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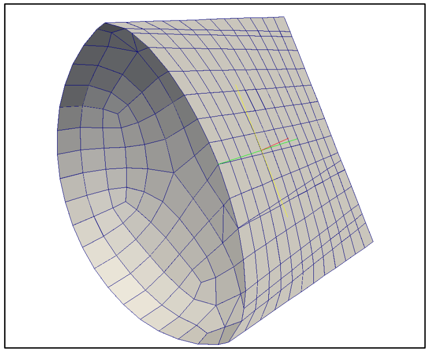

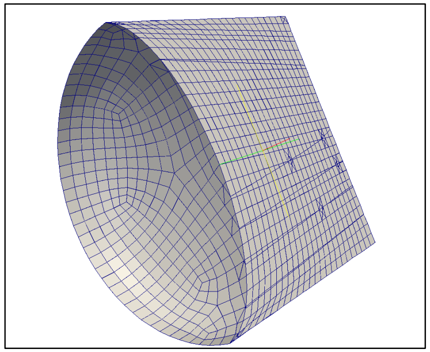

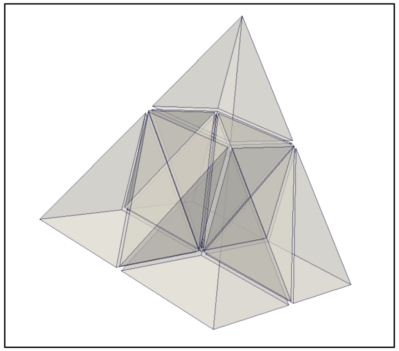

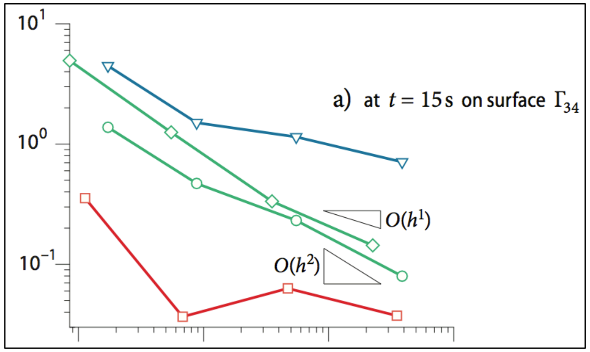

Introduction to Verification

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ESP700

April 2014

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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ESP700: Verification

Overall Goals for Verification

- Identify numerical error and its sources
- Understand and apply models of numerical error
- Understand code verification and assess feature coverage for a given Sierra model
- Quantify numerical error using a mesh refinement study
- Learn about advanced topics such as mesh adaptivity

Motivating Factors for Verification

- Helps answer the questions:
  1. How confident am I in the simulation tools?
  2. What is the accuracy of the results?
- Verification is part of the Predictive Capability Maturity Model (PCMM)
- Verification is part of the Comp/Sim RPP (NW)
- Credibility requires attention to accuracy
- Accuracy should be assessed along with other uncertainties in a model prediction

Sleipner A Offshore Platform

- Descends to a water depth of 82m.
- Concrete gravity base structure consisting of 24 cells, each 12m in diameter.
- Total base area of 16,000m^2; height 110m; concrete volume 75,000m^3.
- Top deck weighs 57,000 tons, supports drilling equipment and accommodation for 200 people weighing 40,000 tons.

Sleipner A Offshore Platform

23 August 1991: During the ballasting to prepare for deck mating in Gandsfjorden outside Stavanger, Norway, the first concrete base structure sprang a leak and sank the platform.

- Structure crushed into debris no larger than 10m, at a depth of 220m.
- Seismic event registering 3.0 on the Richter scale.
- Total economic loss of **$700 million**.

SINTEF investigated the accident, producing 16 reports.

- A cell wall failed, resulting in a crack and a leakage that the pumps were not able to cope with.
- Computed stresses, which were critical to the design of the thickness of the wall had a 47% error.
- The cause was a combination of a serious error in the finite element analysis and insufficient anchorage of the reinforcement in a critical zone.

