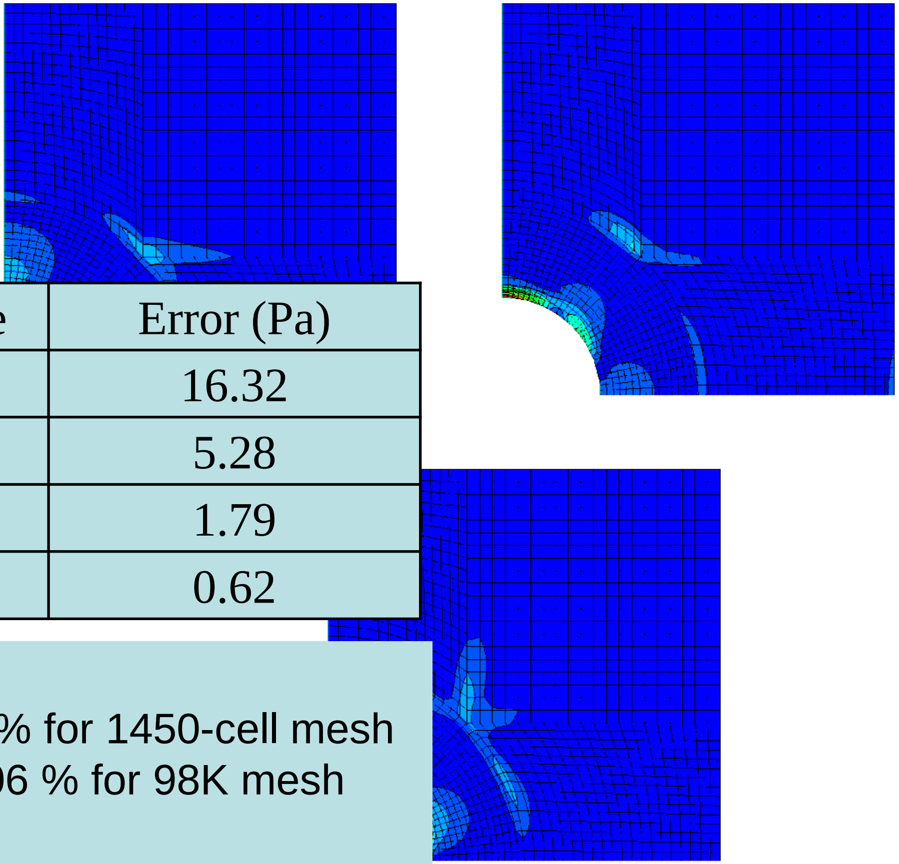
σ_{xx}



σ_{yy}



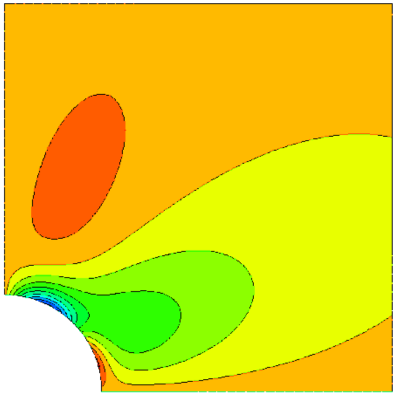
Error



Mesh Size	Error (Pa)
1450	16.32
5800	5.28
23200	1.79
98000	0.62

RMS error

- under 0.2% for 1450-cell mesh
- under 0.006 % for 98K mesh



σ_{xy}

Method of Manufactured Solutions

- Consider, for example, the energy equation:

$$\frac{\partial T}{\partial t}+\frac{\partial u_x T}{\partial x}+\frac{\partial u_y T}{\partial y}=\alpha\left[\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right]+S(x,y,t)$$

- We want to test if its implementation in our code is correct.
- Postulate a known velocity field, and a known temperature field (arbitrarily):

$$u_x=-\cos(\pi x)\sin(\pi y)e^{-2\pi^2 t/\mathrm{Re}} \qquad u_y=\sin(\pi x)\cos(\pi y)e^{-2\pi^2 t/\mathrm{Re}}$$

$$T(x,y,t)=-0.25\left[\cos(2\pi x)+\cos(2\pi y)\right]e^{-4\pi^2\alpha t}$$

- These arbitrary fields will not satisfy the governing equation. Substitute fields into governing equation; find source term required to satisfy equation exactly:

$$S(x,y,t)=0.5\pi\left[u_x\sin(2\pi x)+u_y\sin(2\pi y)\right]e^{-4\pi^2\alpha t}$$

