ParCFD2024
35th International Conference on Parallel Computational Fluid Dynamics
Sep. 02-04, 2024, Bonn, Germany

NekCRF: A Novel GPU-Accelerated Finite-Rate-Chemistry Solver and Application to Hydrogen

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ARTICLE INFO†

Keywords:
NekRS;
Graphics Processing Unit;
Combustion;
Finite-Rate Chemistry;
Hydrogen

ABSTRACT

This paper presents nekCRF, a GPU-accelerated finite-rate chemistry solver for complex combustion problems. An application to hydrogen is shown and especially the performance compared to CPUs is discussed.

1. Introduction

The nekCRF code follows a low MACH (Ma) approach [1, 2] to solve the resulting system of equations for reactive flows. The conservation equation for the gaseous species mass fractions $Y_k, k = 1, \cdots, N$, temperature T, and velocity $\mathbf{v}$ fields result in

$$\frac{1}{\rho}\frac{\partial Y_k}{\partial t} = \mathbf{v}\cdot\nabla Y_k - \nabla\cdot\rho Y_k\mathbf{V}_k + \dot{\omega}_k \qquad k = 1,\cdots,N, \tag{1a}$$

$$\frac{1}{\rho c_p}\frac{\partial T}{\partial t} = -\mathbf{v}\cdot\nabla T + \nabla\cdot\lambda\nabla T + \sum_{k=1}^{N} h_k^0\dot{\omega}_k - \nabla\cdot\rho T\sum_{k=1}^{N} c_{p,k}Y_k\mathbf{V}_k + \frac{dp_0}{dt}, \tag{1b}$$

$$\frac{1}{\rho}\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v}\cdot\nabla\mathbf{v} - \nabla p_1 + \nabla\cdot\mu\left(\underline{\underline{\nabla\mathbf{v}}} + (\underline{\underline{\nabla\mathbf{v}}})^T - \frac{2}{3}(\nabla\cdot\mathbf{v})\underline{\underline{\mathbf{I}}}\right), \tag{1c}$$

$$\nabla\cdot\mathbf{v} = Q_T, \tag{1d}$$

$$p_0 V = nRT, \tag{1e}$$

where t is time, $\mathbf{V}_k, h_k^0, c_{p,k}$ the diffusion velocity, enthalpy of formation and heat capacity of species k, respectively, N the number of the gaseous chemical species, ρ, c_p, λ, μ the mixture density, heat capacity at constant pressure, thermal conductivity and dynamic viscosity, R the ideal gas constant, V volume, and n the total number of moles. The pressure field $p(\mathbf{x},t) = p_0(t) + \gamma Ma^2 p_1(\mathbf{x},t)$ is decomposed in the thermodynamic pressure $p_0(t)$, which can only vary in time, and the hydrodynamic pressure $p_1(\mathbf{x},t)$. Here, $\gamma = c_p/c_v$ is the heat capacities ratio.

Ignoring the Soret and Dufour effects, the species diffusion velocities $\mathbf{V}_k$ are computed by a mixture averaged transport model as

$$\mathbf{V}_k = -\frac{D_k}{X_k}\nabla X_k + \mathbf{V}_c, \tag{2}$$

with X_k being the mole fraction and D_k the mixture-average diffusivity of species k. The correction velocity $\mathbf{V}_c = -\sum_{k=1}^{N} Y_k\mathbf{V}_k$ needs to be introduced [3] to ensure $\sum_{k=1}^{N} Y_k\mathbf{V}_k = 0$, and thus global mass conservation.

The thermal divergence, the non-zero divergence of the velocity field

$$Q_T = \frac{-1}{\rho}\frac{D\rho}{Dt} = \frac{1}{T}\frac{DT}{Dt} + \overline{W}\sum_{k=1}^{N}\frac{1}{W_k}\frac{DY_k}{Dt} + \frac{dp_0}{dt}, \tag{3}$$

with $\overline{W}$ being the mean molecular weight, acts as a constraint and its imposition requires the solution of a variable pressure Poisson equation for the hydrodynamic pressure p_1.

Highly optimized kernels are used to evaluate the costly species production rates as well as the thermodynamic and transport properties. For this purpose, a JIT (just-in-time) kernel generator has been developed, which translates a combustion model (reaction rates, thermodynamic and transport properties) expressed in Cantera format [4] into platform-specific source code.

†This paper is part of the ParCFD 2024 Proceedings. The DOI of this document is 10.34734/FZJ-2025-02504 and of the Proceedings 10.34734/FZJ-2025-02175.

