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# Decoupled Species and Reaction Reduction: An error-controlled method for Dynamic Adaptive Chemistry simulations

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## ABSTRACT

We present a new model reduction method that emphasizes solution error control and is designed for Adaptive Chemistry (i.e. dynamic spatial distribution of smaller, locally-valid reduced models over the course of a simulation, rather than a single, larger reduced model). Species and reaction reductions are performed on-the-fly and in separate steps, allowing better control of model speed and accuracy. We demonstrate its application in combustion CFD with autoignition (1D and 0D) and 2D laminar flame examples. The new Decoupled Species and Reaction Reduction (DSRR) approach is as fast as the Directed Relation Graph (DRG) approach and offers improved solution accuracy control. We also highlight the dependence of the speedup obtainable by mechanism reduction on the Jacobian computation method (analytic or numerical) in the implicit kinetics ODE solver. Analytic Jacobian computation increases the simulation speed (often significantly), but decreases the opportunities for speedup by mechanism reduction. Regardless of the reduction approach, the speedup due to mechanism reduction generally decreases and scales less dramatically with mechanism size when the Jacobians are computed analytically.

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## 1. Introduction

Detailed kinetic mechanisms of hydrocarbon fuels are developed to enable accurate computational prediction of combustion performance as well as emissions. There is a well-recognized need to incorporate detailed chemistry into the modeling of practical combustion technologies, though challenging particularly for multi-dimensional computational domains [1–4]. Major difficulties are due to the large number of chemical species and the wide range of timescales involved in detailed kinetics [4]. Detailed mechanisms for hydrocarbon fuels typically involve tens to thousands of chemical species with chemical timescales ranging from sub-nanoseconds to seconds. In the past decade, significant progress has been made in methodologies and algorithms to reduce the computational cost imposed by the use of detailed chemistry in reacting flow simulations [5–43]. Of the frequently used approaches, Adaptive Chemistry methods have recently gained significant interest.

Adaptive Chemistry methods are developed to exploit the time savings available through the use of various locally-valid skeletal or reduced mechanisms and have been successfully demonstrated

using reduced-model storage and retrieval [31–36], as well as on-the-fly mechanism reduction [37–43]. However, recent efforts have focused on the latter, thanks to the success of the Directed Relation Graph (DRG) approach [5–8], which allows fast mechanism reduction and greatly simplifies the implementation of Adaptive Chemistry. This paper addresses on-the-fly mechanism reduction, commonly referred to as “Dynamic Adaptive Chemistry” (DAC) or “Dynamic Mechanism Reduction”, with particular emphasis on improved accuracy control.

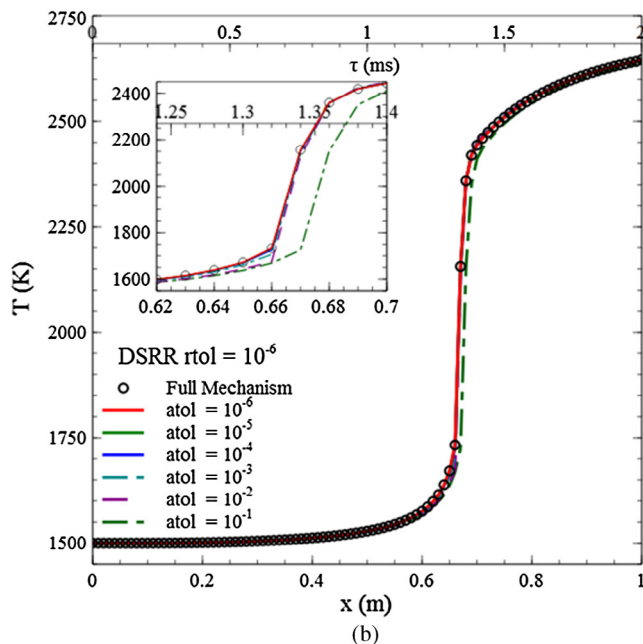
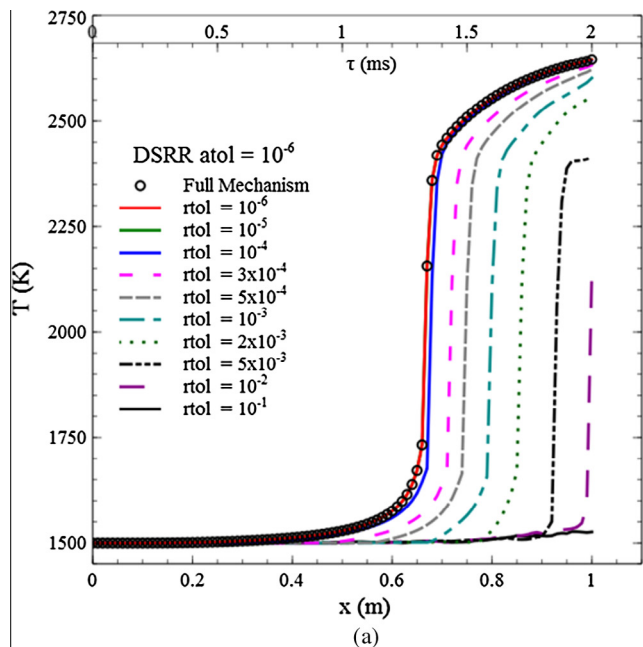
The basic approach of Adaptive Chemistry is to avoid computations for the species and reactions that are “inactive” (i.e. having negligible impact on the kinetics) at each grid point or cell or particle in the computational domain, thus reducing the computational cost. Species and reactions are typically designated as active or inactive at the start of each iteration or time-step in the simulation and assumed to remain as such (active/inactive) until the next iteration or time-step. Adaptive Chemistry is now commonly applied to improve computational efficiency of detailed chemistry simulations and has recently been demonstrated in combination with other methods such as in-situ adaptive tabulation (ISAT) [40,43]. Clearly, in order to minimize computational overhead costs, on-the-fly reduction requires a fast method for mechanism reduction. To our knowledge, DRG-based approaches, and more recently Path Flux Analysis (PFA) [41], are the only

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methods that have been demonstrated to meet this criterion. In this study, we present a new reduction method designed for DAC, in which species and reaction reductions are decoupled. Importantly, the method applies intuitive error controls, alleviating the empiricism typically required in determining appropriate tolerances for mechanism reduction.