- Specify boundary and initial conditions using the “exact” temperature solution

$$T(x,y,t)=-0.25\left[\cos(2\pi x)+\cos(2\pi y)\right]e^{-4\pi^2\alpha t}$$

Method of Manufactured Solutions

- Thus, we have created an “exact” solution.
- The problem:

$$\frac{\partial T}{\partial t}+\frac{\partial u_x T}{\partial x}+\frac{\partial u_y T}{\partial y}=\alpha\left[\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right]+S(x,y,t)$$

$$S(x,y,t)=0.5\pi\left[u_x\sin(2\pi x)+u_y\sin(2\pi y)\right]e^{-4\pi^2\alpha t}$$

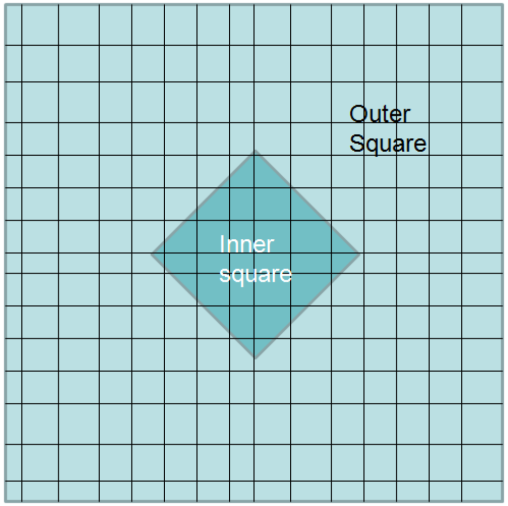
$$u_x=-\cos(\pi x)\sin(\pi y)e^{-2\pi^2 t/\mathrm{Re}} \qquad u_y=\sin(\pi x)\cos(\pi y)e^{-2\pi^2 t/\mathrm{Re}}$$

has the solution

$$T(x,y,t)=-0.25\left[\cos(2\pi x)+\cos(2\pi y)\right]e^{-4\pi^2\alpha t}$$

provided that initial and boundary conditions are specified from T(x,y,t).

Accuracy of Immersed Boundary Method



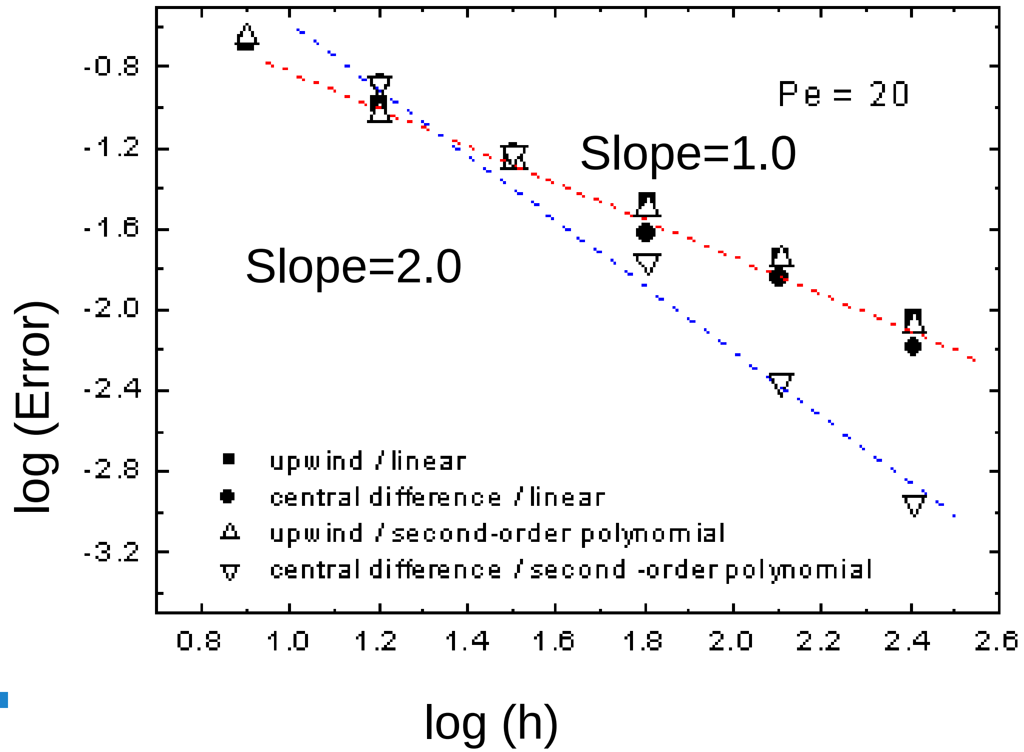
$$u_x = -\cos(\pi x)\sin(\pi y)e^{-2\pi^2 t/\mathrm{Re}}$$