Proper **solution verification** could have avoided the accident.
More careful finite element analysis, made after the accident, predicted that failure would occur with this design at a depth of 62m, which matches well with the actual occurrence at 65m.

Models for Physical Events

- First need to identify different kinds of models:
  - Conceptual/physical model:
    - Continuum mechanics, Cauchy stress, Linear elasticity
  - Mathematical model:
    - Momentum balance equations, boundary conditions
    - Linear elastic constitutive models
  - Numerical model:
    - Finite element shape functions; discrete balance equations
    - Meshes for the domain (8 node hex elements)
  - Computer model:
    - Assembly of nodal forces, stiffness/mass matrices
    - Solution of linear systems, eigenvalue problems

Different Errors for Different Models

- Could say errors or discrepancies
- Errors can arise in all levels of modeling:
  - Conceptual/physical model:
    - Neglected finite strain effects or inertial effects
  - Mathematical model:
    - Wrong boundary condition (neglected friction)
  - Numerical model:
    - Mesh is too coarse for desired accuracy
  - Computer model:
    - Incorrect implementation of material model
- Our focus in this part of the course is on errors from the <u>numerical</u> and <u>computer</u> models.

Quantities of Interest (QoI)

- The models are used to predict something
  - in our case typically a physical event that could potentially be realized experimentally
- It is important to be clear about the precise quantities of interest (QoI) to be predicted:
  - Average displacement (at point, over surface)
  - Max stress/strain in a material
  - Resulting load on a surface (integrated force)
  - Max acceleration over a time interval
- Some QoIs can be computed more accurately than others:
  - Integrated quantities (space/time) are usually more accurate than localized quantities

Back to Numerical Error

- What are the sources of numerical error?
- Approximations made in order to turn the *math model* into something a *computer can solve*
  - Spatial discretization (mesh error)
  - Time integration (discrete time steps)
  - Iterative methods to solve nonlinear equations
  - Numerical integration
  - Truncation of infinite series
  - Finite sampling (uncertainty quantification)
- Numerical error can be reduced with additional computational effort

Models for Numerical Error

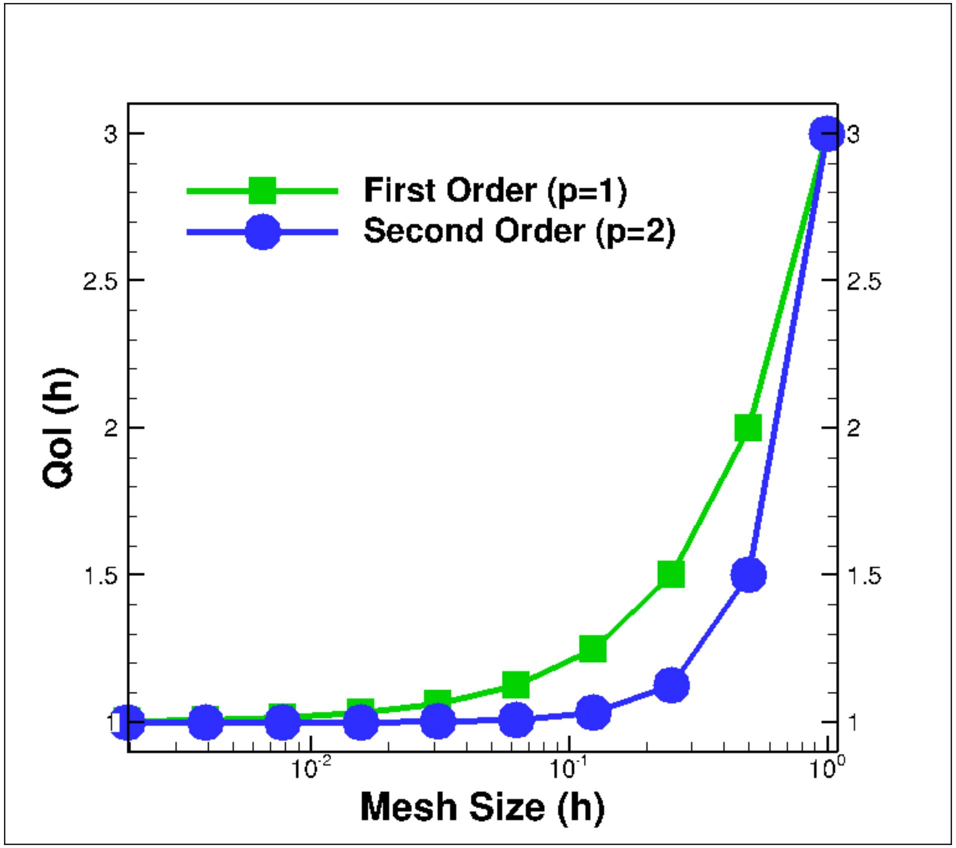
- The most common model you will see:

$$Q(h) = Q + C\,h^p$$

- "Approximate QoI = exact QoI + error term"
- What are all the parameters?
  - Mesh size: *h* or Δx ("delta x")
  - QoI as function of mesh size: *Q(h)*
  - Rate of convergence: *p*
  - Error constant: *C*
- What is h? A measure of the available resolution
  - The size (diameter) of the grid cells used in the mesh
  - The size of the time step

Example: Numerical Error Model

- Compare QoI values for different rates of convergence (p=1 and 2) with exact QoI = 1

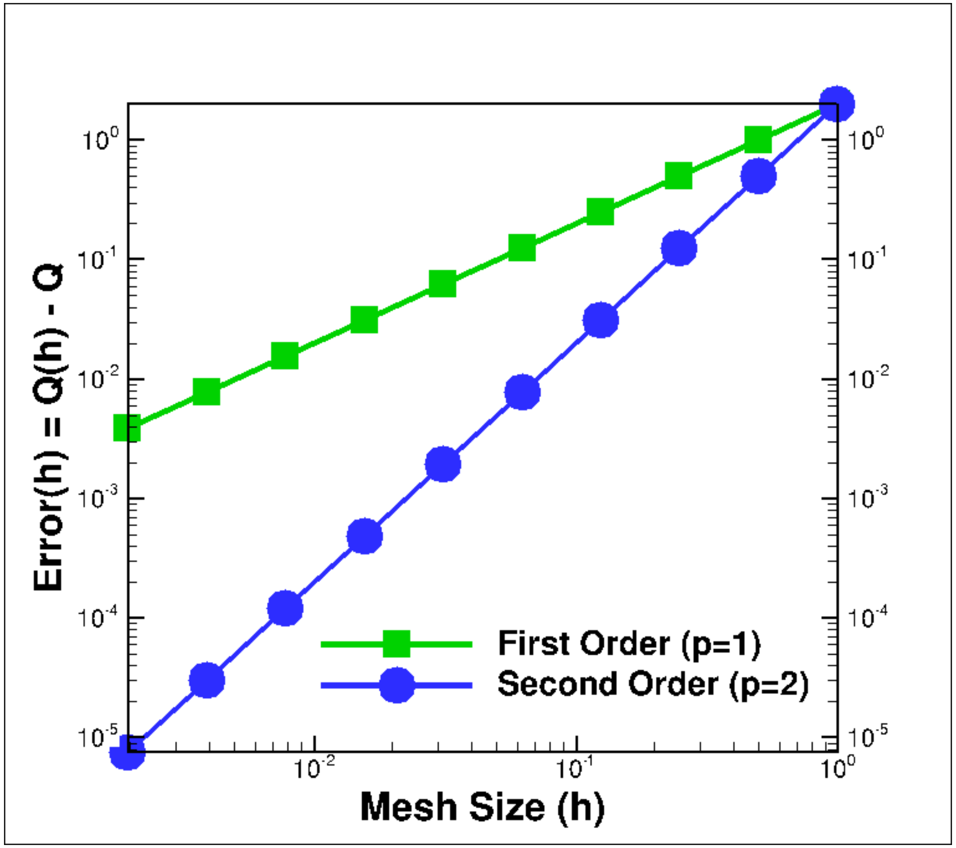


Can you see any difference?

