

Development of a Multiscale Adaptive Reduced Chemistry Solver (MARCS) for Computationally Efficient Combustion Simulations

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Abstract

The Multiscale Adaptive Reduced Chemistry Solver (MARCS) is developed by integrating the Correlated Dynamic Adaptive Chemistry and Transport (CO-DACT) method with the Hybrid Multi-Timescale (HMTS) and G-Scheme methods, and the Full Speed Fluid Solver to conduct the efficient combustion modeling with detailed chemical kinetics. The preliminary results of ignitions and flame propagations in this paper demonstrate that the computational efficiency can be improved by orders of magnitude using CO-DACT method with HMTS and G-Scheme methods. In the final paper, MARCS will be applied to the simulations of a two-dimensional jet flame and an oblique shock inducing auto-ignition with detailed mechanisms and transport to demonstrate the efficiency. Detailed turbulence/chemistry interactions on low temperature ignition and ignition to flame and detonation transition will be investigated.

1 Introduction

Recently, tremendous efforts have been devoted to develop more efficient and lower emission internal combustion engines working at low temperature and high pressure conditions. The optimization and control of fuel injection, ignition timing, and heat release rates at different engine loads requires advanced understanding of turbulence-chemistry coupling. This becomes particularly difficult in the range from low temperature (700 K) to intermediate temperature (1100K) [1] because the low temperature chemistry has to be included in the model increasing the number of species and reactions in the kinetic mechanism. The evaluation of detailed chemical kinetics and transport quantities result of great challenges in combustion models involving hundreds of species and thousands of reactions. Even with the availability of supercomputing capability at petascale and beyond, numerical simulations using such large kinetic mechanisms still remain to be difficult.

The first challenge comes from the size of the chemical mechanism that proportionally increases number of degrees of freedom of the problem. In order to reduce the number of species and reactions involved

several methods have been developed [2][3][4]. Among these methods, the Correlated Dynamic Adaptive Chemistry (CO-DAC) method [5] can provide a locally reduced mechanism on-the-fly without generating overhead CPU time cost.

The second challenge of utilizing detailed chemistry in simulations is the accurate calculation of transport properties for a large number of species. Indeed, these needs to be evaluated in all the cells and at each time step because they vary significantly across the temporal and spatial coordinates due to the rapid species and temperature variations caused by the chemical reactions. Both the traditional multi-component diffusion model [6] and mixture-averaged model [7] become inefficient to be used when a large chemical mechanism is involved. The CO-DAC method [8] makes the calculation of transport properties practically feasible conducting the transport properties calculation in phase space, and reducing the computational cost of two orders of magnitude.

Another challenge comes from the stiffness in the ODE system governing the chemical reactions, indeed, the time integration on the chemical mechanism still remains the most time consuming part in a simulation. Therefore, the use of an advanced time integration method further is required. Several chemical solvers has been developed in last decades, among them, the HMTS method [9] and the G-Scheme method [10] have the potential to be integrated together and provide an efficient integration for the chemical kinetics.

The goal of this paper is to present the MARCS method for an efficient numerical computation of combustion simulations. It integrates a parallel PDE solver, the Full Speed Fluid Solver, with the CO-DAC for on-fly mechanism simplification and evaluation of transport properties, and with HMTS and G-Scheme methods that will be adaptively selected as chemistry solver according to the size of the reduced mechanisms and the local combustion regimes. MARCS method will be here validated solving an oblique shock induced auto-ignition with detailed mechanisms.

2 Multiscale Adaptive Reduced Chemistry Solver (MARCS)

In this section a brief introduction to the methods forming MARCS is provided.

A. Correlated dynamic adaptive chemistry and transport method (CO-DAC)

In a combustion simulation, one cell in adjacent time steps or two different cells in the same time step may have similar thermodynamic conditions, which results in the same local reduced chemical mechanism and/or transport properties. Therefore, detailed calculation in similar cells is redundant. Based on this idea, the CO-DAC method examines computational cells in correlated space spanned by a few phase parameters. Similar cells in the correlated space will be grouped so that the detailed calculation is performed only once.

Due to space limitation, only the implementation of the correlated groups is presented here, the details of phase parameter selection and the validation of the method can be found in [8]. Assuming the phase parameters are: (z_1, z_2, \dots, z_M) , in which each z_i ($i = 1, 2, \dots, M$) is a non-negative parameter in thermodynamic states, such as the temperature and mass or molar fractions, and M is the dimension of the phase space. The phase space, \mathbf{S} , can be constructed by taking the logarithm of the phase parameters: $\mathbf{S} = (\ln(z_1), \ln(z_2), \dots, \ln(z_M))^T$.

As shown in Figure 1, the computation cells in physical domain can be mapped into correlated groups by the following two procedures, time correlation and space correlation.