$$u_y = \sin(\pi x)\cos(\pi y)e^{-2\pi^2 t/\mathrm{Re}}$$

$$\frac{\partial T}{\partial t} + \frac{\partial u_x T}{\partial x} + \frac{\partial u_y T}{\partial y} = \alpha\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right] + S(x,y,t)$$

$$S(x,y,t) = 0.5\pi\left[u_x \sin(2\pi x) + u_y \sin(2\pi y)\right]e^{-4\pi^2 \alpha t}$$

$$T(x,y,t) = -0.25\left[\cos(2\pi x) + \cos(2\pi y)\right]e^{-4\pi^2 \alpha t}$$



Order of Numerical Scheme

- Consider, for example, the diffusion equation:

$$k\frac{d^2T}{dx^2}+S=0 \quad \mathrm{T(0)=T_1}, \quad \mathrm{T(L)=T_2}$$

- A typical central difference discretization of this pde yields

$$\frac{T_{i+1}-2T_i+T_{i-1}}{\Delta x^2}+S_i=0 \qquad \text{truncation error } \mathrm{O}\left(\Delta x^2\right)$$

Order of numerical scheme p =2 in this case

- Other terms would have their own truncation errors. The overall order of the numerical scheme is that of its lowest order truncation error.
- We would like to establish that the implementation in any new code that we write achieves the theoretical order

Richardson Extrapolation

If discrete solution $y(h)$ is a continous and differentiable function of mesh size h, it has a series representation:

$$y(h) = y_{exact} + \alpha_p h^p + O(h^{p+1})$$

y_{exact} = True-but-unknown solution of the pde

$y(h)$ = discrete solution at mesh size h

p = order of convergence

α_p =constant

Three unknowns: $\mathrm{y}_{exact}, p, \alpha_p$

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Richardson Extrapolation (cont)

- The idea of RE is to combine solutions on different meshes to eliminate the leading error terms.
- For example, for a 2nd order accurate solution:

$$y(h) = y_{exact} + \alpha_2 h^2 + O(h^3)$$

$$y\left(\frac{h}{2}\right) = y_{exact} + \alpha_2 \frac{h^2}{4} + O(h^3)$$

- Combining the two solutions to eliminate error, gives

$$RE^2(h, \frac{h}{2}) = \frac{4\,y(h/2) - y(h)}{3} = y_{exact} + O(h^3)$$

Richardson Extrapolation (cont)

- For an arbitrary order p and an arbitrary grid refinement factor r:

$$RE^{p}(h,\frac{h}{r}) = \frac{r^{p}y(h/r) - y(h)}{r^{p}-1} = y_{exact} + O(h^{p+2})$$

- Non-uniform meshes can be used to construct RE, the same mesh generating function was used that depends on a refinement factor *r*.
- If a discrete solution is obtained on *n* different grids, than *n* error terms can be eliminated for a known order of convergence.