Which QoI is computed more accurately (for given mesh size)?

Example: Numerical Error Model (2)

- When we know the exact QoI, we can compute the exact error at each mesh level



Under mesh refinement, higher order methods (with larger rates of convergence) provide superior accuracy

Numerical Error: A Simple Example

- ODE problem for integration of mechanical system (spring)

$$\text{“F=ma”} \iff -kx = m\ddot{x}$$

- We can build a numerical model (central difference)
- Think of this as a simplified version of a solid mechanics code
- We have an exact solution:

$$x(t) = x_0 \cos(\omega\, t), \quad \omega \equiv \sqrt{k/m}$$

$$x_{n+1} = x_n + \Delta t v_n + \frac{1}{2}(\Delta t)^2 a_n$$

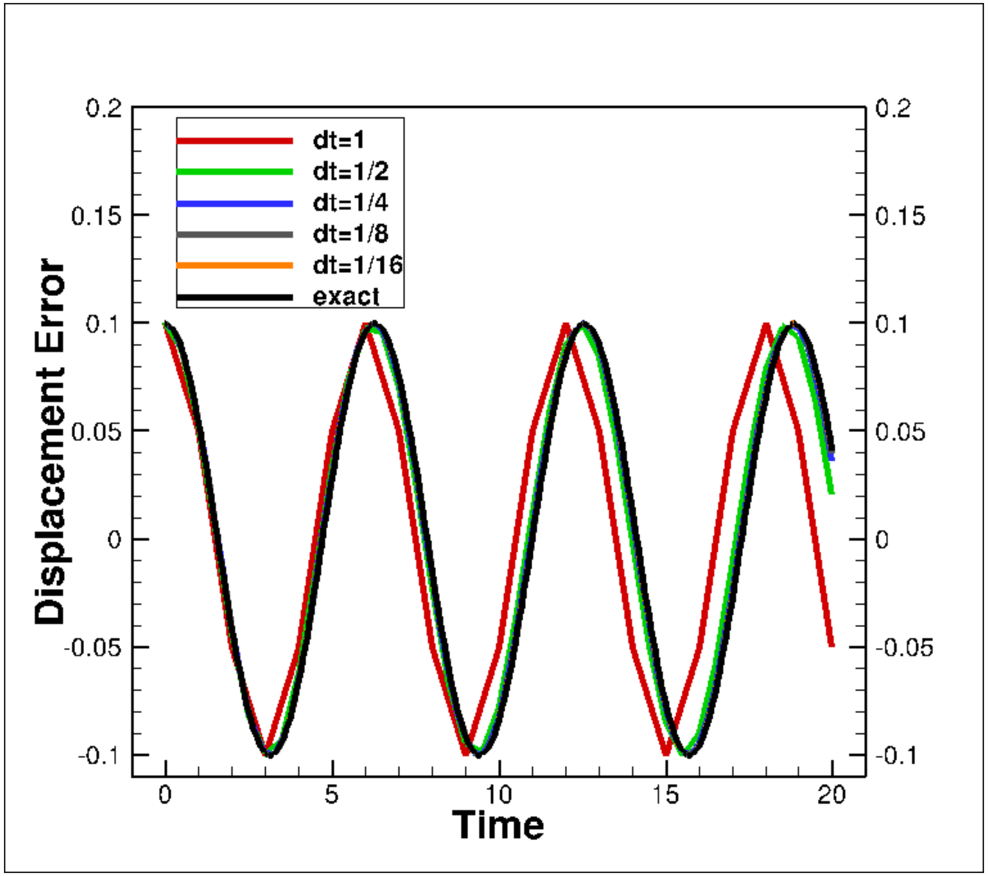
$$v_{n+1} = v_n + \frac{\Delta t}{2}(a_{n+1} + a_n)$$

$$a_{n+1} = m^{-1} F_{n+1} = -\frac{k}{m} x_{n+1}$$

Central Difference Integrator
(the numerical model).
Second order time accuracy.

