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Verification Methods and NRC Regulations: A Brief Overview

Jim Stewart
Sandia National Laboratories

Thanks to Brian Carnes, Francois Hemez, and Rod Schmidt

Why Verification?

- **Reduce risk of high consequence code errors**
- **Reduce development and maintenance costs by finding code implementation errors sooner**
  - Beyond standard Software Quality practices
- **Quantify numerical errors as part of validation and predictions**
- **Reduce numerical errors through mesh adaptivity**
- **Assist in NRC licensing process by providing application-driven evidence of code and solution quality**

Verification: Some Definitions

- **Definition used by AIAA**

  The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.

- **Definition used by ASME**

  The process of determining that a computational model accurately represents the underlying mathematical model and its solution.

- **Definition used by DoD M&S Coordination Office**

  1. The process of determining that a model implementation and its associated data accurately represent the developer's conceptual description and specifications. 2. The process of determining that a model or simulation faithfully represents the developer's conceptual description and specifications. Verification evaluates the extent to which the model or simulation has been developed using sound and established software and system engineering techniques.

Verification Quiz

- **True or False:**

Good agreement with experiment means the equations are being solved correctly.

- *Comparing calculations with experiments does not address verification*
- *Verification addresses mathematical correctness of the software implementation*

More on Verification

Verification answers the questions:

- Is the computational method suitable for this problem?
- Is it implemented correctly?
- Is the computational mesh adequate?
- Is the input data adequate?

Verification has Two Primary Components

- **Code Verification**
  - Numerical Algorithm Verification
    - Verification testing (Order-of-Accuracy Tests)
    - Application-specific Verification Test Suite (VERTS) coverage analysis

- **Solution Verification**
  - Assess adequacy of spatial and temporal discretization
    - Mesh sensitivity studies
    - A Posteriori error estimation
    - Formal mesh refinement (e.g., Richardson extrapolation)
  - Assure correctness of user-input algorithm parameters

Code Verification Practices

- **Document all mathematical model equations and numerical models**
- **Implement support for Method of Manufactured Solutions (MMS), including**
  - User-defined source terms
  - Initial/boundary conditions
  - Material properties
- **Construct and regularly run a suite of order-of-convergence tests using the MMS approach**

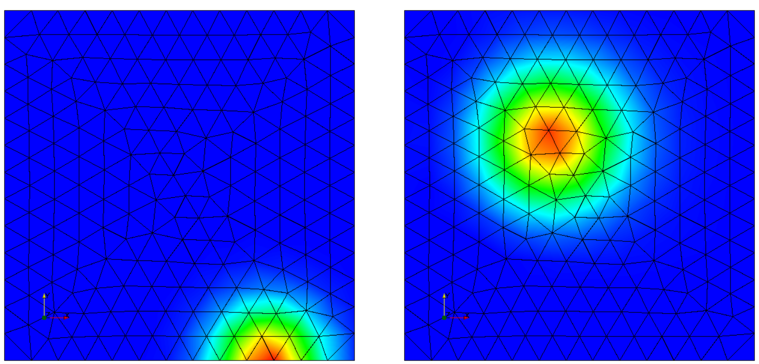
Code Verification Example

- **Goal: Verify theoretical convergence rates on test problem**
- **Compare numerical solution with reference (analytic) solution using error metrics**

$$||u - U|| \qquad \mathcal{Q}(u) - \mathcal{Q}(U)$$

- **Fit error model (steady/transient) to errors on different grids**

$$E(h,k) = C\,h^{\alpha} + D\,k^{\beta},$$



Transient diffusion problem with source term chosen to produce advecting exponential solution (left is t=0, right is t=1)

Transient order of converge parameters for error in gradients. Linear finite elements and second order time integration.

Level	C	D	alpha	beta
1	4.42	-0.752	0.618	0.566
2	6.22	0.137	0.976	2.48
3	8.01	0.531	1.07	2.82
4	5.68	0.691	0.970	2.81
5	6.99	0.857	**1.02**	**2.58**

More on Solution Verification

Solution verification addresses the following questions:

- **In the context of *model validation*:**
  - Are numerical errors obscuring or undermining comparisons of calculations with experimental data?
- **In the context of *predictions*:**
  - Is the solution accuracy adequate for the intended application?

