Improving accuracy and performance of Rotating Detonation Engine simulations

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1 Introduction

Nowadays, many laboratories over the world conduct their experiments on the rotating detonation and Rotating Detonation Engine (RDE) [1][2]. In Poland experimental works are conducted at Institute of Heat Engineering of Warsaw University of Technology and from 2010 also at Institute of Aviation. The latest result of cooperation of these two institutes is the project started in 2010 in the framework of Operational Programme Innovative Economy entitled "Turbine engine with detonation combustion chamber".

Parallel to the experimental group, the numerical group has been established. Researchers are developing numerical tools that are necessary for simulations of processes being investigated. Codes that have been validated with the experimental data can be further used as a cheap alternative for experiments or for better understanding of processes with wider range of parameters that are hardly available from experimental results.

This work presents results of three-dimensional simulations of the detonation propagating in candidate combustion chamber of RDE turboshaft engine shown in Fig. 1, which is the subject of the aforementioned project. The assessment of the two techniques of improving performance and / or accuracy of numerical simulations of RDE combustion chamber will be presented, namely the Adaptive Mesh Refinement (AMR) and parallelization of computationally expensive parts of the code in CUDA Fortran.

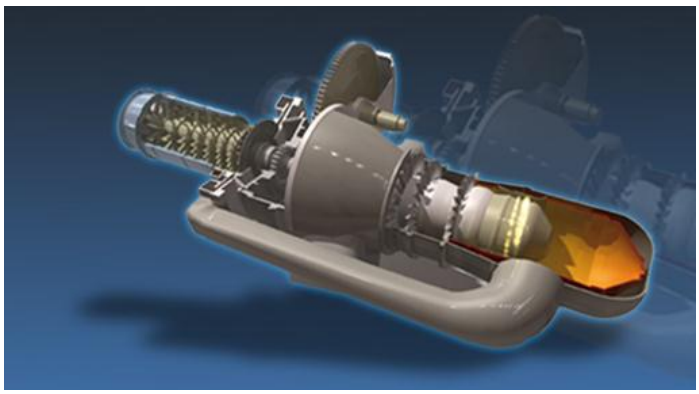

Figure 1. Turboshaft Rotating Detonation Wave Engine.

2 Mathematical and numerical model

Simulations are based on the classical Euler equations, extended to describe the motion of a multicomponent reacting gas, discretized on unstructured grid, in the form:

$$\frac{\partial}{\partial t}\int_V \underbrace{\mathbf{U}}_{\substack{\text{vector of}\\ \text{conserved}\\ \text{variables}}} dV + \sum_{j=1}^{N_{faces}} \underbrace{\mathbf{T}}_{\substack{\text{transformation}\\ \text{matrix}}}{}^{-1} \int_{A_j} \underbrace{\mathbf{F}^j}_{\substack{\text{vector of}\\ \text{convective}\\ \text{flux at face j}}} dA_j = \int_V \underbrace{\mathbf{S}}_{\substack{\text{source term}\\ \text{for chemistry,}\\ \text{injection etc.}}} dV \ .$$

Numerical fluxes **F** are evaluated by HLLC (Harten-Lax-van Leer-contact) approximate Riemann Problem solver [3]. Convective terms are integrated in time by use of the explicit Euler method. The source term **S** is chemical composition change rate resulting from the chemical reactions. The production rate of chemical compounds ω_i is an overall sum of the production and destruction rates for a given chemical compound in all reactions taken into account in the chemistry model:

$$\omega_i = \frac{d\rho_i}{dt} = W_i \left[\sum_{k=1}^{m} \pm \nu_{i,k} \alpha \left(k_{k,for} \prod_j C_j^{\upsilon_{jk}} - k_{k,back} \prod_j C_j^{\upsilon_{jk}} \right) \right].$$

The chemical reaction sources are integrated by the quasi-equilibrium solver CHEMEQ2 or DVODE [4]. The model described above is a widely accepted approach of modeling gaseous detonations. The model is implemented into the in-house code REFLOPS USG [5,6].

In the particular case presented in this work, combustion of hydrogen is described by one reversible reaction:

$$H_2 + 2O_2 \Leftrightarrow 2H_2O\,.$$

The forward reaction rate is calculated by use of classical Arrhenius equation with the reaction rate constants tuned for a reference case, and verified against the Petersen 20-step mechanism [7]:

$$k = AT^n \exp\left(-\frac{E_a}{RT}\right),$$

while the backward reaction rate is calculated from the assumption of local chemical equilibrium.

3 Simulations

The stepped combustion chamber of RDE investigated in Institute of Aviation consists of two annular sections of different heights. The computational model of the stepped chamber was build up from 190 000 elements, and the smallest cell size is 2.2 mm. The study has been conducted on very simple model of inviscid flow with premixed gas.

