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Parallel Adaptive High-Resolution Simulation of Rotating Detonation Engines in 3D

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ABSTRACT

Simulations of rotating detonation engines are still dominated by solvers on uniform or statically refined meshes. Here, we demonstrate the application of 3D parallel block-structured adaptive mesh refinement to this problem class. The computations employ a generic shock-capturing curvilinear high-speed combustion solver within the parallel adaptive mesh refinement framework AMROC. The ability to not only capture the rotating waves effectively, but to resolve sub-scale phenomena down to the cellular structures, intrinsic to detonation propagation, demonstrates the potential of the approach.

1. Introduction

Rotating detonation engines (RDEs) employ one or multiple detonation waves to burn continuously injected propellants at the base of an annular chamber. Each detonation spins circumferentially, creating a self-sustained reaction front followed by high-pressure gas. As the burned gases are exhausted in the axial direction, they generate thrust. RDEs are of considerable interest nowadays as they have the potential to operate thermodynamically more efficiently than conventional pressure-constant combustion engines. RDEs can also operate over a wide range of speeds and pressures, which makes them attractive for use in a variety of applications, e.g., in aerospace propulsion and land-based power generation systems.

Investigating the internal flow field of RDEs in experiments is very challenging as it is difficult to capture the details of waves propagating at velocities of about 2000 m/s. Numerical simulations provide an alternative, however they also face serious obstacles. To be sufficiently sensitive for reliable detonation prediction, it is necessary to employ detailed chemical reaction models. Since practical RDEs generally mix propellants only in the combustion chamber, diffusion cannot be neglected. While using the Navier-Stokes equations with full chemistry models seems paramount, the resolution requirements to capture the instationary detonation waves accurately make in particular reliable 3D simulations very expensive.

An effective approach in mitigating the computational cost is dynamic adaptive mesh refinement (AMR). Because of the need to handle an annular cylindrical chamber, the number of reported 3D simulations of RDEs, that have applied on-the-fly mesh adaptation techniques, is comparatively small. Simply assuming all propellants to be premixed, usually the inviscid Euler equations have been solved, in most cases with a simplified one-step reaction model. Only recently, Pal et al. [1] adopted the commercial CFD code CONVERGE with a full chemistry model for unsteady Reynolds-averaged Navier-Stokes equations, albeit with a cut-cell Cartesian AMR method.

2. Methods

Here, we conduct 3D numerical simulations of an RDE using an extended version of our parallel bock-structured finite volume AMR framework AMROC [2]. AMROC has recently been extended for body-fitted curvilinear meshes defined by a mapping function [3]. For RDE simulation, the multi-component Navier-Stokes equations with a detailed chemical model are solved as governing equations. The HLLC (Harten-Lax-van Leer contact) scheme is applied to approximate the inviscid fluxes, where facet-dependent rotation matrices are used to rotate the velocities to align with the 3D curvilinear mesh. A second-order-accurate MUSCL-Hancock method with mapping-dependent spatial reconstruction is applied for the temporal update. The viscous fluxes are calculated at each face in physical space through the coordinate transformation and are incorporated with a conventional second-order-accurate finite volume approach. As it is common for detonation problems, the chemically reactive source terms are integrated cell-wise in an operator

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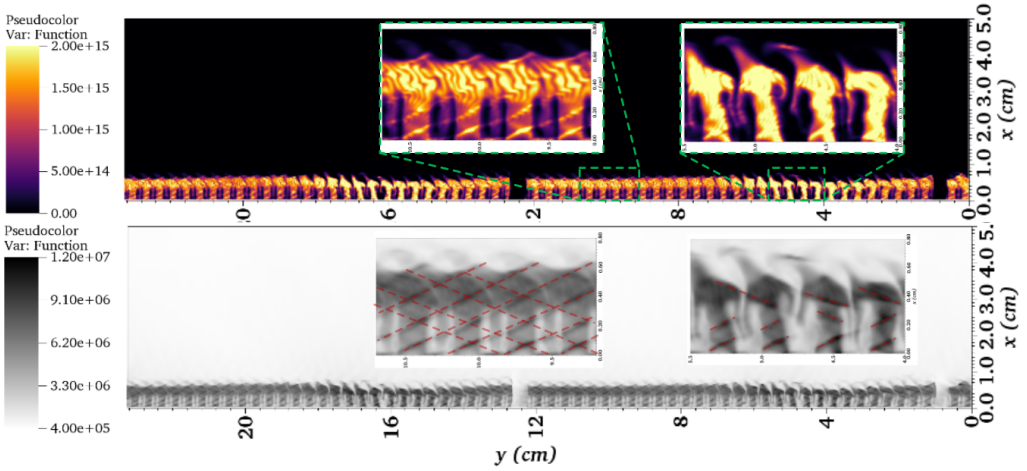

Figure 1: Unwrapped slices of pressure (bottom) and heat release rate (top) during half a rotation cycle.

splitting scheme. A semi-implicit generalized Runge–Kutta method of fourth order (GRK4A) is adopted to integrate the chemical kinetics [4].

