Computational Physics and Methods

Consistent and Meta-Stable Equation of State Models for Hydro and Solid Dynamics

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Simulations of real engineering interest require the use of thermodynamic constitutive models that go beyond simple analytic equations of state. In this talk we discussed the complications that arise from using general equations of states for fluids and solids. Issues that need to be addressed include equilibrium and non-equilibrium treatments for mixed and separated species and robust treatments for incompatible mixtures such as metals in tension and gases.

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Background and Motivation

Simulations of real flows introduce many complications that are not present in typical academic simulations of ideal gases. The need to produce simulation results that can be used for engineering design require that the physical properties of the materials in the relevant flows be represented as realistically as possible. Our basic background here is to solve the compressible Euler equations for a possible mixture of materials:

$$\frac{\partial \rho}{\partial t} + \nabla \bullet \left(\rho \mathbf{u}\right) = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \bullet \left(\rho \mathbf{u} \otimes \mathbf{u}\right) + \nabla P = 0$$

$$\frac{\partial \rho \left(\frac{1}{2}u^2 + e\right)}{\partial t} + \nabla \bullet \left[\rho \mathbf{u}\left(\frac{1}{2}u^2 + e\right) + P\mathbf{u}\right] = 0$$

This model assumes that at the micro-scale the materials in the flow are separated by well-defined interfaces. In practice however the complete resolution of such interfaces is not practical and is replaced by one of several types of mixture closures. The use of such closures is unavoidable for real applications and the choice of a suitable model and some of its ramifications on the computation of the numerical solution are central to designing effective compressible simulation tools.

Description

The physical properties of a material that are relevant to a compressible flow are expressed by an equation of state (EOS) that relates the thermodynamic properties of the material, in our case the pressure, density, temperature, and specific internal energy [1, 2]. A major issue for applications using real equations of state is the finite domain of the intended EOS model. For example the SESAME [3] database for material properties list the equation of state properties as tabulated pressures and specific internal energies as functions of a tabulated list of densities and temperatures. Attempts to evaluate the EOS at densities or temperatures outside the tabulated ranges leads to extrapolations off the table and can produce unexpected results. A major issue for the hydrodynamic solver is the detect these out of domain evaluations and apply some “fix” to the results to ensure a stable solution. A second issue is the requirement that the EOS model be thermodynamically stable, this is a restriction on on the free energies that define the EOS to satisfy appropriate convexity conditions. Fundamentally a hydrodynamic solver needs for the thermodynamic isothermal bulk modulus (derivative of the pressure with respect to the log of the denstiy at constant temperature) to always be non-negative. Enforcing these conditions for a working hydro code that uses a variety of equations of state is a fundamental code design issue.

Mixtures are also a major issue to be handled by a robust multi-material hydro code. One of the most common closure models assumes that the materials in a computational cell are in equilibrium at a common temperature and density. Given the total specific internal energy

and specific volume of the mixture, together with the mass fractions of the material components in the cell, the cell pressure and temperature is computed using the condition that the total cell quantities for specific volume and energy are the mass average of the component values:

$$e = \sum_{k=1}^{N} \mu_k e_k\left(P,T\right),\ V = \sum_{k=1}^{N} \mu_k V_k\left(P,T\right)\ .$$

A similar model for gas mixtures assumes that the components are mixed at a molecule level and hence occupy the entire volume simultaneously. In this case we are given the component specific volumes, mass fractions, and the total specific volume and energy in the cell and the cell temperature is computed by solving:

$$e = \sum_{k=1}^{N} \mu_k e_k\left(V_k,T\right),\ P = \sum_{k=1}^{N} P_k\left(V_k,T\right)\ .$$

In both cases a major issue is to handle the out of domain evaluations in some reasonable way the does not produce "bad" mixed cell properties. A good example of this is when the materials include metal-gas mixtures that are approaching cavitation.

Beyond these two models for fully mixed cells there are a great number of extensions to non-equilibrium mixtures. These extensions all involve the imposition of additional dynamic equations for the component volumes or entropies in order to close the partial differential equations for the flow. A broad equilibrium pressure and non-equilibrium temperature closures in common usage [4] is the uniform strain (or uniform compression) model that asserts that each separate component in a material volume experiences the same relative compression. Mathematically this property is expressed by the condition that the volume fractions for the components are conserved. A corresponding model assumes that the components are thermally isolated so the each component entropy advects with the flow. Further non-equilibrium extensions may relax the condition of pressure equilibrium as well as temperature. Such extensions are important for metal-gas mixtures where the physical equilibrium property is normal stress across the separating interface.

Anticipated Impact

Treating general equations of state, especially for mixtures, is a daunting task and is a major source of simulation failures for high-energy flows. There is a continuing effort to improve the robustness of flow solvers subject to equation of state errors and deficiencies. Improvement in such treatments, including the identification of when they occur, is critical for conducting predictive simulations of high-speed flows. Improving the efficiency of the EOS evaluations is another important objective. Indeed, for purely hydrodynamic simulations using real equations of state like SESAME, the overhead for the EOS evaluations is likely to be the single largest factor in the simulation time to completion.

Path Forward

Better schemes for extracting the EOS domain of validity are perhaps the leading deficiency in the use of use models in engineering applications. Error handling for out of domain evaluations is also essential. Improving the efficiency of tabulated EOS evaluations is greatly needed as well.

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