Solution Verification Practices

- Insure at least ***two to three grid resolutions*** are available for any problem.
- Quantify <u>non grid-related</u> numerical error (iterative solver controls, contact tolerances)
- Quantify grid-related errors in response functions using Richardson extrapolation (if possible)
- Consider using *a posteriori* error estimation and adaptivity

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Solution Verification Example

- **Goal:** ***Estimate discretization error*** **on real problems**
- **Richardson Extrapolation:** **Compare numerical response quantities computed on three different grids/time steps**

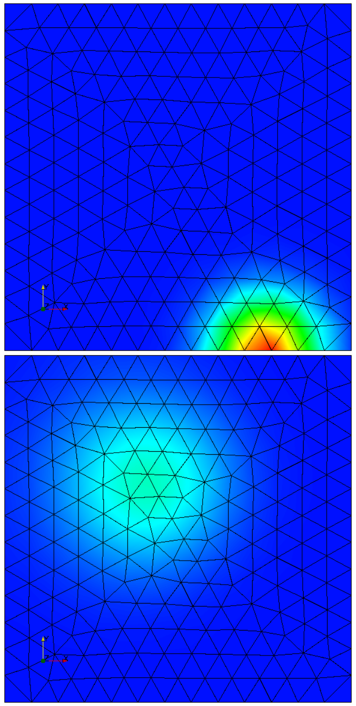
$$E(h,k) = Ch^{\alpha} + Dk^{\beta} = Q - Q(h,k)$$

Steady state requires 3 grids *Transient requires 3 grids/time steps*

Level	C	D	alpha	beta	Q
1	-0.15919	1.5491	1.7424	10.212	0.055312
2	-0.32215	-1.3289	2.8858	2.2447	0.056667
3	-0.16251	-2.0058	2.7479	2.4672	0.056614
4	-0.074378	-1.0142	**2.4408**	**2.1968**	0.056621

Transient advection-diffusion problem with exponential IC. Exact solution Q unknown.

Rates are approaching 2^{nd} order in space and time.



Limitations of Richardson Extrapolation

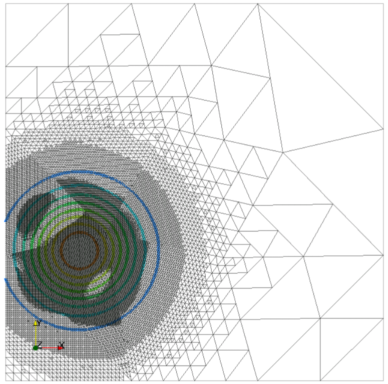
- **Running on multiple grid scales is costly**
- **Errors can change significantly as model parameters are varied**
  - Calibration, validation, uncertainty quantification
- **May not reach asymptotic regime**
- **Quantities may be non-monotone as grid is refined**
- **Realistic problems often do not exhibit theoretical converge rates**

Error Estimation and Adaptivity

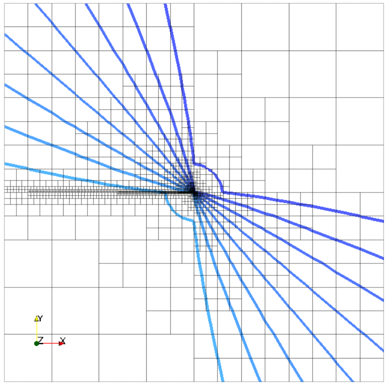
- **Outcomes**
  - Quantitative error estimates for a given grid
  - Reduction of numerical error through adaptivity
- **Goal-oriented approach**
  - Direct estimates of error in quantities of interest
  - Requires *intrusive* implementation (solver, PDE residuals, numerical method)
  - Rough cost: 20-50% of original simulation
- **Adaptivity**
  - For non-smooth problems (complex geometry, multiple materials) efficiency improves by orders of magnitudes
  - Implementation can benefit from existing libraries