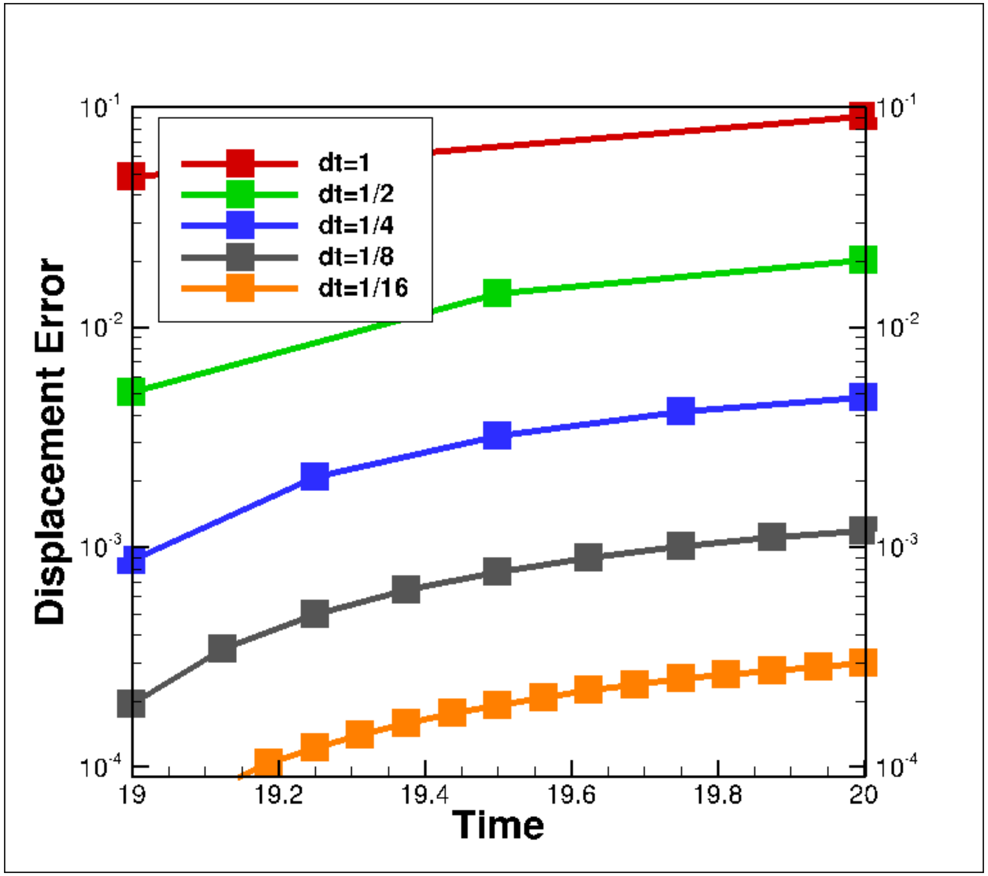
Simple Example: Position Output

- We plot position versus time for exact and numerical solutions
- We can observe phase errors and some loss of peak displacement
- How can we verify that the computer model (the implementation of the central difference integrator) is correct?



