

DNS of Intrinsically Unstable 3D Flames Using Deficient Reactant Thermochemistry: Validation and Scaling in NekRS

Hamid Kavari^{a,*}, Pasquale Eduardo Lapenna^a, Mathis Bode^b, Daniel Mira^c and Francesco Creta^a

^aSapienza University of Rome, Department of Mechanical and Aerospace Engineering, Via Eudossiana 18, 00184 Rome, Italy

^bForschungszentrum Jülich GmbH, Jülich Supercomputing Centre, Wilhelm-Johnen-Straße, 52428 Jülich, Germany

^cBarcelona Supercomputing Center (BSC-CNS), Plaça d'Eusebi Güell, 1-3, Les Corts, 08034 Barcelona, Spain

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ABSTRACT

Understanding the intrinsic instabilities of hydrogen flames is crucial for achieving net zero emissions. Direct Numerical Simulation (DNS) serves as a pivotal tool for this purpose, despite its high computational cost. With advancements in High Performance Computing (HPC) shifting towards GPUs, the deficient reactant model has been integrated into the NekRS framework to improve efficiency. This study validates the deficient reactant thermochemical model within the low-MACH number governing equations in NekRS. In addition, we present the strong scaling performance of this implementation.

1. Introduction

The use of hydrogen as an alternative to carbon-based fuels presents unique challenges due to intrinsic premixed flame instabilities that can profoundly impact flame characteristics [1]. To explore these instabilities Computational Fluid Dynamics (CFD) can be a pivotal tool, where using high fidelity Direct Numerical Simulation (DNS) plays a crucial role in analyzing flame morphology. However, achieving a practical implementation of DNS in complex combustion simulations requires substantial computational resources. Hence, all of the physical scales of flow and flame have to be resolved, and using High Performance Computing (HPC) capabilities becomes crucial [2]. NekRS [3] is a state-of-the-art GPU-accelerated CFD solver that relies on the high-order Spectral Element Method (SEM). In the present study, validation and scaling of the deficient reactant thermochemical model [1, 4] within the low-MACH number governing equations [5] implemented and coupled to NekRS, based on a well-established 2D DNS data set [1, 4, 6, 7] of intrinsic instabilities of premixed flames is presented.

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*Corresponding author

✉ hamid.kavari@uniroma1.it (H. Kavari);

pasquale.lapenna@uniroma1.it (P.E. Lapenna); m.bode@fz-juelich.de (M. Bode); daniel.mira@bsc.es (D. Mira); francesco.creta@uniroma1.it (F. Creta)

ORCID(s): 0009-0000-1122-5342 (H. Kavari); 0000-0002-1966-8743 (P.E. Lapenna); 0000-0001-9922-9742 (M. Bode); 0000-0001-9901-7942 (D. Mira); 0000-0003-1923-0810 (F. Creta)

2. Numerical method

The deficient reactant model employs a single-step, irreversible reaction with constant transport properties, integrated into the low-MACH equations, coupled with the equation of state to solve through high-order SEM. The dimensionless transport equations are expressed as follows [6]

$$\rho \frac{Du}{Dt} = -\nabla p_2 + \frac{1}{Re} \nabla \cdot \left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right), \quad (1)$$

$$\rho \frac{D\theta}{Dt} = \nabla \cdot (\delta_c \nabla \theta) + \frac{\Omega}{\delta_c}, \quad (2)$$

$$\rho \frac{DY}{Dt} = \nabla \cdot \left(\frac{\delta_c}{Le} \nabla Y \right) - \frac{\Omega}{\delta_c}. \quad (3)$$

The continuity equation is represented by the non-zero velocity divergence resulting from both the heat release rate and thermal diffusion, as a restriction on velocity divergence, becomes

$$\nabla \cdot \mathbf{u} = (\sigma - 1) \left[\nabla \cdot (\delta_c \nabla \theta) + \frac{\Omega}{\delta_c} \right], \quad (4)$$

$$\rho = (\theta(\sigma - 1) + 1)^{-1}, \quad (5)$$

$$\Omega = \frac{Ze^2}{2Le} Y \exp \left(\frac{Ze(\theta - 1)}{1 + (1 - \sigma^{-1})(\theta - 1)} \right), \quad (6)$$

where Ω represents the source or sink term based on a single-step Arrhenius reaction and $\mathbf{I}$ is the identity tensor. Also variables including the velocity $\mathbf{u}$, the hydrodynamic pressure p_2 , temperature $\theta = (T - T_u)/(T_{ad} - T_u)$, the mass fraction of the deficient reactant Y are non-dimensionalized. In addition, the LEWIS number Le , ZELDOVICH number Ze , REYNOLDS number Re , the unburnt-to-burned density ratio

