Topic number 5

Parallel computing of multidimensional hypersonic re-entry flows considering a state-to-state description

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The present study aims at assessing and improving the scalability of the recently developed SPARK code. Accurate predictions of hypersonic re-entry flows, surrounding an inter-planetary exploratory spacecraft, are still extremely difficult due to the high coupling between non-equilibrium processes, radiation and the near-flow field during the entry of a spacecraft in a planetary atmosphere. A high-fidelity simulation of these stringent aerothermodynamics conditions is still CPU limited and requires parallel computations. In the framework of the preparatory access to PRACE research infrastructure (Partnership for Advanced Computing in Europe), a 2D-axyssimetric simulation with state-specific chemical description was performed in order to access SPARK scalability tests in extremely demanding computational conditions. Both the numerical simulations and the code scalability tests will be presented.

1. Introduction

Physical-chemical processes occuring in extremely nonequilibrium atmospheric entry flows can only be adequately modelled through a state-to-state description. Yet, coupling of CFD models with state-specific descriptions remains a daunting task.

SPARK aims at improving the prediction capability of numerical simulations of a wide range of applications. For instance, aerothermodynamics properties for hypersonic re-entry flows and thermal heat fluxes have been numerically studied in by [1] using SPARK. Two distinct classes of physical models are implemented in SPARK, enabling the simulation of gas thermodynamics in non-equilibrium conditions considering either multi-temperature models or state-specific models.

2. Numerical setup

The model is implemented in the in-house SPARK solver (Software Package for Aerodynamics, Radiation and Kinetics) [1] dedicated to compressible aerothermodynamics simulations with detailed chemistry, multi-temperature models and state-specific species characterization. SPARK is written in Fortran 03/08 and explores newly supported object-oriented features, enabling the encapsulation of different physical models, numerical methods, mesh-related operations and interface communications by means of derived-types and type-bound procedures.

A 2D-axisymmetric computational domain of a sphere-cone aero-shell geometry is considered. About 10 thousand volume cells are used for the computational domain discretization. A first convergence run is performed using an initial uniform mesh in order to adapt the mesh at the shock boundary layer. It then follows a second convergence run for the final mesh configuration. The mesh is divided into multiple blocks, which allows for multicore parallel computation. Each block having the same computational load, characterized by an evenly distributed number of volume cells. A second-order finite volume scheme is used for spatial discretization. Time integration of convective terms is performed explicitly using a second-order scheme. The system is marched in time towards convergence. A 5-species air mixture (N2, O2, NO, N and O) with a vibrational state-specific description of the molecular species is considered. The chemical model requires handling over 150 internal states and over 15 000 reactions. A very small CFL is required due to the stiffness of the chemical source terms near the shock boundary layer. The code is parallelized using Coarray Fortran feature, based on the Simple Program Multiple Data model, where each replication of the program is called an image.

3. Acknowledgements

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3. References

[1] B. Lopez and M. Lino da Silva, 46th AIAA Thermophysics Conference, 13–17 June 2016, Washington, D.C, 2016-4025.