Examples of Error Estimation and Adaptivity

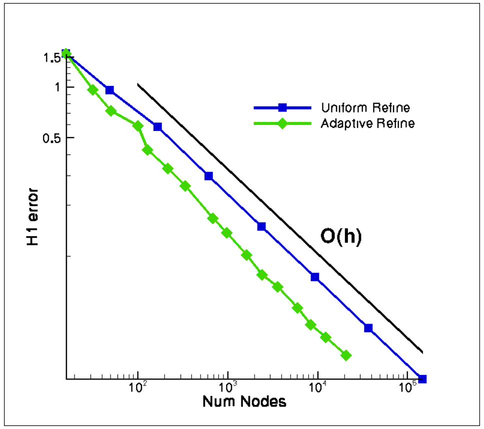
- **Test problems with exact solutions: (1) Smooth exponential (2) Non-smooth multi-material problem**



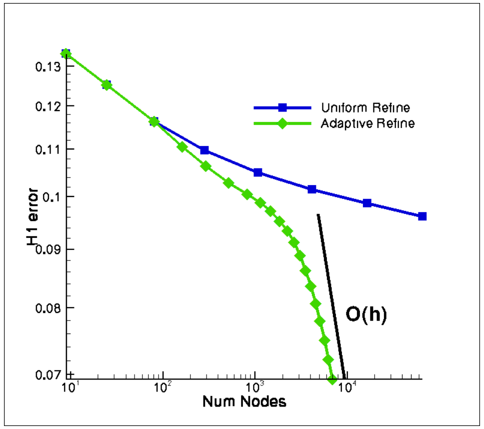
(1) Adaptivity based on error in gradients effectively resolves the solution



(2) Adaptivity is dramatic – six orders of magnitude in local mesh size.



(1) For smooth problems we get fractional increase in efficiency



(2) For non-smooth problems we get orders of magnitude increase in efficiency

Verification: When and Who?

When is verification done?

- Code Verification is done *before* Solution Verification
- …which is generally done *before* Uncertainty Quantification

Who has the primary responsibility?

- For code verification, the *code developers*
- For solution verification, the *code users*
- *To be effective, these activities are integrated, team efforts supporting the Born-Assessed framework*

Verification: What is Still Needed?

- **Development of manufactured solutions for the wide range of NEAMS applications**
- **Improved means of measuring adequacy and maturity of code verification testing**
  - Improved measures of code and feature coverage

    …*line coverage in regression testing is inadequate*
  - Coverage tools deployable to NEAMS IPSCs
- **Less expensive and more robust methods for estimating spatial and temporal discretization error**
  - Numerical error estimators for nonlinear parabolic and hyperbolic PDEs
  - Methods to handle the couplings across multiple physics and scales that NEAMS IPSCs will contain

VU-Related NRC Regulatory Requirements

Rodney C. Schmidt (SNL), "A review of NRC regulatory requirements and statements concerning verification, validation and uncertainty quantification of computer codes used in support of nuclear reactor license applications," ***FY09 NEAMS VU Milestone (SNL)***

NRC Regulatory Requirements Overview

- Construction and operational licenses for Nuclear Reactors require *detailed safety analysis* that is governed by NRC regulations and policies.

- *V&V and UQ are important topics* in regulatory documents describing safety analysis requirements.

- A clear understanding of the requirements and regulations that relate to V&V and UQ should guide the development of advanced modeling and simulations tools.

NRC Publications and Documents

Title 10, Code of Federal Regulations Part 50
Domestic Licensing of Production and Utilization Facilities

These are the regulations that must be officially satisfied

Regulatory Guides

These describe acceptable methods, procedures, etc. which, if followed, will meet regulatory requirements where applicable.

NUREG Reports

These address specific technical and programatic issues that may affect both the NRC and potential Licensees

Other

SECY
NRC Policy Statements

Title 10 Part 50 -- Domestic Licensing of Production and Utilization Facilities

Title 10 part 50 has ~1700 pgs, 50 "parts," and many appendices. Five sections were identified as important to code V&V and UQ.

