Journal of Computational Physics 272 (2014) 842–864

Contents lists available at ScienceDirect

Journal of Computational Physics

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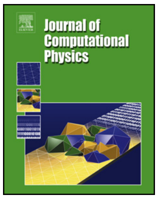

WAMR: An adaptive wavelet method for the simulation of compressible reacting flow. Part II. The parallel algorithm

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ARTICLE INFO

Article history:
Received 20 August 2012
Received in revised form 27 March 2014
Accepted 28 March 2014
Available online 4 April 2014

Keywords:
Wavelet
Adaptive
Compressible reacting flow
Newtonian fluid
Detailed kinetics
Multicomponent diffusion
Detonation
Bubble ignition

ABSTRACT

The Wavelet Adaptive Multiresolution Representation (WAMR) algorithm is parallelized using a domain decomposition approach suitable to a wide range of distributed-memory parallel architectures. The method is applied to the solution of two unsteady, compressible, reactive flow problems and includes detailed diffusive transport and chemical kinetics models. The first problem is a cellular detonation in a hydrogen–oxygen–argon mixture. The second problem corresponds to the ignition and combustion of a hydrogen bubble by a shock wave in air. In both cases, results agree favorably with previous computational results.

1. Introduction

Reacting flows typically consist of a multicomponent mixture of gases, undergoing some form of reaction process, which may include any combination of combustion, ionization, or even nuclear reactions. In such flows, reactions often act as energy sources (or sinks), driving, or otherwise altering, the bulk fluid motion of the mixture. Conversely, the rate and extent of reactions depend on the local fluid state, coupling fluid motion and reactive sources. In the continuum limit, these problems are described by the reactive compressible flow equations. The flow equations consist of a set of coupled partial differential equations (PDEs) governing the conservation of mass, momentum, energy, and evolution of species mass fractions, and, with constitutive equations and appropriate boundary and initial conditions, define specific problems.

The present work is primarily concerned with the simulation of high-speed flows, where compressibility effects and the presence of phenomena such as shock waves are important. In addition, we consider flows where chemical reactions occur. The reactive source typically consists of exothermic oxidation reactions, resulting in the occurrence of detonations. As a result of the stringent resolution demanded by detonations, it is common practice to use reduced or simplified models. The most common simplifications are those applied to diffusive effects and to the reactive source. In the first case, diffusive transport of mass, momentum, and energy are neglected, with the *a priori* assumption that small-scale effects associated with diffusion are negligible. The omission of diffusive effects leads to purely "inviscid" solutions, and also "removes" their associated fine resolution requirements. However, the removal of diffusion effects makes the governing equations purely hyperbolic with the smallest length scale being identically zero. Their solution requires appropriate numerical methods to

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http://dx.doi.org/10.1016/j.jcp.2014.03.059

provide an artificial smallest length scale through a numerical viscosity to retain solution stability and monotonicity near shock or detonation fronts [1].

Detailed chemical reaction mechanisms consist of a number of species undergoing a set of elementary reactions with prescribed rate constants typically of an Arrhenius form. The reaction mechanism enters the system of equations as a species production rate. However, detailed reaction terms are often computationally costly due to two aspects. The first is purely the expense of computing the numerous species and rate constants; detailed mechanisms for a simple hydrocarbon such as methane contains 30 species and 300 reactions [2], while larger hydrocarbons like iso-octane contain 860 species and 3600 reactions [3]. The prediction of mass fractions of species necessitates the solution of their corresponding evolution equations. Furthermore, as the rate constants are dependent on the local state, they need to be evaluated at every grid point at each time step. Both aspects lead to a large computational cost. A second factor is due to the inherent stiffness of chemically reacting systems. Each reaction in the mechanism proceeds at varying rates, with some occurring over very short time scales; which, in turn, limits the integration time-step that can be used. Due to these factors, reduced or simplified models are often employed instead of the full detailed chemical kinetics. The degree of reduction is highly dependent on the specific information that one desires to address. In general, reduced chemistry models used in detonation simulation consist of a small number of easily evaluated kinetic steps, calibrated to approximate overall effects of chemical reactions [4–12].

The construction of simplified reaction models is an active field of research [13–16]. However, the use of most such models introduces significant error into simulations. Simplified models, especially phenomenological models such as the one- and two-step reactions, do not capture all relevant dynamics inherent in the full mechanism [17]. The loss of these dynamics and the coupled nature of the fluid dynamics and chemistry, generally leads to simulations relying on reduced models having only, at best, qualitative similarity to the true physics [18,19]. Furthermore, such models cannot provide important kinetic details that could lead to improvement in fuel efficiency, or cannot provide predictions regarding minor species, which are key to pollution reduction. However, recent approaches do show promise to provide accurate, reduced models through multiscale analysis [20–30]. In the present work we use only hydrogen mixtures for reactive problems. For a simple fuel such as hydrogen, detailed reaction mechanisms contain usually 9 species and at most 40 or so reactions. A mechanism of this size is sufficiently small to be utilized on today's modern computers. The relative simplicity of the chemical kinetics and its common use in experiments has led to a large number of investigators concentrating on reacting flows using hydrogen mixtures.

Because of the true multiscale nature of compressible reacting flows, the use of adaptive methods to simulate them almost always offers an essential advantage. A number of adaptive mesh refinement (AMR) packages and libraries have been developed and applied to various problems. AMROC [31] is an implementation of the Berger–Oliger AMR scheme using modified DAGH [32] subroutines for grid operations and data management in parallel computing environments. It has been applied to simulations of detonations propagating through channels in 2- and 3-dimensions (2- and 3-D) using the reactive Euler equations with detailed chemical kinetics [33,34]. The PARAMESH [35] library provides routines for parallel AMR using a subdivision scheme. It has been applied to a variety of problems including cellular detonations in carbon [36], magnetohydrodynamics, and astrophysical hydrodynamics [37]. A similar subdivision AMR scheme with a novel data structure is described in [38], and used extensively by Oran and coworkers for studying laminar flame propagation [39], cellular detonation structure [40], and deflagration-to-detonation transition (DDT) [7,41] in channels.

The current work extends the work discussed in Part I [42]. It addresses the development of an efficient parallel adaptive wavelet-based collocation method for the simulation of compressible, reactive flows. As demonstrated in Part I, the amplitudes in the wavelet transform used in the method provide a direct measure of the local error at each collocation point. Subsequently, spatial grid adaption can be driven by removing points with small wavelet amplitudes resulting in a minimal loss of accuracy while greatly reducing the number of unknowns. Coupled with the efficient use of widely available distributed memory parallel architectures, the method presented in this work provides a tool for producing solutions of multidimensional problems using an adaptive verified numerical simulation (VNS). Though this work is focused on the simulation of reactive flows, the method developed is equally applicable to many multiscale problems encountered in other disciplines.

2. Governing equations

The numerical simulation of reactive flows consists of the solution of a set of governing equations which model the physics and chemistry along with associated initial and boundary conditions using a numerical method. Here we solve the unsteady, compressible, reactive balance equations for a K-component mixture in a d-dimensional problem in conservation form. Details are given in Part I [42]. Briefly, the set of equations describes conservation of mass, linear momentum, and total energy, and includes $K-1$ evolution equations for the species' partial densities.

The system of balance equations are closed by additionally defining constitutive relationships for the equations of state based on thermodynamic relations, diffusive transport based on a Newtonian fluid, Fourier and Ficks' laws with Sorét and DuFour effects, and chemical kinetics based on the law of mass action and the Arrhenius form of reaction rate temperature dependence. For complete details the reader is referred to Part I [42].