A sparse stiff chemistry solver based on dynamic adaptive integration for efficient combustion simulations

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ABSTRACT

A sparse stiff chemistry solver based on dynamic adaptive hybrid integration (AHI-S) is developed and demonstrated for efficient combustion simulations. In a previous study, a dynamic adaptive method for hybrid integration (AHI) was developed to speed up the time integration of chemically reacting flows with detailed chemistry. The AHI method solves the fast subcomponent of chemistry implicitly and the slow subcomponent of chemistry and transport explicitly, and it was shown that AHI is more accurate and efficient than the operator-splitting schemes when there are significant radical sources from the transport term. In the present study, the AHI method is first improved to minimize the number of nontrivial entries in the Jacobian. Sparse matrix techniques are further integrated into AHI to achieve high computational efficiency. The performance of the new AHI-S solver is investigated in constant-pressure auto-ignition systems using different mechanisms that consist of 9–2878 species. It is shown that the computational cost of the AHI-S solver is overall linearly proportional to the mechanism size and is comparable to that of evaluating reaction rates using CHEMKIN-II subroutines. The AHI-S solver achieves speed-up factors ranging from approximately 10, for the 9-species hydrogen mechanism, to approximately 3000, for the 2878-species biodiesel mechanism, compared with the fully implicit VODE solver with Jacobian evaluated through numerical perturbations and factorized with dense matrix operations. It is further found that for mechanisms with less than approximately 100 species, the time saving of AHI-S is primarily attributed to the reduced size of the implicit core of the governing equations, while for mechanisms with more than 100 species, the computational cost of VODE is dominated by the dense LU factorization, such that the time saving of AHI-S is mostly attributed to the sparse LU factorization. The AHI-S solver is then applied to unsteady perfectly stirred reactors involving extinction and re-ignition. Speed-up factors from 50 to 30,000 are achieved compared with the Strang splitting scheme with the chemistry substeps implicitly integrated with VODE, while speed-up factors of 10–100 are achieved compared with the Strang splitting scheme implemented with the sparse stiff LSODES solver. In the end, the performance of AHI-S is investigated in one-dimensional (1-D) unsteady freely propagating laminar premixed flames for a methane/air mixture, for which the time step size in AHI-S is limited by the fastest transport process. A speed-up factor of approximately 200 is achieved compared with the Strang splitting scheme for fixed time step sizes between 10^{-8}s and 10^{-6}s.

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1. Introduction

Detailed chemical kinetics is important for accurate prediction of combustion processes such as ignition, extinction and flame propagation, while it may involve a large number of species and reactions [1]. Recent progress in mechanism reduction, e.g. using directed relation graph (DRG) based methods [2–7], makes it possible to obtain accurate yet still comprehensive skeletal mechanisms with less than a few hundreds of species for practical engine fuels. However chemical stiffness may remain in skeletal and even reduced mechanisms due to the highly reactive radicals and their short timescales, such that the high-cost implicit solvers for ordinary differential equations (ODE), e.g. VODE [8] and DASAC [9], are typically required for time integration of combustion systems using reasonably large time steps.

To alleviate this problem, dynamic stiffness removal [10] was developed to eliminate short chemical timescales for compressible flow simulations using direct numerical simulations (DNS), such that the low-cost explicit solvers can be employed with time step sizes up to approximately 20 ns. Implicit solvers are typically

required for combustion simulations involving even larger time steps. For multidimensional flows, the operator-splitting schemes are widely used to separate chemistry integration from that of transport processes to avoid the high computational cost for solving fully coupled implicit equations [11–15]. Splitting schemes however can incur significant errors in certain cases. For example, it was found in Ref. [16] that, when significant radical sources are present in the transport term, $O(1)$ splitting errors may occur in ignition processes unless small time steps comparable to those required for explicit solvers are taken. A dynamic adaptive hybrid integration (AHI) method [16] was then developed for effective error control in such cases. Significant speed-up was achieved as well using AHI compared with the splitting schemes for small and moderately large mechanisms, say with less than about 100 species, by solving only the fast subcomponent of chemistry implicitly.

Nevertheless, for large mechanisms, Jacobian evaluation and factorization can dominate the computational cost in implicit solvers, such that analytical Jacobian evaluation [17], sparse matrix techniques [18–20], and adaptive preconditioning methods [21,22] can significantly speed up stiff chemistry solvers. As reported in Refs. [18,20], the computational cost for chemistry integration can be reduced to approximately a linear function of the number of species, N, using sparse matrix techniques, while it can scale as $O(N^2)$ to $O(N^3)$ using dense matrix operations. The sparse matrix techniques are also applicable to AHI to further reduce the computational cost, particularly when large mechanisms are involved.

In the present study, a sparse AHI solver (AHI-S) is developed to further reduce the size of the fast chemistry subcomponent, such that sparser Jacobian can be obtained for improved efficiency. The performance of the AHI-S solver is first investigated in auto-ignition using mechanisms with 9, for hydrogen, to 2878 species, for a biodiesel surrogate. AHI-S is compared with other solvers for numerical efficiency in a variety of combustion systems including auto-ignition, unsteady perfectly stirred reactors (PSRs) and 1-D freely propagating premixed flames. It will be shown that AHI-S can achieve similar per-step computational cost to that of fully explicit solvers.

