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Discrete Lagrange equations for reacting thermofluid dynamics in arbitrary Lagrangian–Eulerian frames

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Abstract

Interest in the development of multiscale methods has focused attention on the marked differences in the numerical modeling techniques typically applied at different scales. Most continuum dynamics models construct approximate solutions to partial differential equations, while most nanoscale models employ a discrete Hamiltonian approach. Previous research has demonstrated that the introduction of entropies or internal energies as generalized coordinates, along with separation of the discretization and model formulation steps, allows general thermomechanical models to be developed, at the continuum scale, using a nonholonomic Hamiltonian or Lagrange equation formulation. With the introduction of additional state variables and nonholonomic constraints, the latter work may be further extended in order to model reacting systems. Employing a finite element interpolation and a Lagrangian, an Eulerian, or an ALE mesh, the new formulation has been validated by solving several one-dimensional reacting shock physics problems. The result is a continuum dynamics modeling approach highly compatible with the discrete energy methods normally used at the nanoscale.

Keywords: Lagrange's equations; ALE; Reacting systems; Detonation

1. Introduction

In previous work the authors and co-workers [1–3] have developed new discrete energy methods for continuum fluid dynamics modeling. Employing entropies or internal energies as generalized coordinates, and a finite element interpolation of the flow field, the cited works formulated discrete Hamiltonian or Lagrange equation formulations for viscous compressible fluid dynamics in Lagrangian, Eulerian, and arbitrary Lagrangian–Eulerian (ALE) frames. The ODE models were developed without reference to any partial differential equations, and were validated by solving a set of shock physics problems. The latter work established the feasibility of applying typical nanoscale modeling methods to thermomechanical continuum dynamics simulations, for both open and closed systems, and therefore offers opportunities for the development of multiscale simulation techniques based on a unified energy-based modeling methodology. This paper extends the aforementioned work to reacting flows, including the strong chemical–thermomechanical coupling associated with detonations.

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The chemical dynamics included in a reacting flow model is normally quantified by modeling processes which occur on a scale much smaller than that required to model the fluid dynamics. At the molecular level energy based modeling methods are the norm [4], while at the system level the use of energy methods is relatively rare [5]. Both finite difference [6,7] and finite element methods have been employed to model reacting systems. Explicit methods [8–10] are typically used to model fast flows, such as detonations, while implicit methods [11] have been effectively employed in modeling slower systems. Oran and Boris [12] and Powers [13] review various methods used in numerical simulation of reactive flow and detonations, including multi-scale modeling.

In general the introduction of finite-rate chemistry leads to significant complications. Additional state variables are needed, one for each chemical species, as well as species continuity relations with source terms. The choice of chemical kinetic model, including the number of modeled reactions and their rate constants, largely determines computational cost. For example in combustion chemistry, computational requirements increase with the size of the fuel molecule. Hydrogen–air combustion models typically involve approximately 10 species and 30–60 reaction equations, if nitrogen is considered inert. Including nitrogen chemistry can double the number of species and reactions. Methane and ethane based models may again double the number of species and reactions, while octane models may include 800 species and 3000 reactions [12]. At very high temperatures, modeling the free electrons in an ionizing flow may be required. Stiffness problems may arise in systems involving fast reactions of species with small concentrations [12,14,6]. In view of these complications, simulations of detonation are often limited to one spatial dimension [13,15–17], sometimes as a prelude to more expensive two and three dimensional simulations [18]. In some previous work, the assumption of simplified one-step kinetics (two species and a single, irreversible reaction equation) has allowed for very efficient modeling of reacting shocks [12,19–23]. It has also allowed for the study of unstable 1-D detonations [22,24,18,25]. In these models resolution requirements may influence predictions of detonation stability [15,17]; the same may be true when more detailed kinetics [26,27] are included. Modeled instabilities are often described as pulsating or galloping, characterized by regular, short-period, low-amplitude oscillations.

The formulation of the system level model developed in this paper may be outlined as follows. First a simple finite-element interpolation is introduced and the state variables are chosen (they include the mesh coordinates). Having adopted an ALE frame of reference, a set of constraints describing the mesh motion is then specified [3]. Then the kinetic and potential energies are formulated, the latter as a simple sum of the element internal energies. Next, the conservation of mass and energy relations and the species evolution equations are introduced, as nonholonomic constraints. A virtual work expression is then developed, which includes the effects of momentum and energy convection. Finally the canonical Lagrange equations are introduced, and are specialized to obtain the final state equations for the system. To validate the model, a number of example problems are solved, which include: (1) Eulerian, Lagrangian, and ALE meshes, (2) both open and closed systems, (3) simplified as well as relatively detailed chemical kinetics, and (4) stable as well as unstable pulsating overdriven detonations. Note that species diffusion effects are neglected, as is typically the case for shocked flow and detonation simulations [28,12,7].

2. Discretization

The finite element interpolation adopted here employs piecewise constant velocity gradients, with mass densities and internal energy densities also uniform on an element. In the one dimensional models described in this paper, these elements are two-noded lines; they are of course three-noded triangles or four-noded tetrahedra in two and three dimensions. On external boundaries open to flow, the total pressure and total enthalpy are taken to be piecewise constant.

The system level model is composed of n_e elements and n_n nodes. The extensive state variables for each element are the total mass $m^{(i)}$, the total internal energy $U^{(i)}$, and the species masses $s_k^{(i)} (k = 1 \dots N_s - 1)$ for a mixture of N_s chemical species where

$$\sum_{k=1}^{N_s} s_k^{(i)} = m^{(i)}. \tag{1}$$

In one dimension the global mass, species mass, and internal energy vectors are (with superscript T the transpose)

$$\mathbf{m} = [m_1 m_2 \dots m_{n_e}]^T, \quad \mathbf{s} = [\mathbf{s}^{(1)T} \mathbf{s}^{(2)T} \dots \mathbf{s}^{(n_e)T}]^T, \quad \mathbf{U} = [U_1\ U_2 \dots\ U_{n_e}]^T \tag{2}$$