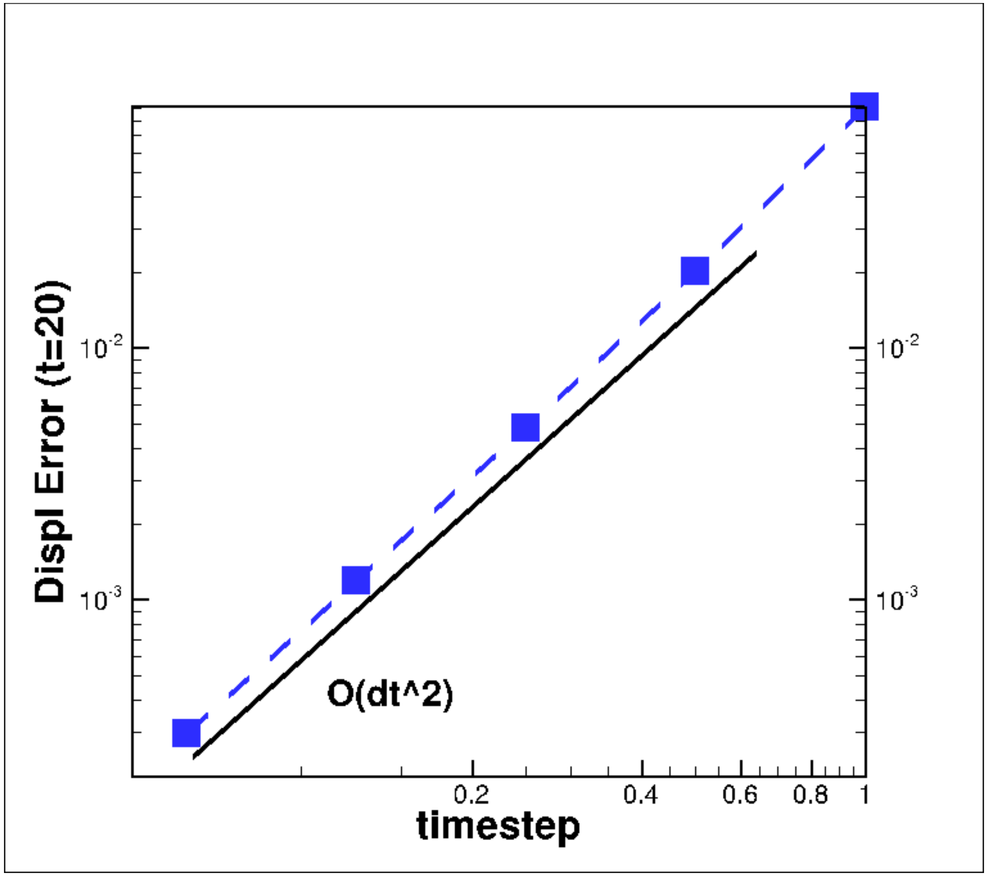
Simple Example: Position Errors

- Since we have the exact solution, we can plot the difference (errors) between numerical solutions and the exact solution
- We clearly see the errors reducing with time step size (here near final time)
- Is this enough evidence?