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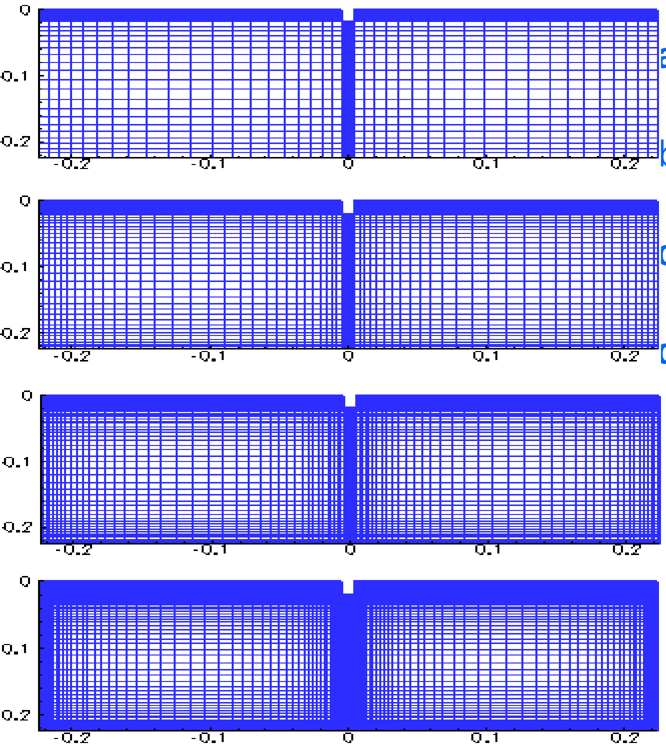
Example of 2D RE