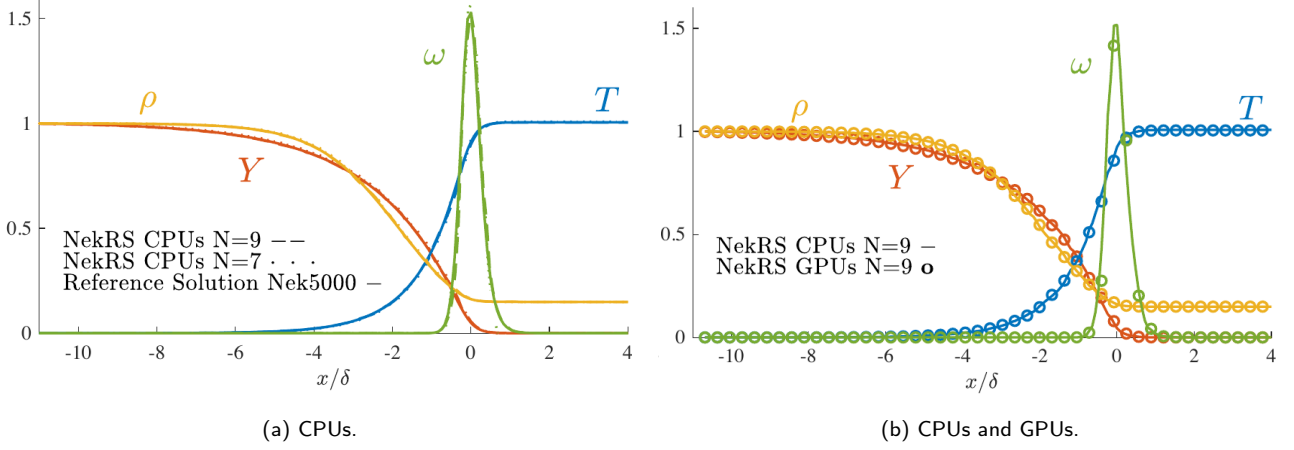


Figure 1: Validation of the EoS independent formulation in NekRS for CPUs and GPUs.

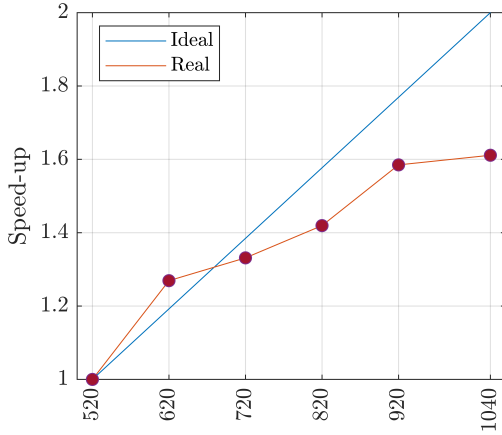


Figure 2: Strong scaling on JUWELS BOOSTER.

$\sigma = \rho_u/\rho_b$ are non-dimensional parameters (see [4] for further details). The only distinction with [6] lies in scaling the non-dimensional flame thickness δ_c , with respect to the cut-off wavelength λ_c rather than the reference hydrodynamic length L , as further detailed in [8].

3. Results

The deficient reactant model has been implemented and extensively utilized in various references [1, 4, 6] within Nek5000, employing a reference solution of a 1D laminar lean hydrogen-air premixed flame to validate the NekRS code. In the Fig. 1a the results of 1D solution, for SERIAL back-end which uses CPUs taking advantage of the MareNostrum 4 cluster at Barcelona Supercomputing Center (BSC), for two different polynomial order of $N = 7$ and $N =$

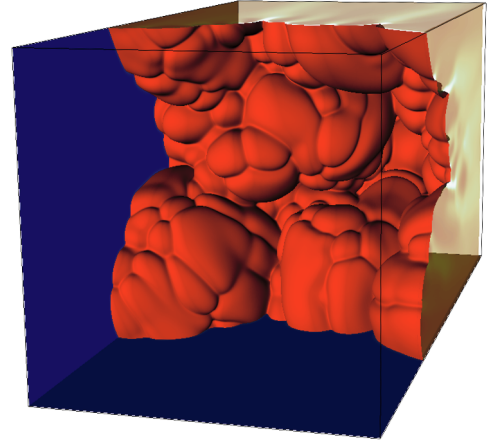


Figure 3: Isosurface of the progress variable of the flame simulation.

9, were compared with the reference solution of Nek5000. The comparison shows a good agreement for T, Y, ω, ρ for all three cases. Also, Fig. 1b compares the results of CUDA back-end using CTE-POWER cluster at BSC, with the validated SERIAL back-end with consistent validation results.

In order to perform a strong scaling of the code, a test case of thermo-diffusive unstable flame with around 18.5 M spectral elements of polynomial order of 7, translating into 6.3 B grid point has been tested on JUWELS Booster cluster in Forschungszentrum Jülich. Each node of this cluster is equipped with four NVIDIA A100, 40GB GPUs and the least amount of nodes needed for the test case to fit the device memory is 130 which has 520 MPI rank. To compare the speed-up across different MPI ranks, we selected a time

instance where the flame is corrugated, as a restart point. The calculation time for a single time-step, averaged over one thousand time-steps, is selected as the speed-up metric. As it can be seen in Fig. 2 different MPI ranks speed-up reported and the baseline is the 130 nodes, where the speed-up is compared to it. As can be seen in Fig. 2 the MPI rank 920 is the highest rank which is close to the ideal speed-up line, while increasing the rank will lead to efficiency reduction. In addition, to demonstrate the domain and flame, Fig. 3 represents an isosurface of progress variable of 0.7, showing a corrugated flame.

4. Conclusions

This study emphasizes the importance of understanding hydrogen flame instabilities for achieving net zero emissions. DNS is crucial despite its computational demands. Implementing the deficient reactant model in NekRS enhances efficiency and offers insights into flame behavior. The validation of a low-MACH formulation alongside strong scaling analysis showcases promising performance gains across different computational architectures, advancing our understanding of complex combustion dynamics. In addition, to advance this study and consider species effects in hydrogen flames, NekCRF [9], a detailed kinetic chemistry solver, will be employed for comparative analyses. This approach is expected to yield deeper insights into flame behavior and enhance our understanding of these complex combustion processes.

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