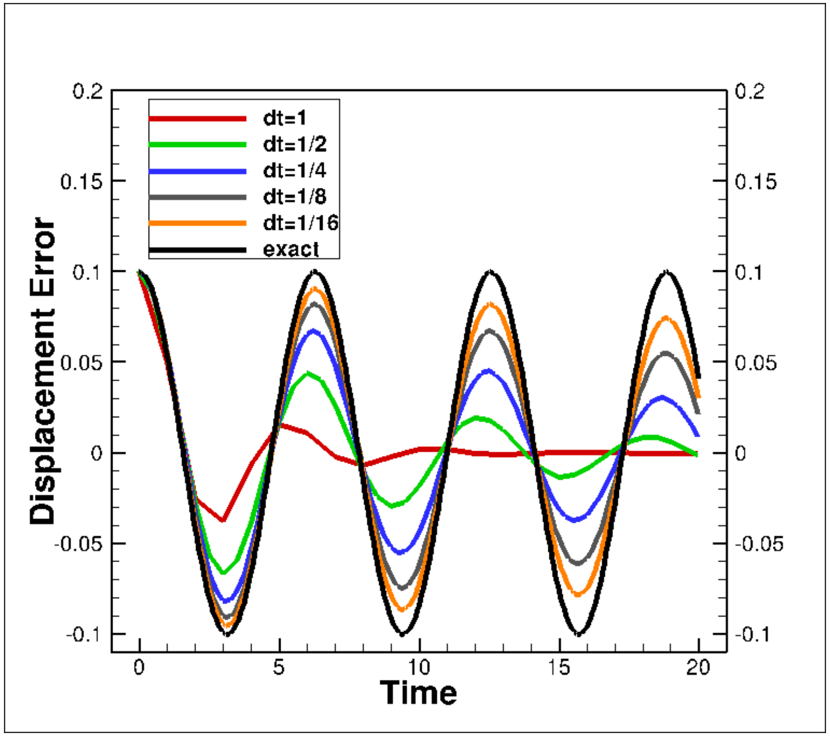
Simple Example: Rate of Convergence

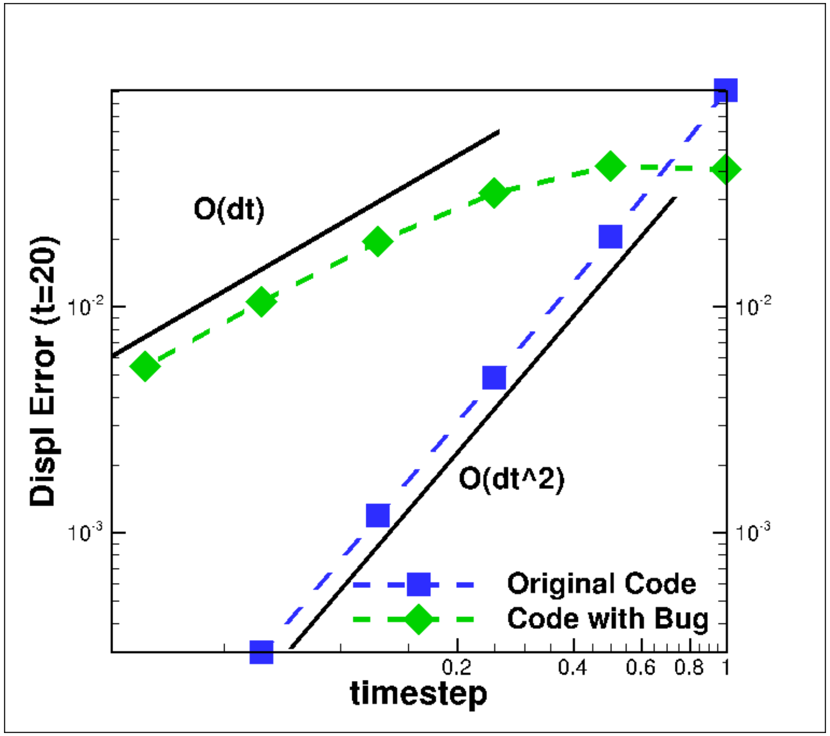
- We plot the errors versus the time step at final time (log-log scale)
- Now we see the second order slope and have verified that the implementation appears to deliver as promised
- Later we will discuss extrapolation when the exact solution is unknown



Simple Example: Code Verification

- Suppose we made a code mistake: $v_{n+1} = v_n + \Delta t\, a_{n+1}$
- We can get larger errors, lower convergence rates, sometimes no convergence at all!





Code and Solution Verification

Code Verification is the activity of ensuring that the code correctly implements the numerical model.

- Errors in computer models are called code defects or bugs
- The code developers/testers have primary responsibility for identifying and eliminating code bugs

Solution Verification is the quantification and reduction of numerical error.

- Done in the context of the overall uncertainty budget.
- Error may or may not need to be reduced.

Examples of Theoretical Convergence Rates

- We will use solid mechanics as an example
- Assume we are using linear finite elements (8-node hex)
- Modal analysis:
  - Eigenvalues and eigenvectors: p=2
- Static problems:
  - Displacements: p=2
  - Strains and stresses: p=1
- Dynamic problems (with second order time integrator)
  - Velocities: p=2 (other variables same as static case)
- These are the <u>optimal</u> rates. In practice, geometric and material irregularities will reduce the actual rate!

Outline of Class

- Part I: Introduction
- Part II: Code Verification
- Part III: Solution Verification
- Part IV: Adaptivity and Advanced Topics