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Sensitivity and uncertainty quantification techniques applied to systems of conservation laws

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Abstract

Uncertainty quantification techniques are increasingly important in the interpretation of data and numerical simulations. Such techniques are typically employed either on data with poorly characterized underlying dynamics or on values from highly idealized model evaluations. We examine the application of these techniques to an intermediate case, in which data are generated from coupled, nonlinear partial differential equations—conservation laws—that admit discontinuous solutions. The values we analyze are generated from the numerical solution of the PDEs, in which we systematically vary both (i) fundamental modeling parameters and (ii) the underlying numerical algorithms. A number of sensitivity tests will be performed in order to assess the relative importance of such different types of uncertainty and we draw preliminary conclusions and speculate on the implications for more complex simulations.

Keywords: Conservation laws, compressible flow, sensitivity analysis, uncertainty quantification, statistical effect screening

1. Main text

We examine the application of sensitivity analysis and uncertainty quantification techniques to study the behavior underlying the set of coupled, nonlinear partial differential equations (PDEs) that govern compressible flow. In particular, we examine the sensitivity of the computed solution output to the structural parameters involved in determining the equations, to the parameters associated with the algorithms used to integrate the equations, and to the choice of the algorithms themselves. The approach we take examines different parameter sampling schemes (full factorial, quasi Monte Carlo, Latin Hypercube) and different tools with which to quantify the system's sensitivities, from screening to Sobol' method to emulation-based analysis.

The conservation laws of one-dimensional, inviscid, non-heat-conducting compressible flow can be written as

$$u_t + f_x(u) = 0 \tag{1}$$

where subscripts denote partial derivatives, u is the array of conserved variables (mass, momentum, and energy) $u = [\rho,\ \rho v,\ E]^{\mathrm{T}}$, with ρ the mass density, v the velocity, $E = \rho e + (1/2)\rho v^2$ is the total energy, with e the specific

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internal energy, and $f(u)$ is the flux function $f = [\rho v, \rho v^2+p, (E+p)u]^1$, with p the pressure. Augmenting these PDEs are an equation of state, $p = p(\rho,e)$, which characterizes the material response, and initial and boundary conditions. The proper solutions to these conservation laws are weak solutions that are chosen by the application of vanishing viscosity. These equations have extremely broad application; there are many references on numerical integration schemes for them, e.g., the monograph by LeVeque (2002). Notably, these PDEs admit discontinuous solutions (e.g., shock waves) and complex wave dynamics.

We consider problems that correspond to an idealized shock-tube configuration, described by Sod (1978), in which two constant but different initial states are allowed to interact under the dynamics of (1): $u(t=0) = u_1$ for $x < x_I$ and $u(t=0) = u_2$ ($\neq u_1$) for $x > x_I$. Only the stiffened gas equation of state is considered: $p = (\gamma-1)\rho e + \gamma p_\infty$, with free parameters γ and p_∞.

To solve the PDE system, the equations are discretized. The numerical solution of this discrete system provides an *approximate* solution to the PDE system. The computational algorithm that defines the discretization in space and time, for which there are several choices, can be viewed as a model in the uncertainty quantification context, and, thus, introduces many more parameters. For example, the computational mesh over which the solutions are obtained is apportioned into N cells, onto which (1) is discretized. Output values are generated as functions of the numerical solution and are smooth in nature. These shock physics simulations will be performed in ALEGRA, described by Robinson et al. (2008).

In addition to a large set of continuous and discrete parameters, there are model structure choices associated with the numerical solution of these equations. We consider full factorial design Latin Hypercube Sampling (LHS) and quasi Monte Carlo (QMC) sampling to sample the parameter/model space: in particular, it will be interesting to evaluate the effectiveness of QMC versus the other methods. We use a variety of techniques to characterize the sensitivity of the computed results to the parameters tested: (i) screening methods are very interesting, especially in view of extending the application for more complex simulation contexts; (ii) Sobol' method will provide easy and accurate computation of variance based measures, provided a sufficient number of model evaluations is affordable; (iii) testing and checking the effectiveness and performance of emulation based analysis, in combination with screening, is a very useful test per se and especially for any application where the Sobol' approach is not affordable. We will compare the results of the analysis produced by each method and the computational burden associated with their application. We expect that the results will depend most sensitively on the equation of state, the number of mesh cells used, and the finite difference approximation used for the first derivative in Equation (1).

We also anticipate that this work will be a useful guide and benchmark for more complex simulation studies.

2. References

LeVeque R., 2002: *Finite Volume Methods for Hyperbolic Problems*, Cambridge University Press, Cambridge, UK.

Robinson, A. et al., 2008: "ALEGRA: An Arbitrary Lagrangian-Eulerian Multimaterial, Multiphysics Code", AIAA-2008-1235, *Proceedings of the 46th AIAA Aerospace Sciences Meeting and Exhibit*, 7–10 January 2008.

Sod G., 1978: "A Survey of Several Finite Difference Methods for Systems of Nonlinear Hyperbolic Conservation Laws", *Journal of Computational Physics*, 27 (1), pp. 1–31.