Time correlation: The time correlation between current and previous time step is examined and applied first. For any cell, if the thermodynamic states in the current and the previous time step fall into one

correlated group in the phase space, the cell at the adjacent time steps is correlated. So, the local reduced mechanism or the transport properties at previous step will be directly passed to the current time step. Here we only consider the time correlation between two adjacent time steps to limit the memory and CPU-time cost of data storage.

Space correlation: For the cells which are not in the time correlated groups, we apply the space correlation. A set of group indexes, (l_1, l_2, \dots, l_M) will be assigned to each cell, where $l_i = [(\ln(z_i) - \ln(z_{i,min}))/2\varepsilon] + 1$, ($i = 1, 2, \dots, M$), and ε is a user specified threshold value to discretize the phase space.

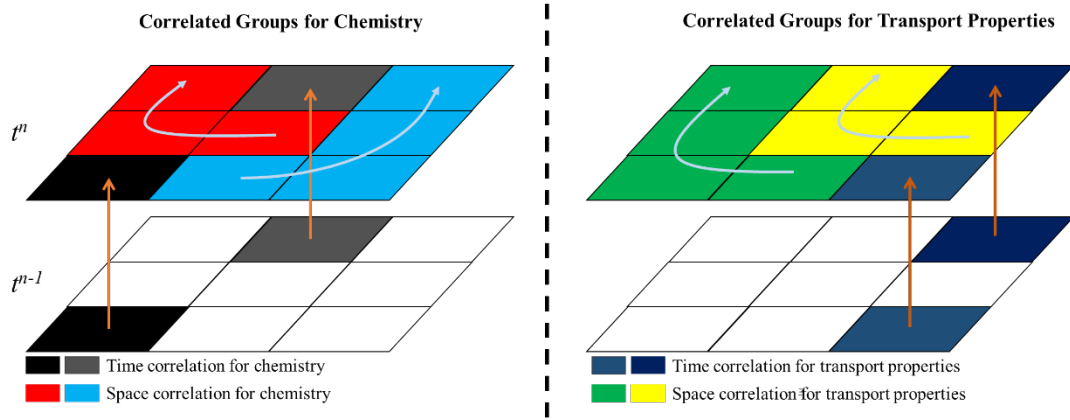


Figure 1. Schematic of time and space correlations in chemistry and transport properties.

According to the group index in phase space, the existing correlated groups will be recorded by a hash table. The key in the hash table is the group index l and the corresponding value, v , is the physical index of the first cell in this group. If the group index of a computation cell already exists, this cell will use the local reduced mechanism or the transport properties in cell v . Otherwise, the reduced mechanism or the transport properties in this cell will be calculated by the detailed model and a new key-value mapping will be added in the hash table.

B. Hybrid Multi-Timescale (HMTS) and G-Scheme methods

Based on the locally reduced mechanism from the CO-DACT method, the chemical reactions are integrated by HMTS or G-Scheme method. The solver automatically determines which method to use based on the combustion regime and the size of mechanism.

In the HMTS method, the species equations are integrated with their own characteristic time scales. The timescale of n -th species, τ_n , is estimated as[9]:

$$\tau_n = - \left[\frac{\partial}{\partial Y_n} \left(\frac{dY_n}{dt} \right) \right]^{-1} = \left(\frac{\partial D_n}{\partial Y_n} \right)^{-1} \quad (1)$$

where Y_n and D_n are the mass fraction and the destruction rate of n -th species, respectively. The species having a difference of timescale in one order of magnitude, are grouped into an integration group. The group index of the n -th species, G_n can be obtained as:

$$G_n = \left\lceil \log_{10} \left(\frac{t_{base}}{\tau_n} \right) \right\rceil + 1 \quad (2)$$

where t_{base} is the base time step in DNS calculations.

With the definitions of the timescale and group index, each the groups is integrated separately based on its own timescale. Moreover, when it is not interested in the detailed history of the fast modes, the implicit Euler method can applied to further increase the efficiency. The HMTS method has been demonstrated to be more efficient than the VODE solver [9].

In G-Scheme method [10], projects the system of ODEs in a phase space and exploits the possibility for reduction from the manifestation of spectral gaps. The modes are automatically spited into slow, active and fast modes by evaluating their own timescale and the relative contribution to the vector field. For slow and fast modes, the regular perturbation and standard perturbation are applied, respectively, to correct the results. The detailed integrations are only applied to the active modes. By doing this, the G-Scheme method removes the stiffness of the system using the time scale of the active modes for time integration.

The HMTS and G-Scheme have their own advantages depending on the mechanism size and the combustion regimes. Therefore, adaptively selecting the locally most efficient solver according to the local conditions, so that higher computational efficiency can be achieved.