Grids



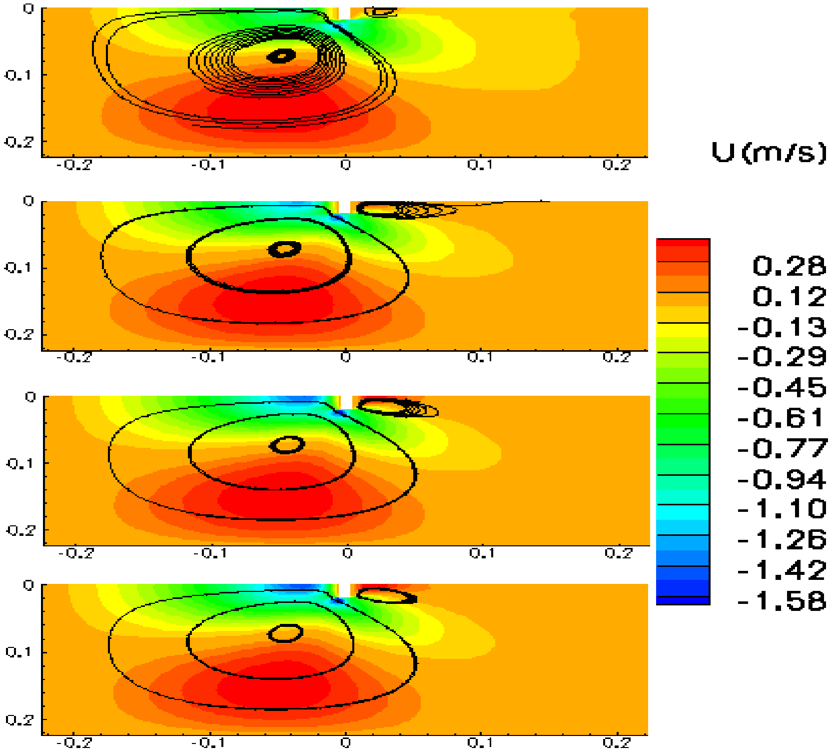
a) **31x46-19x31-31x46**
Total: 3,441

b) **41x61-25x41-41x61**
Total: 6,027

c) **51x75-31x51-61x91**
Total: 9,333

d) **61x91-37x61-61x91**
Total: 13,359

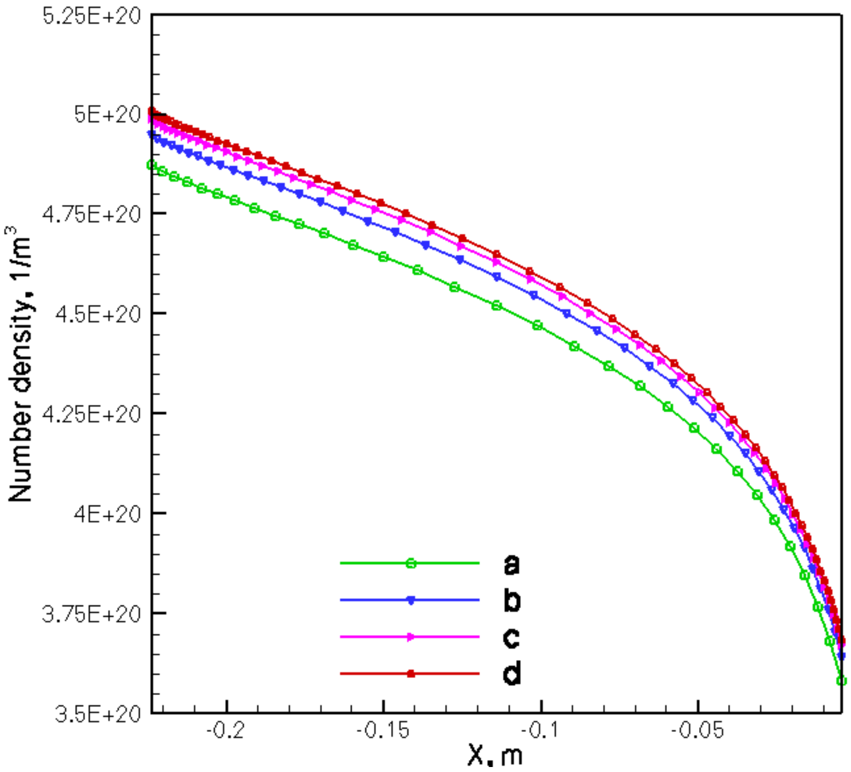
X-velocity and streamlines



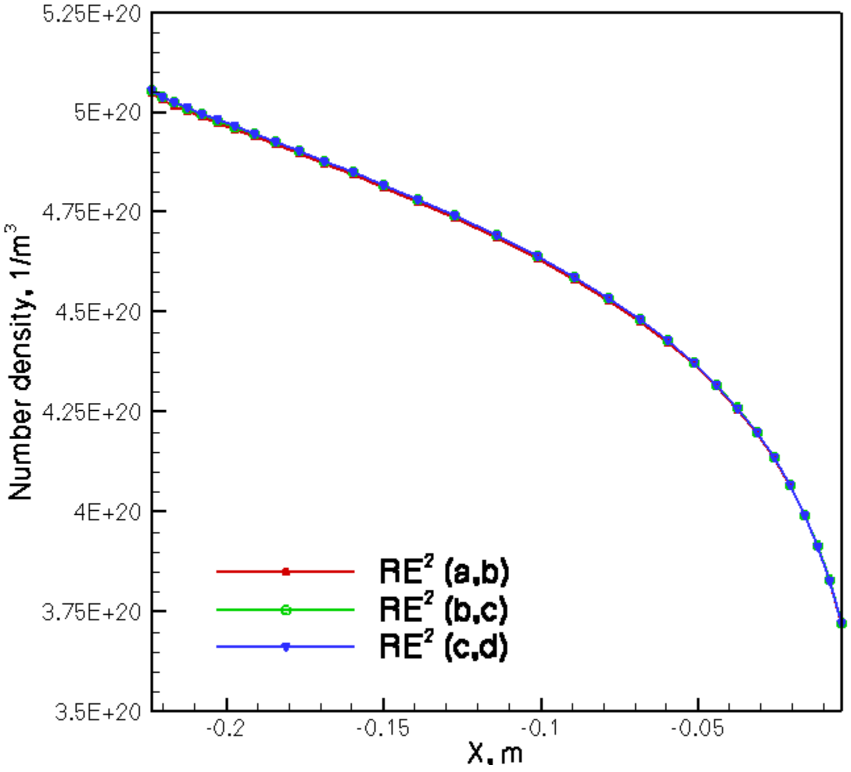
- Radiometric flow: outer walls at 300 K, left and right plate surfaces are at 410 and 450 K, respectively, with Argon gas at 2 Pa.
- 3-block non-uniform meshes with power-law distribution of nodes.
- 2nd-order discrete-ordinate mehod for ES model kinetic equation is applied.