The paper is organized as follows. In Section 2, the AHI method is reviewed and the AHI-S method is formulated, results from the AHI-S method for various combustion systems are presented and compared with other solvers in Section 3, and conclusions are drawn in Section 4.

2. Methodology

2.1. Review of the AHI method

The spatially discretized governing equations for typical reacting flows can be expressed as the following ODEs:

$$\frac{d\mathbf{\Phi}}{dt} = \mathbf{S}(\mathbf{\Phi}) + \mathbf{M}(\mathbf{\Phi}) \tag{1}$$

where $\mathbf{\Phi}$ is the vector of dependent variables of dimension n_Φ, including, e.g. temperature and species concentrations, and $\mathbf{S}$ and $\mathbf{M}$ represent the chemistry and transport terms, respectively. Note that in a multi-grid system, $\mathbf{\Phi}$ consists of variables at all grid points. In the AHI method [16], fast species and reactions are first identified on-the-fly based on reaction timescales defined in a recent analytic formulation of computational singular perturbation (CSP) [23]:

$$\tau_i \equiv \left| \frac{\partial \Omega_i}{\partial \mathbf{c}} \cdot \mathbf{v}_i \right|^{-1},$$

$$\frac{\partial \Omega_i}{\partial \mathbf{c}} = \left[\frac{\partial \Omega_i}{\partial c_1}, \frac{\partial \Omega_i}{\partial c_2}, \ldots, \frac{\partial \Omega_i}{\partial c_N} \right], \quad \mathbf{v}_i = [v_{1,i}, v_{2,i}, \ldots, v_{N,i}]^T \tag{2}$$

where τ_i is the timescale of the ith reaction, Ω_i is the reaction rate, N is the number of species, c_k is the mole concentration of the kth species, and $v_{k,i}$ is the stoichiometric coefficient of the kth species in the ith reaction. The ith reaction is considered to be fast if

$$\tau_i < \tau_c/\beta \tag{3}$$

where τ_c is a threshold timescale that is typically comparable to the integration time step Δt, and β is a safety factor. The kth species is considered to be fast if the following criterion is satisfied for any fast reaction i,

$$\left| \frac{\partial \Omega_i}{\partial c_k} \right| > \beta \tau_c^{-1}. \tag{4}$$

Note that the safety factor is typically mechanism-dependent and different safety factors can be optionally used for the identification of fast species and reactions.

The governing equations (Eq. (1)) can then be rewritten as:

$$\frac{d\mathbf{\Phi}}{dt} = \mathbf{S}_f(\mathbf{\Phi}) + \mathbf{g}_s(\mathbf{\Phi}), \qquad \mathbf{\Phi} = \begin{bmatrix} \mathbf{\Phi}_f \\ \mathbf{\Phi}_s \end{bmatrix}$$

$$\mathbf{S}_f = \sum_{i=1}^{m} \mathbf{v}_i \Omega_i$$

$$\mathbf{g}_s = \sum_{i=m+1}^{n_r} \mathbf{v}_i \Omega_i + \mathbf{M} \tag{5}$$

where $\mathbf{\Phi}_f$ and $\mathbf{\Phi}_s$ are the fast and slow variables of dimension n_f and $n_\Phi - n_f$, respectively, n_r is the total number of reactions, and m is the number of fast reactions. It is assumed that sufficiently small integration time steps are taken, such that the transport term and the energy equation are not stiff. In AHI, the ODE system in Eq. (5) is temporally discretized using a first-order scheme:

$$\begin{bmatrix} \mathbf{\Phi}_f^{n+1} - \mathbf{\Phi}_f^{n} \\ \mathbf{\Phi}_s^{n+1} - \mathbf{\Phi}_s^{n} \end{bmatrix} \frac{1}{\Delta t} = \mathbf{S}_f \left(\mathbf{\Phi}_f^{n+1}, \ \mathbf{\Phi}_s^{n} \right) + \mathbf{g}_s \left(\mathbf{\Phi}_f^{n}, \ \mathbf{\Phi}_s^{n} \right) \tag{6}$$

where the superscript n indicates the nth time step. The fast variables $\mathbf{\Phi}_f^{n+1}$ are solved implicitly using the first n_f equations of Eq. (6). The slow variables can then be solved explicitly from the remaining equations.

2.2. A sparse AHI solver (AHI-S)

2.2.1. Sparse Jacobian for the fast chemistry subcomponent

The chemical Jacobian is typically sparse for most practical fuels involving large mechanisms. The sparse pattern of the chemical Jacobian is first demonstrated using constant-pressure auto-ignition governed by

$$\frac{dy_k}{dt} = \frac{\omega_k W_k}{\rho}, \quad k = 1, 2, \ldots, N \tag{7}$$

$$\frac{dT}{dt} = -\frac{1}{\rho c_p} \sum_{k=1}^{N} h_k \omega_k W_k \tag{8}$$

$$\rho = p \left/ \left(R_u T \sum_{k=1}^{N} \frac{y_k}{W_k} \right) \right. \tag{9}$$

where the subscript k indicates the kth species, y is mass fraction, ω is species molar production rate, W is molecular weight, h is specific enthalpy, c_p is the mixture-averaged specific heat capacity, ρ is density, p is pressure, T is temperature, and R_u is the universal gas constant.