AMROC employs a patch-wise refinement strategy, where the entire domain comprises a collection of smaller discrete elements known as blocks. Within these blocks, cells are dynamically flagged using specified refinement criteria. These flagged cells are subsequently grouped into a region of various-sized rectangular blocks. Once the refined cells are created from their parent, namely coarser cells, a hierarchy of embedded grid patches with multiple levels is established. Data between different refinement levels is transferred by averaging and prolongation operations that consider the geometric mapping. To ensure a fully conservative scheme, a flux correction approach is applied and equally extended to handle facets of variable area [3].

For distributed memory parallelization with MPI, the hierarchical mesh is partitioned on-the-fly to processors using a space-filling curve in computational space [2]. A rigorous domain decomposition approach is applied, in which higher refinement levels follow the distribution of the base level cells, however increased workload from spatial and temporal refinement is considered whenever the hierarchical mesh is recreated. The regridding and redistribution process occurs at a specified frequency, ensuring that the region of interest is dynamically captured by the highest-level mesh.

3. Results

A 3D annular model of an RDE running on ethylene and oxygen is simulated. The outer diameter of the chamber is 75 mm, the channel width is 1 mm and the axial height is 50 mm. This chambers corresponds to an actual experiment from our laboratory [5], although the detailed plenum geometry and also plug and aerospike nozzles at the exit are not considered. Initially, the chamber is filled with air at atmospheric conditions. A layer of stoichiometric ethylene-oxygen is initialized with a height of 10 mm. A patch with an analytic 1D detonation wave solution is then used to artificially generate a single detonation wave in the first cycle. A stoichiometric ethylene-oxygen mixture with 20% nitrogen dilution is injected from slots at the head plane. A reduced ethylene/oxygen reaction mechanism [6] with 10 species and 10 reactions is utilized to model the chemistry. Nitrogen is treated as an inert gas. A velocity inlet is used for the injection and the top side is set as an extrapolation outflow boundary condition. The diluted mixture is injected at 300 K and 2 bar, with an inflow velocity of 200 m/s. The average combined inlet mass flow rate is measured at 42.1 g/s. All other boundaries are treated as adiabatic slip walls, thereby neglecting any viscous boundary layers. Because detonation waves in gases propagate at a velocity of around 2000 m/s, this is a justifiable and common simplification in RDE simulations.

Figure 1 depicts the unwrapped plane in the middle of the channel, showcasing two distinct structures observed during the detonation propagation process throughout half of a rotation cycle. The discrete injection leads to flow disturbances ahead of the detonation, and the mixing between the mixture jets and their interval determines the detonation strength locally. The reflected waves are enhanced in the region where the mixture is present. The computational resolution is sufficient to capture the “cells” formed by pressure waves propagating at regular intervals perpendicular to the detonation front. Their size is estimated to be 1.5 mm. These numerical "soot foils" offer a visual representation of the internal wave structure. Weaker reflected waves are observed

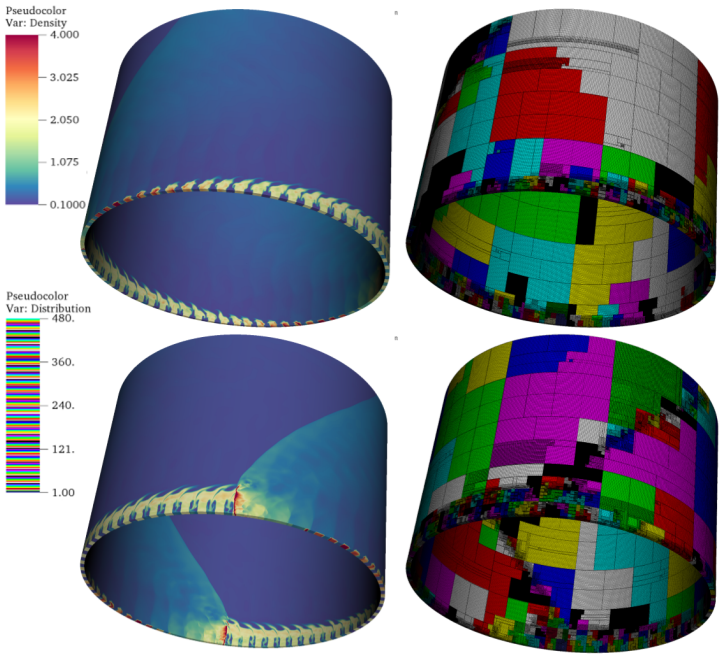

Figure 2: Two snapshots of the evolving density (left) and processors distribution (right) in the 3D RDE.

in regions where mixing is incomplete, which leads to the disappearance of the cellular structure.

The computation was run with two additional refinement levels and it uses approximately 11.6 M to 12.3 M instead of 94.4 M cells in the uniform case. The calculation is performed on 480 cores (Intel Xeon E5-2670 2.0GHz). Typical run times for a simulated time of 1 ms were approximately 12 days wall clock time. Two snapshots of density and processor distribution are displayed in Fig. 2. The images visualize how, after a transient early state without clear detonation (upper row), two stable detonation waves have developed again (lower row). The adaptive mesh clearly follows the fronts at the highest level (right) and most processors are utilized in regions where the workload is high. Note that the number of self-sustaining periodic waves dependent critically but sensitively on the flow conditions and it is one of the most important predictions of RDE simulations.

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