Example of RE

Number density at Y=0



Solution on different grids

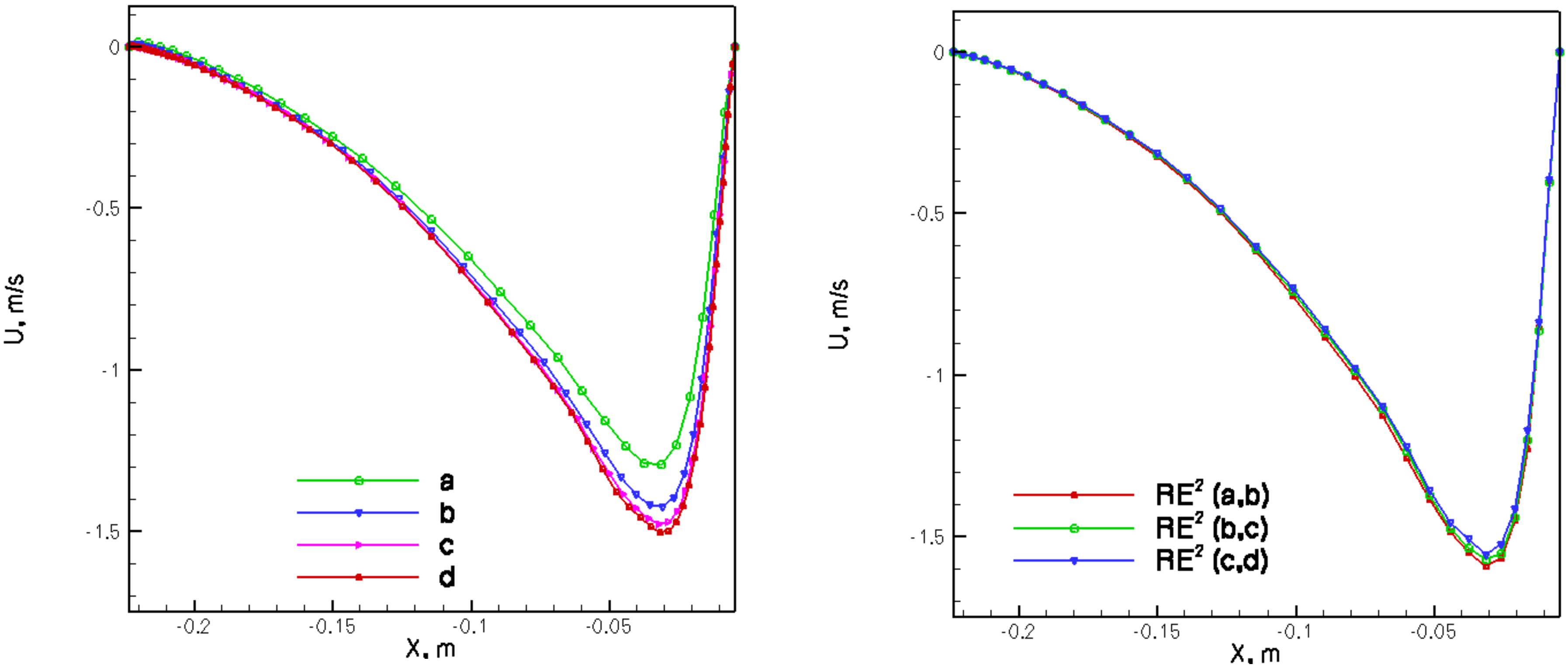


Richardson Extrapolation

- Number density solutions on coarse and finest grids differ by about 3%.
- Richardson extrapolation for all three cases is within 0.15% which indicates that the grid sizes are in asymptotic regime.

Example of RE

X-velocity at Y=0



Solution on different grids

Richardson Extrapolation

- X-velocity solutions on coarse and finest meshes differ by as much as 18%.
- Richardson extrapolation for all three cases is within 2.7%.

Example of RE

- In radiometric flow calculations the quantity of interest is the radiometric force on the plate.
- Richardson extrapolation can be used to assess the numerical accuracy of the force prediction by the numerical solution.
- In order to apply RE for integrated quantities, for example, force or drag coefficient, the order of quadrature has to be the same or higher than the order of the method.

Grid	**Force, μN**	**Est. Error,%**
A	86.31	4.84
B	88.23	2.76
C	89.13	1.76
D	89.5	1.35
RE^2(a,b)	90.7	
RE^2(b,c)	90.73	

Order of Convergence (Cont’d)

To find order of convergence, we use computations at 3 mesh resolutions,

$h_C, h_M, h_F.$

Solving for the unknowns, we find:

$$p = \frac{\log\left(\dfrac{y(h_M) - y(h_C)}{y(h_F) - y(h_M)}\right)}{\log(r)} \qquad y_c = \frac{r^p y(h_F) - y(h_M)}{r^p - 1}$$

where $r = \dfrac{h_C}{h_M} = \dfrac{h_M}{h_F}$

Furthermore, we define the Grid Convergence Index (GCI):

