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Faster solvers for large kinetic mechanisms using adaptive preconditioners ☆

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Abstract

The adaptive preconditioners developed in this paper substantially reduce the computational cost of integrating large kinetic mechanisms using implicit ordinary differential equation (ODE) solvers. For a well-stirred reactor, the speedup of the new method is an order of magnitude faster than recent approaches based on direct, sparse linear system solvers. Moreover, the new method is up to three orders of magnitude faster than traditional implementations of the ODE solver where the Jacobian information is generated automatically via finite differences, and the factorization relies on standard, dense matrix operations. Unlike mechanism reduction strategies, the adaptive preconditioners do not alter the underlying system of differential equations. Consequently, the new method achieves its performance gains without any loss of accuracy to within the local error controlled by the ODE solver. Such speedup allows higher fidelity mechanism chemistry to be coupled with multi-dimensional fluid dynamics simulations.

Keywords: Chemical kinetics; Sparse matrix; Preconditioner; Ordinary differential equation

1. Introduction

Accurate chemistry modeling in reacting flows is vital to many engineering applications. One of the most important is the design of high-efficiency, clean-combustion engines for transportation. For these advanced engine operating modes, modeling the chemical kinetics is essential to guide the design effort [1]. Detailed kinetic mechanism have recently been developed for accurate gasoline surrogates [2], biodiesel surrogates [3] and the next generation of diesel surrogates [4]. These mechanisms include thousands of species along tens of thousands of reaction paths to provide a robust and accurate model of fuel oxidation.

Resolving the detailed chemistry within a computational fluid dynamics (CFD) simulation has traditionally relied on dense matrix based ordinary differential equation (ODE) solvers [5]. The traditional approach still remains in wide use because it is straightforward to implement and effective for sufficiently small mechanisms (fewer than 50 species). However, with dense solvers, as the number of species grows into the hundreds,

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the overall simulation cost is dominated by the dense matrix operations. In fact, the cost of solving a single chemically reacting cell with the 7172-species mechanism for a diesel component [6] is on the order of one day. Recent approaches [7–9] have updated the traditional ODE solver to yield an order of magnitude or more speedup. However, further work is still needed to reduce the computational cost to a level where the detailed mechanisms are widely-used in multidimensional CFD engine simulations.

For several decades, a considerable amount of research has focused on reducing the size of the kinetic mechanisms in order to reduce the cost of simulating chemistry (see the review by Lu and Law [10]). The disadvantage of global reduction techniques is that they often require a high-level of expertise to understand the limitations and range of accuracy of the new, smaller mechanisms. To combat these challenges, Liang et al introduced an on-the-fly mechanism reduction technique in [11] that allows for more automation when combined with the appropriate error controls. Other researchers have extended this effort to reduce mechanisms in the context of species transport [12], and to remove the stiffness in the ODE system caused by the chemical kinetics [13]. Mechanism reduction, however, is not the only means to reduce the computational cost of solving detailed chemical kinetics.

There are a number of strategies based on advances in applied mathematics and algorithm design that deliver computational speedup without any loss of accuracy. The improvements generally apply to two main categories: thermochemical calculations and ODE solvers. In the first category, the computational time to evaluate the chemical system derivatives can be reduced by avoiding high-cost functions such as the exponential and logarithm terms in the species production rate. Some strategies to achieve this include: precomputation and interpolation of expensive functions [9], direct elimination of redundant exponentiation [10], and *in situ* adaptive tabulation (ISAT) [14].

In the second category, there is some ongoing research in new classes of integrators for chemical systems (*e.g.* exponential-type [15]). However, many recent advances for chemical system integration focus on the matrix operations that underpin the common backward difference formulation (BDF) approximating the ODE system [16]. The construction of the Jacobian matrix and the linear system solvers used for each non-linear iteration are updated to take advantage of the sparse structure of large kinetic mechanism. In [7], automatic differentiation software is used to construct analytical Jacobian matrices well-suited for direct, sparse linear system solvers. Similarly, in [9], the chemical system derivatives are derived to produce an analytical Jacobian approximation that is able to take full advantage of sparse solvers, which yields a speedup over traditional dense methods of an order of magnitude or more for large mechanisms.

The approach in this paper follows a similar path that seeks to reduce the computational cost through improvements to the linear system solver. The direct sparse solvers implemented in the recent approaches [7,15] are replaced with an iterative linear solver based on the generalized minimum residual (GMRES) method [17]. Specifically, this paper uses the scaled preconditioned GMRES method as implemented in the CVODE solver [18].

This paper develops preconditioners to accelerate the convergence rate of the GMRES method when used as part of the ODE solver for large kinetic mechanisms. In particular, a class of adaptive preconditioners related to on-the-fly mechanism reduction is constructed. These preconditioners are then applied to the time integration of a constant volume, well-stirred reactor (WSR) containing a stoichiometric fuel–air mixture using nine kinetic mechanisms. The mechanisms range in size from hydrogen (10 species [19]) to the biodiesel component 2-methylnonadecane (7172 species [6]). The average computation time for the WSR is then compared to the traditional ODE solver based on dense matrix operations. For the largest mechanism tested, the new adaptive preconditioners are three orders of magnitude faster than the traditional approach. The adaptive preconditioners are also an order of magnitude faster than recent advanced solvers that use analytical Jacobians and direct sparse solvers.

2. Approach

The aim of this investigation is to reduce the computational cost of combustion simulation and enable the use of more detailed chemistry in engine design. The particular approach is to find effective preconditioners for integrating large kinetic mechanisms using the GMRES-based solver in CVODE. Before discussing what is meant by an effective preconditioner, first consider the BDF time discretization and associated Jacobian matrices used to solve the ODE system.

For a general N-dimensional ODE system, $dx_i/dt = f_i(x_1, \ldots, x_N, t)$ for $1 \leqslant i \leqslant N$, its Jacobian matrix J is defined as

$$J_{ij} = \frac{\partial f_i}{\partial x_j}, \tag{1}$$

and the linear system used in the non-linear solver is

$$B = I - \alpha \Delta t J, \tag{2}$$

where I is the identity matrix, and α is a constant related to the method order and previous time-steps and Δt is the current step size. The matrix

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