The rest of the paper is organized as follows: the methodology of Decoupled Species and Reaction Reduction is described in Section 2. Its performance in combustion simulations is demonstrated in Section 3. Finally, conclusions are presented in Section 4.



**Fig. 1.** Steady-state temperature profiles in 1D methane ignition problem. A secondary horizontal axis (residence time, “ $\tau$ ”) was added to quantify the ignition delay times. For mechanism reduction, (a) DSRR  $atol$  is fixed at  $10^{-6}$  while  $rtol$  is varied between  $10^{-1}$  and  $10^{-6}$ . Predictions at relative tolerances of  $10^{-5}$  and  $10^{-6}$  match the full mechanism prediction very closely. Solution accuracy degrades as  $rtol$  is increased and no ignition is predicted at a tolerance of  $10^{-1}$ ; (b) DSRR  $rtol$  is fixed at  $10^{-6}$  while  $atol$  is varied between  $10^{-1}$  and  $10^{-6}$ . The reduced-model predictions approximate the full mechanism solution well for all  $atol$  values in this range, since the relative error tolerance is kept low.

## 2. Methodology

We consider a reacting gas-phase mixture consisting of  $N_S$  chemical species, composed of  $N_E$  elements. The thermo-chemical state of the mixture at a given location and time is determined by the pressure  $p$ , the mixture temperature  $T$ , and the  $N_S$ -sized vector  $\mathbf{Y}$  of species mass fractions. The species composition generally evolves through three processes: advection, diffusion and chemical reaction. Here we focus on the class of solution methods in which a splitting scheme is used to account for these processes in separate fractional solution steps. At each flow iteration or time-step, the split equations are solved separately and then “reassembled” using any of various available schemes, to approximate the full equations [44–49]. We are concerned with the efficient solution of the (adiabatic and isobaric) reaction step, in which the composition  $\Phi \equiv \{\mathbf{Y}, T\}$  of each computational cell evolves according to  $N_{eq}$  ( $=N_S + 1$ ) coupled nonlinear stiff ordinary differential equations (ODEs) resulting from chemical kinetics,

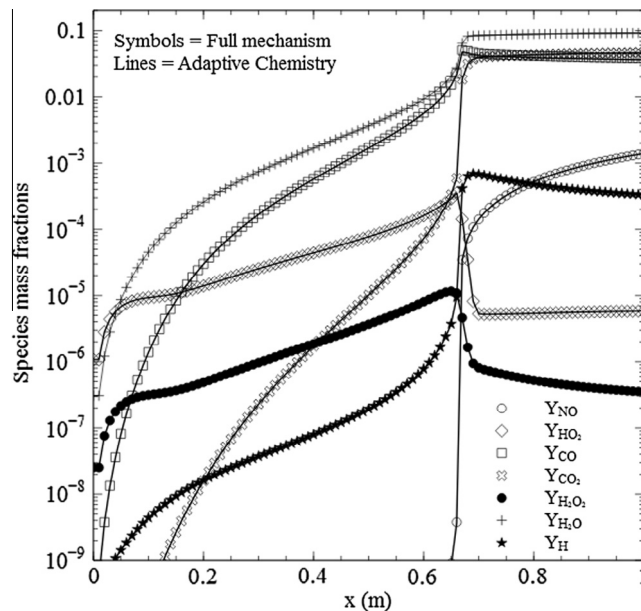
$$\frac{d\phi_k}{dt} = R_k(\omega) \quad \forall k = 1, 2 \dots N_{eq} \quad (1)$$

Here,  $R_k$  is the rate of change of species  $k$  due to chemical reactions, with contributions from the  $N_{rxn}$  elementary reactions in the mechanism. The net reaction rate of the  $i$ th elementary reaction is given by the phenomenological expressions

$$\omega_i(\phi) = k_{f,i} \prod_{j=1}^{N_s} C_j^{v_{f,j}^i} - k_{r,i} \prod_{j=1}^{N_s} C_j^{v_{r,j}^i} \quad i = 1, 2 \dots N_{rxn}, \quad (2)$$

where  $k_{f,i}$  and  $k_{r,i}$  are the forward and reverse rate constants (respectively) of reaction  $i$ ;  $C_j$  is the molar concentration of species  $j$ ; and  $v_{j,i}$  is the stoichiometric coefficient of species  $j$  in reaction  $i$ .

The task in the reaction fractional step is to solve the chemical kinetics initial value problem (IVP) in Eq. (1) over a flow time step  $\Delta t$  (i.e. given an initial state  $\phi(t_0) = \phi_0$ , solve for  $\phi(t_0 + \Delta t)$ ). The flow time step may be constant or variable in space and time, but is often several orders of magnitude larger than the smallest timescale in the chemistry sub-problem. So, Eq. (1) is typically stiff and is most often solved using an implicit ODE solver, such as VODE, DVODE, DASAC and CVODE. The most expensive computations encountered in solving Eq. (1) are due to: (1) the



**Fig. 2.** Steady-state species profiles in error-controlled DAC simulation of 1D methane ignition problem (DSRR  $atol = 10^{-6}$ ,  $rtol = 10^{-6}$ ). DAC solution matches the full mechanism solution for all species.

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