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A study of direct and Krylov iterative sparse solver techniques to approach linear scaling of the integration of chemical kinetics with detailed combustion mechanisms

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ABSTRACT

The integration of the stiff ODE systems associated with chemical kinetics is the most computationally demanding task in most practical combustion simulations. The introduction of detailed reaction mechanisms in multi-dimensional simulations is limited by unfavorable scaling of the stiff ODE solution methods with the mechanism's size. In this paper, we compare the efficiency and the appropriateness of direct and Krylov subspace sparse iterative solvers to speed-up the integration of combustion chemistry ODEs, with focus on their incorporation into multi-dimensional CFD codes through operator splitting. A suitable preconditioner formulation was addressed by using a general-purpose incomplete *LU* factorization method for the chemistry Jacobians, and optimizing its parameters using ignition delay simulations for practical fuels. All the calculations were run using a same efficient framework: SpeedCHEM, a recently developed library for gas-mixture kinetics that incorporates a sparse analytical approach for the ODE system functions. The solution was integrated through direct and Krylov subspace iteration implementations with different backward differentiation formula integrators for stiff ODE systems: LSODE, VODE, DASSL. Both ignition delay calculations, involving reaction mechanisms that ranged from 29 to 7171 species, and multi-dimensional internal combustion engine simulations with the KIVA code were used as test cases. All solvers showed similar robustness, and no integration failures were observed when using ILUT-preconditioned Krylov enabled integrators. We found that both solver approaches, coupled with efficient function evaluation numerics, were capable of scaling computational time requirements approximately linearly with the number of species. This allows up to three orders of magnitude speed-ups in comparison with the traditional dense solution approach. The direct solvers outperformed Krylov subspace solvers at mechanism sizes smaller than about 1000 species, while the Krylov approach allowed more than 40% speed-up over the direct solver when using the largest reaction mechanism with 7171 species.

1. Introduction

The steady increase in computational resources is fostering research of cleaner and more efficient combustion processes, whose target is to reduce dependence on fossil fuels and to increase environmental sustainability of the economies of industrialized countries [1]. Realistic simulations of combustion phenomena have been made possible by thorough characterization and modeling of both the fluid-dynamic and thermal processes that define local transport and mixing in high temperature environments, and of the chemical reaction pathways that lead to fuel oxidation and pollutant formation [2]. Detailed chemical kinetics modeling of complex and multi-component fuels has been achieved through extensive understanding of fundamental hydrocarbon chemistry [3] and through the development of semi-automated tools [4] that identify possible elementary reactions based on modeling of how molecules interact. These detailed reaction models can add thousands of species and reactions. However, often simple phenomenological models are preferred to even skeletal reaction mechanisms that feature a few tens/hundreds of species in "real-world" multidimensional combustion simulations, due to the expensive computational requirements that their integration requires, even on parallel architectures, when using conventional numerics. The stiffness of chemical kinetics ODE systems, caused by the simultaneous co-existence of broad temporal scales, is a further complexity factor, as the time integrators have to advance

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the solution using extremely small time steps to guarantee reasonable accuracy, or to compute expensive implicit iterations while solving the non-linear systems of equations [5].

Many extremely effective approaches have been developed in the last few decades to alleviate the computational cost associated with the integration of chemical kinetics ODE systems for combustion applications, targeting: the stiffness of the reactive system; the number of species and reactions; the overall number of calculations; or the main ordinary differential equations (ODE) system dynamics, by identifying main low-dimensional manifolds [6–16]. A thorough review of reduction methods is addressed in [2]. From the point of view of integration numerics, some recent approaches have shown the possibility to reduce computational times by orders of magnitude in comparison with the standard, dense ODE system integration approach, without introducing simplifications into the system of ODEs, but instead improving the computational performance associated with: (1) efficient evaluation of computationally expensive functions, (2) improved numerical ODE solution strategy, (3) architecture-tailored coding.

As thermodynamics-related and reaction kinetics functions involve expensive mathematical functions such as exponentials, logarithms and powers, approaches that make use of data caching, including in situ adaptive tabulation (ISAT) [17] and optimal-degree interpolation [18], or equation formulations that increase sparsity [19], or approximate mathematical libraries [20], can significantly reduce the computational time for evaluating both the ODE system function and its Jacobian matrix. As far as the numerics internal to the ODE solution strategy, the adoption of sparse matrix algebra in treating the Jacobian matrix associated with the chemistry ODE system is acknowledged to reduce the computational cost of the integration from the order of the cube number of species, $O(n_s^3)$, down to a linear increase, $O(n_s)$ [21–23].

