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Identifying and Treating Numerical Uncertainties in the Code Verification Process

Scott W. Doebling[1], Diane E. Vaughan[2] and James R. Kamm[3]

[1] Computational Physics Division, Los Alamos National Laboratory
PO Box 1663, Los Alamos, New Mexico, USA, doebling@lanl.gov
[2] Computational Physics Division, Los Alamos National Laboratory
PO Box 1663, Los Alamos, New Mexico, USA, dev@lanl.gov
[3] Computational Physics Division, Los Alamos National Laboratory
PO Box 1663, Los Alamos, New Mexico, USA, jrkamm@lanl.gov

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The purpose of this research is to identify, analyze, and quantify the impact of numerical uncertainties in the process of performing code verification on a computational physics simulation code. We address uncertainties arising from both: (a) The computation of the test problem result in the physics simulation code; and (b) the calculations involved in the code verification analysis.

The most common approach to code verification proceeds as: (1) Select a verification test problem that has a well-characterized solution (typically an analytic, semi-analytic, or other highly accurate solution); (2) Set up and solve that problem in the computational physics code that is being assessed; and (3) Analyze the accuracy of the solution from the computational physics code using the well-characterized solution as the reference "correct answer." It is also common to vary the spatial mesh resolution and assess both the absolute solution error and its observed order of convergence.

Each of the above steps involves the selection of numerical models, numerical treatments, and associated parameters. We use the modifier "numerical" to distinguish these models, treatments, and parameters from the "physical" models and parameters that represent the actual conservation equations and closure relations used in the simulation code. We refer to the quantitative impact of these numerical factors on the computed results as "numerical uncertainty."

For example: In the process of performing a computational hydrodynamics simulation, the numerical choices include widely discussed and apparent factors such as mesh resolution and time step. There are also choices that can be less obvious to the user but potentially just as influential on the numerical uncertainty such as: The framing of the equations (Lagrangian, Eulerian, ALE); the underlying numerical scheme, including the discretization of the conservation equations using staggered-grid vs. cell-centered variables; assumptions of problem symmetry (e.g. spherically or axially symmetric); formulation of the numerical dissipation models (such as artificial viscosity) including selection of reference velocity, coefficients, and limiters; and inclusion of ancillary models such as mesh stabilization treatments. The user (knowingly or unknowingly) makes choices about all of these numerical factors, and the variation in these choices is a source of numerical uncertainty.

Likewise, when performing the code verification analysis, the user must make many choices, for example: How to map the computed and reference solutions onto a common domain; the choice of global verification metric (e.g. L1 or L2 norm); the weighting factors for the metric (e.g. volume, mass, unit); the method for computing the reference spatial dimension; the form of the error model; the method for estimating the parameters in the error model; the value for the expected convergence rate, etc. These choices also introduce numerical uncertainty into the process of code verification.

The approach employed here uses verification test problems to study the impact of these numerical choices on the code verification analysis of one or more hydrodynamics codes. The physics of interest for this study are limited to shock hydrodynamics of an ideal gas. The quantities of interest from such calculations include accuracy and spatial convergence of physical variables such as density, pressure, internal energy, temperature, and material velocity, and more general properties such as preservation of symmetry.