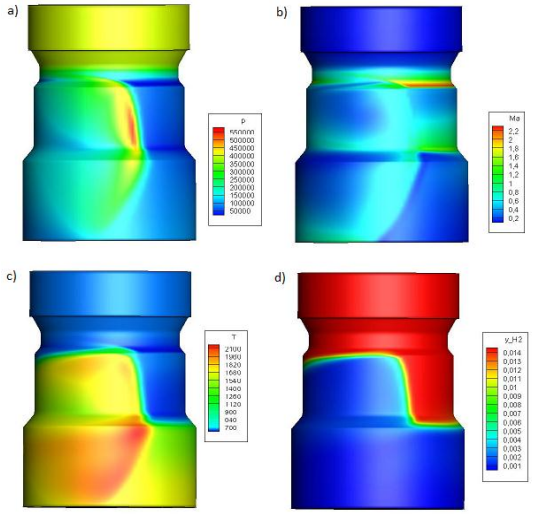

Figure 2. Results of simulations with premixed H_2/Air mixture. Contours of pressure(a), Mach number(b), temperature(c), mass fraction of H_2(d) for λ=2 and p_{in}=4 bar.

Chemeq2 on GPU

The performance of GPU implementation of Chemeq2 procedure [6] during RDE simulations has been assessed. The procedure is suited for the existing in-house code REFLOPS USG and was written in CUDA Fortran, which allows programmer to exploit the computational power of GPU in Fortran. To date not much has been done in parallelizing chemical kinetics procedures. Moreover, the effort undertaken by the authors of developing GPU implementation of chemical kinetics ODE solver CHEMEQ2 is one of the only two described in scientific publications so far ([6][8]).

Adaptive Mesh Refinement

AMR technique, which allows automatic local refinement of grids in regions is implemented in REFLOPS USG. Any good refinement criterion should detect regions of high errors in solution a-priori and apply local mesh refinement in these regions. The error is the highest in proximity of discontinuities and in regions of high gradients. Several refinement criterions have been tested and compared using the proposed method of quantitative assessment of performance and accuracy.

In case of each tested criterion, measurement of execution time of serial code and error analysis for single time step has been performed for some values of refinement threshold and different maximum levels of refinement allowed. Subsequently, for each refinement criterion, plots of execution time versus error have been composed and are subject to further analysis (see Fig. 3).

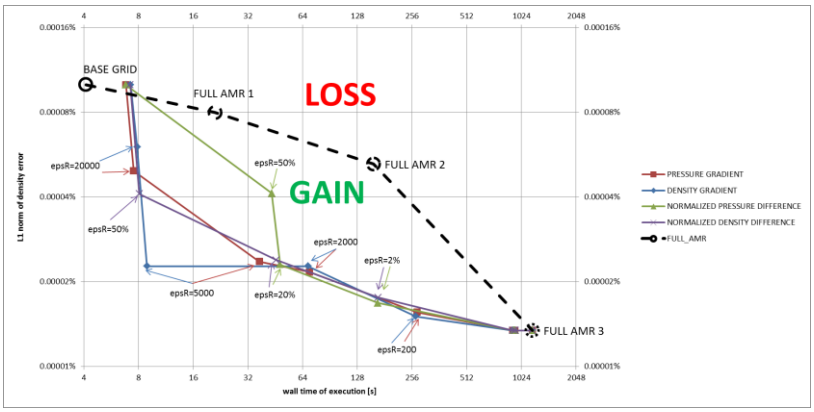

Figure 3. Comparison of performance of refinement criterions (maximum 3levels of refinement allowed)

4. Summary

The results of the implementation of GPU version of chemical kinetics ODE solver CHEMEQ2 are very promising, and speedups are of order of 20 times comparing to single CPU thread. It must be however pointed out, that the practical use of the GPU technology demands parallelization of other parts of CFD codes that are the minor performance bottlenecks of the code.
Research on the performance of AMR refinement criterions has shown that criterions based on density give the highest performance benefit for a given error, and if refinement criterion threshold is properly selected, the performance gain can be about 4 times with only a little bit lower accuracy (what is confirmed in Fig. 3).
Results of accuracy and performance measurements will be further presented and discussed in detail in the full paper.

Acknowledgements

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References

[1] Wolanski P. (2010). Development of the continuous rotating detonation engines. Progress in Pulsed and Continuous Detonations. Edited by Roy GD and Frolov SM. Moscow: Torus Press.
[2] Wolanski P. (2013). Detonative propulsion. Proceedings of the Combustion Institute. 34: 125.
[3] Toro EF. (2010). Riemann Solvers and Numerical Methods for Fluid Dynamics. 3rd edition. Berlin: Springer.
[4] Brown PN, Byrne GD and Hindmarsh AC. (1989). VODE: A Variable Coefficient ODE Solver. SIAM J. Sci. Stat. Comput. 10: 1038.
[5] Kobiera A, Swiderski K, Folusiak M, Wolanski P. (2009). REFLOPS - a New Parallel CFD Code for Reactive Euler Flow Simulation. Archivum Combustionis. 29: 111.
[6] Folusiak M, Swiderski K, Kobiera A, Wolanski P. (2011). Graphics Processors as a Tool for Rotating Detonation Simulations. Irvine, USA: ICDERS.
[7] Petersen EL and Hanson RK. (1999). Reduced Kinetics Mechanisms for Ram Accelerator Combustion. Journal of Propulsion and Power. 15: 591.
[8] Shi Y, Green WH, Wong HW, Oluwole OO. (2012). Accelerating multi-dimensional combustion simulations using GPU and hybrid explicit/implicit ODE integration. Combustion and Flame. 159:7:2388.