C. Full Speed Fluid Solver

The HMTS and G-Scheme methods are implemented into an in-house parallelized code, Full Speed Fluid Solver [11] to simulate unsteady, compressible and reactive flows. The code is based on curvilinear coordinates and uses cell-centered collocated storage arrangement on semi-block structured grid for all quantities. The convection and diffusion terms are discretized with 3rd-order AUSMPW+ and central difference schemes respectively. A modified fully implicit lower-upper symmetric Gauss-Seidel (LU-SGS) scheme with Newton-like sub-iterations in pseudo time is taken as time marching method for solving the Navier-Stokes equations. The corresponding Courant number is under unit for most of the grid cells. Ten steps of sub-iteration are performed in each computational step, which guarantees that the residual decreases of about three orders of magnitude in the inner iteration so that the LU-SGS can achieve second order accuracy. This solver has been validated with several real-geometric cases [11].

3 Results and Discussion

The preliminary results presented in this section are used to demonstrate the capability of the Full Speed Fluid Solver, CO-DACT and HMTS, G-Scheme methods, respectively. The results of the 2D jet flame and oblique shock induced ignition will be included in the full length paper and final presentation.

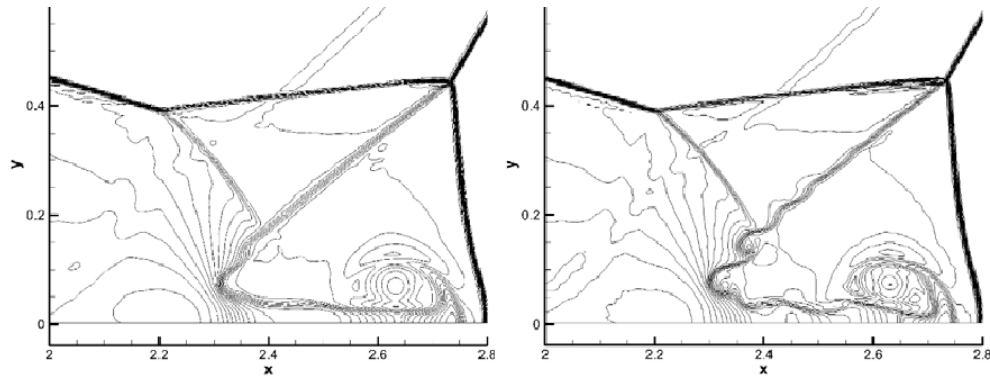


Figure 2. Density contours of the double Mach reflection problem at $t = 0.2$, calculated by (left) AUSM+ and (right) AUSMPW+ schemes respectively.

The double Mach reflection case [12] is a widely used benchmark to test the ability of shock capturing and the small scale structure resolution of a flow solver. In the present simulation, the computational domain is $[0, 4] \times [0, 1]$. The lower boundary is set to be reflecting wall starting from $x = 1/6$. At $t = 0$, a right-moving 60° inclined Mach 10 shock is positioned at $[1/6, 0]$. The upper boundary is set to describe the exact motion of the Mach 10 shock. The left boundary at $x = 0$ is assigned with post-shock values. An outflow condition with zero gradients is set at $x = 4$. Fig. 2 shows the density contours at $t = 0.2$ obtained with AUSM+ and AUSMPW+ schemes, respectively. It is seen that the shock waves as well as the small structures near the up-rolling region are well captured by both schemes. However, only the AUSMPW+ scheme adopted in the present solver can resolve structures along the contact line, which implies that this method is more accurate and less dissipative near discontinuities.

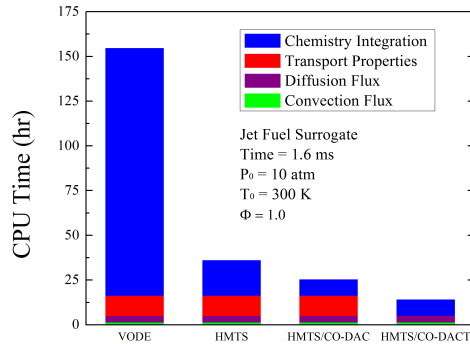


Figure 3. CPU time comparisons for CO-DACT.

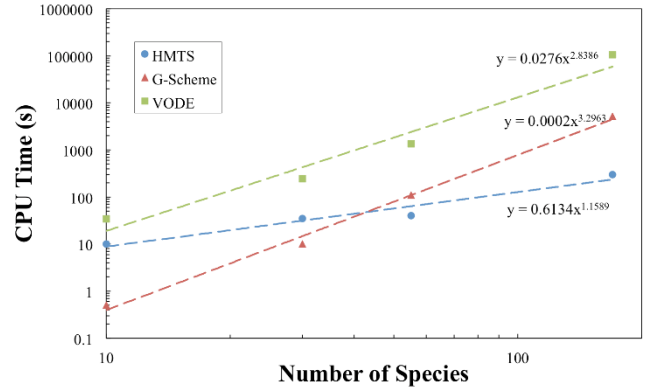


Figure 4. CPU time comparison of HMTS and G-Scheme.