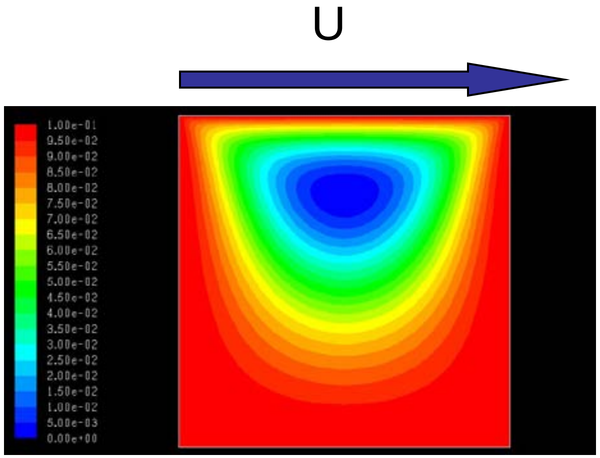
$$\mathrm{GCI} = 100 \left|\frac{y(h_C) - y(h_M)}{y(h_C)}\right| \left(\frac{\beta}{r^p - 1}\right)$$

where β is a safety factor, $1 \le \beta \le 3$.

Verification: Summary

- *Code verification* refers to establishing that coding in your solver is done correctly. This is done by comparing to exact solutions and/or using MMS, and establishing that the correct order of convergence *p* is obtained.
- *Solution verification* is performed when we are using an established code to do simulations
- Here we want to ensure that our mesh is fine enough to give us a good approximation to the pde solution
- The grid convergence index is a means to do that.
- Small GCI values indicate that the numerical solution is close to the pde solution.
- Typically, values under 1% are sought.

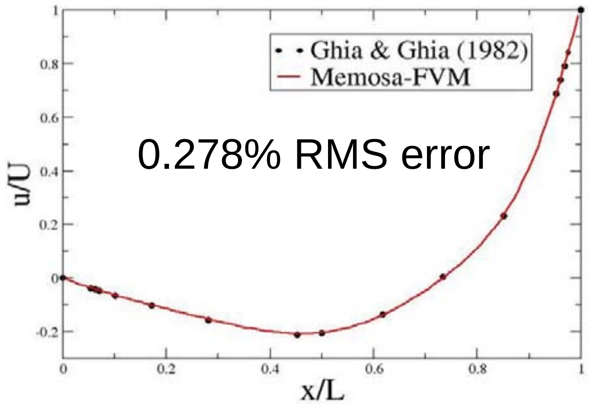
MEMOSA-FVM Verification Example



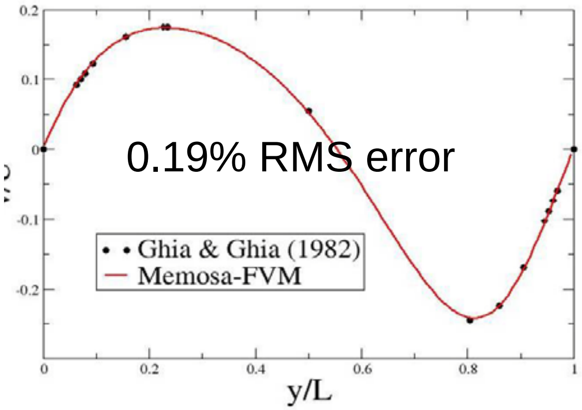
Lid Driven Cavity At Re=1-100

- Classical benchmark test for CFD codes
- Comparison to benchmark solution of Ghia et al. for Re=100
- Grid convergence tests for Re=1

Re=100



0.278% RMS error



0.19% RMS error

Solution shows good agreement with benchmark at Re=100

Order of convergence is approximately second-order. GCI is very low value, establishing mesh independence.

Grid	64x64	128x128	256x256	Order	GCI* (%)
ψ_{max} (Re=1)	0.099918	0.100028	0.100061	1.746	0.01388

***medium to fine**

Ghia,et al, JCP 48, 38 (1982)

References

- Francois M. Hemez, “Uncertainty Quantification and the Verification and Validation of Computational Models”, Los Alamos Natl Lab Report LA-UR-03-8491. http://institute.lanl.gov/ei/model_v/pubs/Hemez_03-8491.pdf
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- PRISM Center tools and reference material at MemsHUB http://memshub.org