- **§ 50.34 "*Contents of applications; technical information*" requires**
  - PSAR for construction license, FSAR for operational license, and QA
- **§ 50.36 "*Technical Specifications*" requires that safety limits, limiting control settings, etc. be based on the safety analysis.**
  - Defines why UQ is important because margins cannot be determined without UQ.
- **§ 50.46 "*Acceptance criteria for emergency core cooling systems for light-water nuclear power reactors*"**
  - Code validation and UQ requirements, key safety metrics (SRQs) specified

Title 10 Part 50 -- Domestic Licensing of Production and Utilization Facilities (Cont.)

- **Appendix B to Part 50** “***Quality Assurance Criteria for Nuclear Power Plants and Reprocessing Plants***”
  - States that QA requirements “apply to all activities affecting the safety related functions . . .” ;
- **Appendix K to Part 50 -- “*ECCS Evaluation Models*”**
  - Defines acceptable and required features of the ECCS evaluation models called for in §50.46, including
    - Code documentation
    - Spatial and temporal convergence studies
    - Code validation
    - Sensitivity Studies
    - Uncertainty Quantification

Key NRC Regulatory Guides

- **Regulatory Guides describe specific methods, processes, analysis and modeling, etc. that are considered acceptable by the NRC.**
  - Regulatory Guides are NOT regulations
  - Other methods may be used but may require a potentially long approval process
- **Over 200 active Regulatory Guides are in the Power Reactors section**

Key NRC Regulatory Guides (Cont.)

- **Ten were identified as particularly relevant, including:**
  - 1.70 Standard Format and Content of Safety Analysis Reports for Nuclear Power Plants (LWR Edition)
    - Describes all parts of an acceptable SAR, including V&V and UQ requirements
  - 1.157 Best-Estimate Calculation of Emergency Core Cooling System Performance
    - Effectively defines the current regulatory position on best-estimate calculations and UQ
  - 1.200 An Approach for Determining the Technical Adequacy of Probabilistic Risk Assessment Results for Risk-Informed Activities
    - V&V and UQ in the context of PRA
  - 1.203 Transient and Accident Analysis Methods
    - A central document describing NRC position on code V&V and UQ.

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Key NUREG Reports

NUREG Reports address specific technical/programmatic issues that may affect NRC and/or potential Licensees. Four of note:

- **NUREG-0800 -- Standard Review Plan for the Review of Safety Analysis Reports for Nuclear Power Plants**
  - The reviewers “Bible.” 315 separate pdf files organized into nineteen chapters and an appendix.
  - Eight sections are particularly relevant to V&V and UQ
- **NUREG/CR-5249 -- Quantifying Reactor Safety Margins: Application of Code Scaling, Applicability, and Uncertainty Evaluation Methodology to a Large-Break, Loss-of-Coolant Accident (CSAU)**
  - First rigorous effort (1989) for UQ of best-estimate computer codes.
  - Referenced in many key regulatory guides and NUREG reports

Key NUREG Reports (Continued)

- **NUREG-1855 -- Guidance on the Treatment of Uncertainties Associated with PRAs in Risk-Informed Decision Making**
  - Addresses both *aleatory* and *epistemic* uncertainty in the context of PRA
  - Very recent (March, 2009)
- **NUREG-1737 -- Software Quality Assurance Procedures for NRC Thermal Hydraulic Codes**
  - Defines V&V activities in five of the six "Elements of Software Quality Assurance" described.

Summary
Verification and Licensing Support

- **Verification**: Develop test problems, new methods, and software tools

- **Validation**: VU will collect validation datasets and identify database gaps as required by the born-assessed and licensing missions

- **Calibration, SA, UQ:** Develop and deploy new capabilities and software tools for the NEAMS IPSCs

- **Licensing:** Serve as the primary interface to the NRC for support of licensing using NEAMS science-based M&S tools and capabilities

Extra Slides

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Calibration, Validation, Prediction: *Where Does Verification Occur?*