Implicit, backward-differentiation formula methods (BDF) are among the most effective methods for integrating large chemical kinetics problems [24,25] and packages such as VODE [26], LSODE [27], DASSL [28] are widely adopted. Recent interest is being focused on applying different methods that make use of Krylov subspace approximations to the solution of the linear system involving the problem's Jacobian, such as Krylov-enabled BDF methods [29], Rosenbrock–Krylov methods [30], exponential methods [31]. As far as architecture-tailored coding is concerned, some studies [32,33] have shown that solving chemistry ODE systems on graphical processing units (GPUs) can significantly reduce the dollar-per-time cost of the computation. However, the potential achieveable per GPU processor is still far from full optimization, due to the extremely sparse memory access that chemical kinetics have in matrix–vector operations, and due to small problem sizes in comparison to the available number of processing units. Furthermore, approaches for chemical kinetics that make use of standardized multi-architecture languages such as OpenCL are still not openly available.

Our approach, available in the `SpeedCHEM` code, a recently developed research library written in modern Fortran language, addresses both issues through the development of new methods for the time integration of the chemical kinetics of reactive gaseous mixtures [18]. Efficient numerics are coupled with detailed or skeletal reaction mechanisms of arbitrarily large size, e.g., $n_s \geqslant 10^4$, to achieve significant speed-ups compared to traditional methods especially for the small-medium mechanism sizes, $100 \leqslant n_s \leqslant 500$, which are of major interest to multi-dimensional simulations. In the code, high computational efficiency is achieved by evaluating the functions associated with the chemistry ODE system throughout the adoption of optimal-degree interpolation of expensive thermodynamic functions, internal sparse algebra management of mechanism-related quantities, and sparse analytical formulation of the Jacobian matrix. This approach allows a reduction in CPU times by almost two orders of magnitude in ignition delay calculations using a reaction mechanism with about three thousand species [34], and was capable of reducing the total CPU time of practical internal combustion engine simulations with skeletal reaction mechanisms by almost one order of magnitude in comparison with a traditional, dense-algebra-based reference approach [35,36].

In this paper, we describe the numerics internal to the ODE system solution procedure. The flexibility of the software framework allows investigations of the optimal solution strategies, by applying different numerical algorithms to a numerically consistent, and computationally equally efficient, problem formulation. Some known effective and robust ODE solvers, as LSODE [27], VODE [26], DASSL [28], used for the combustion chemistry integration [18], are based on backward differentiation formulae (BDF) that include implicit integration steps, requiring repeated linear system solutions associated with the chemistry Jacobian matrix, as part of an iterative Newton procedure. Based on the same computational framework and BDF integration procedure, the effective efficiency of the sparse direct and preconditioned iterative Krylov subspace solvers reported in Table 2 was studied. To consider the effects of reaction mechanism size, a common matrix of reaction mechanisms for typical hydrocarbon fuels and fuel surrogates, spanning from $n_s = 29$ up to $n_s = 7171$ species was used, whose details are reported in Table 1.

The paper is structured as follows. A description of the modeling approach adopted for the simulations is reported, including the major steps of the BDF integration procedure. Then, a robust preconditioner for the chemistry ODE Jacobian matrix is defined, as the result of the optimization of a general-purpose preconditioner-based incomplete *LU* factorization [37,38]. Integration of ignition delay calculations at conditions relevant to practical combustion systems is compared for the range of reaction mechanisms chosen, at both solver techniques and with different BDF-based stiff ODE integrators. Finally, the direct and Krylov subspace solvers are compared for modeling practical internal combustion engine simulations.

Table 1
Overview of the reaction mechanisms used for testing in this study.

Mechanism	n_s	n_r	Fuel	Composition	Ref.
ERC n-heptane	29	52	n-Heptane	$[nC_7H_{16} : 1.0]$	[39]
ERC PRF	47	142	PRF25	$[nC_7H_{16} : 0.75, iC_8H_{18} : 0.25]$	[40]
Wang PRF	86	392	PRF25	$[nC_7H_{16} : 0.75, iC_8H_{18} : 0.25]$	[41]
ERC multiChem	128	503	PRF25	$[nC_7H_{16} : 0.75, iC_8H_{18} : 0.25]$	[42]
LLNL n-heptane (red.)	160	1540	n-Heptane	$[nC_7H_{16} : 1.0]$	[43]
LLNL n-heptane (det.)	654	2827	n-Heptane	$[nC_7H_{16} : 1.0]$	[44]
LLNL PRF	1034	4236	PRF25	$[nC_7H_{16} : 0.75, iC_8H_{18} : 0.25]$	[44]
LLNL mehtyl-decanoate	2878	8555	Methyl-decanoate	$[md : 1.0]$	[34]
LLNL n-alkanes	7171	31669	Diesel surrogate	$[nC_7H_{16} : 0.4, nC_{16}H_{34} : 0.1, nC_{14}H_{30} : 0.5]$	[45]