In order to demonstrate the computational efficiency of the CO-DACT method, the CPU time comparisons between VODE, HMTS, HMTS/CO-DAC and HMTS/CO-DACT methods in a premixed spherical propagating flame calculation is plotted in Figure 3. It shows that for the VODE method the computational cost is mostly due to the chemistry integration cost. This cost is reduced by one order of magnitude using HMTS and even further using HMTS/CO-DAC. In this latter case the evaluation of the transport properties is larger than the chemistry integration cost, however, using HMTS/CO-DACT this becomes negligible.

Figure 4 shows the comparison of the computational cost between HMTS and G-Scheme methods with different chemical mechanisms. It demonstrates that the dependency of CPU time on the mechanism size is first order and third order, respectively for HMTS and G-Scheme method. Therefore, the solver automatically switches to G-Scheme method when the local reduced mechanism is smaller than 40 species and select HMTS method when the mechanism is larger, so that it can be more efficient.

4 Conclusion

The capability of the in-house Full Speed Fluid Solver and the efficiency of the CO-DACT, HMTS and G-Scheme methods are demonstrated in the preliminary results. The parallel Full Speed Fluid Solver can handle large scale and multi-dimensional simulations. The CO-DACT, HMTS and G-Scheme methods are able to accelerate the combustion modeling by orders of magnitude. Therefore, by integrating them together, the proposed MARCS method has the promising potential to conduct combustion modeling in

large domain and multi-dimensional geometry with detailed chemical kinetics in order to investigate complicated coupling between chemistry and transport.

References

- [1] F. Zhao, T. N. Asmus, D. N. Assanis, J. E. Dec, J. A. Eng, and P. M. Najt, "Homogeneous Charge Compression Ignition (HCCI) Engines." 2003.
- [2] W. Sun, Z. Chen, X. Gou, and Y. Ju, "A path flux analysis method for the reduction of detailed chemical kinetic mechanisms," *Combust. Flame*, vol. 157, no. 7, pp. 1298–1307, Jul. 2010.
- [3] M. Valorani, F. Creta, D. A. Goussis, J. C. Lee, and H. N. Najm, "An automatic procedure for the simplification of chemical kinetic mechanisms based on CSP," *Combust. Flame*, vol. 146, no. 1, pp. 29–51, 2006.
- [4] T. Grenga, S. Paolucci, and M. Valorani, "G-Scheme-based simplification and analysis methodology for hydrocarbon ignition," in *Eastern States Section of the Combustion Institute*, 2016.
- [5] W. Sun, X. Gou, H. a. El-Asrag, Z. Chen, and Y. Ju, "Multi-timescale and correlated dynamic adaptive chemistry modeling of ignition and flame propagation using a real jet fuel surrogate model," *Combust. Flame*, vol. 162, no. 4, pp. 1530–1539, 2015.
- [6] C. F. Curtiss and J. O. Hirschfelder, "Transport Properties of Multicomponent Gas Mixtures," *J. Chem. Phys.*, vol. 17, no. 6, p. 550, 1949.
- [7] R. B. B. J.O. Hirschfelder, C.F. Curtiss, *Molecular Theory of Gases and Liquids*. John Wiley and Sons, New York, 1954.
- [8] W. Sun and Y. Ju, "Multi-timescale and Correlated Dynamic Adaptive Chemistry and Transport Modeling of Flames in n-Heptane/Air Mixtures," *53rd AIAA Aerosp. Sci. Meet.*, 2015.
- [9] X. Gou, W. Sun, Z. Chen, and Y. Ju, "A dynamic multi-timescale method for combustion modeling with detailed and reduced chemical kinetic mechanisms," *Combust. Flame*, vol. 157, no. 6, pp. 1111–1121, Jun. 2010.
- [10] M. Valorani and S. Paolucci, "The G-Scheme: A framework for multi-scale adaptive model reduction," *J. Comput. Phys.*, vol. 228, no. 13, pp. 4665–4701, 2009.
- [11] S. Fu and L. Wang, "RANS modeling of high-speed aerodynamic flow transition with consideration of stability theory," *Prog. Aerosp. Sci.*, vol. 58, pp. 36–59, Apr. 2013.
- [12] P. Woodward and P. Colella, "The numerical simulation of two-dimensional fluid flow with strong shocks," *J. Comput. Phys.*, vol. 54, no. 1, pp. 115–173, Apr. 1984.