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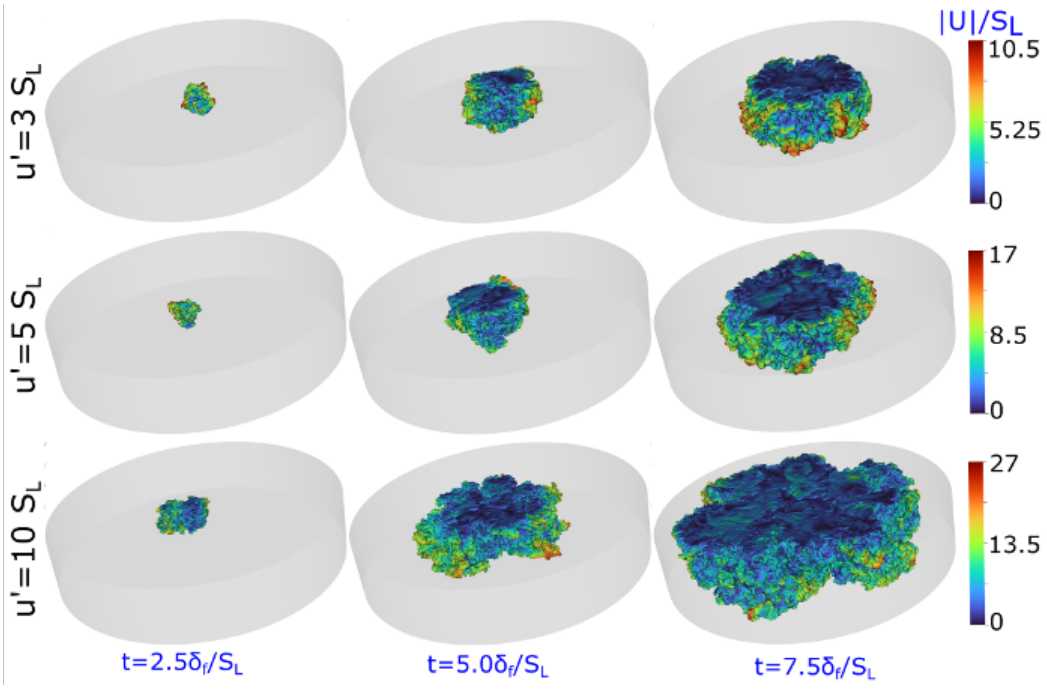

Figure 1: Overview of confined flame kernel simulations at different turbulent intensities. The flame surfaced is colored by the local speed relative to the laminar burning velocity.

2. Application

Flame kernels are important benchmark configurations to better understand complex combustion effects such as thermo-diffusive instabilities. They are often calculated with periodic boundary conditions, but nekCRF also allows to handle confined geometries effectively.

Lean hydrogen flame kernels in confined geometry were calculated under three different turbulent conditions for this work. The turbulent intensity was fixed relative to the laminar burning velocity s_L and varied between $u' = 3, 5, 10 s_L$. The mixture corresponded to $\phi = 0.4$, the ambient temperature was $T_u = 700\,\mathrm{K}$, the wall temperature $T_w = 450\,\mathrm{K}$ and the pressure $p_0 = 2\,\mathrm{atm}$. The mechanism considered 9 species. Figure 1 shows the development of the flame kernels at different times. The effect of confinement is made clear by the selected coloring. In addition, the coloring illustrates the faster expansion speed at higher turbulence. A similar effect can also be observed for the internal heat release rate, which increases with increasing turbulent intensity and is significantly higher than the heat release rate of a laminar flame in all cases.

3. Discussion and conclusions

The application of the lean hydrogen flame kernels demonstrates that nekCRF is capable of performing large-scale simulations of reactive flows. The accuracy of nekCRF [5] was also compared with other codes as well as Cantera (cf. Fig. 2) and showed that the accuracy of the results is in line with the models used. Finally, the performance of nekCRF as a GPU-accelerated code compared to an implementation on CPUs will be discussed. For this purpose, a test case with nekCRF and nek5000 with LAVp (this corresponds to the same models once on GPU and once on CPU) was calculated and the theoretical and practical (due to cache effects and resulting limited throughput) performance compared. Theoretically, nekCRF is up to 22 times faster. Practically still 14 times faster. This means that a simulation for which nek5000 needs two weeks with LAVp can be calculated by nekCRF in one day. This is a significant game

T	H2	O2	H2O	H
1.64e-6	9.48e-6	9.05e-06	9.00E-06	7.35E-04

O	OH	HO2	H2O2	N2
2.46E-03	2.82e-04	1.65e-03	9.33e-06	9.02e-6

Figure 2: Resulting maximum differences between nekCRF and Cantera for a premixed test case.

changer both for the realization of beyond the state-of-the-art simulations and for model development due to much faster iteration times.

Acknowledgment

The authors acknowledge computing time grants for the project TurbulenceSL by the JARA-HPC Vergabegremium provided on the JARA-HPC Partition part of the supercomputer JURECA at Jülich Supercomputing Centre, Forschungszentrum Jülich, the Gauss Centre for Supercomputing e.V. (www.gauss-centre.eu) for funding this project by providing computing time on the GCS Supercomputer JUWELS at Jülich Supercomputing Centre (JSC), and funding from the European Union's Horizon 2020 research and innovation program under the Center of Excellence in Combustion (CoEC) project, grant agreement no. 952181. Support by the EuroHPC Inno4Scale program acknowledged.

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