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IMPLEMENTATION AND VALIDATION OF A COMPUTATIONALLY EFFICIENT DNS SOLVER FOR REACTING FLOWS IN OPENFOAM

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Abstract. To meet future climate goals, the efficiency of combustion devices has to be increased. This requires a better understanding of the underlying physics. The simulation of turbulent flames is a challenge because of the multi-scale nature of combustion processes: relevant length scales span over five orders of magnitude and time scales over more than ten. Because of this, the direct numerical simulation (DNS) of turbulent flames is only possible on large supercomputers.

A DNS solver for chemically reacting flows implemented in the open-source framework OpenFOAM is presented. The thermo-chemical library Cantera is used to compute detailed transport coefficients based on kinetic gas theory. The multi-scale nature of time scales, which are much lower for the combustion chemistry than for the flow, are bridged by an operator splitting approach, which employs the open-source solver Sundials to integrate chemical reaction rates.

Because the direct simulation of turbulent flames has to be performed on supercomputers, special care has been taken to improve the computational performance. A tool was developed which generates highly optimized C++ source code for the computation of chemical reaction rates. Additionally, a load balancing approach specifically made for the computation of chemical reaction rates is employed. In total, these optimizations can reduce total simulation times by up to 70%. The accuracy of the new solver is assessed from different canonical testcases: 2D and 3D Taylor-Green vortex simulations show that the solver can reach up to fourth order convergence rates and that results differ by less than 1% when compared to spectral DNS codes. Molecular diffusion and chemical reaction rates are compared to solutions of 1D flames from Cantera, showing perfect agreement.

The solver is used to simulate the Sydney/Sandia burner. The simulation is performed on one of Germany's largest supercomputer on 28 800 CPU cores, employing 150 million cells and a chemical reaction mechanism with 19 species and about 200 reactions. Comparison with experimental data shows excellent agreement for time averaged and RMS values.

1 INTRODUCTION

The detailed simulation of turbulent flames is an important task for advancing our understanding of combustion processes and going toward a sustainably energy supply in the future. However, combustion phenomena are governed by a large range of length and time scales, which makes it a multi-scale problem: The residence time of reacting gases in combustion devices may be in the order of seconds, while fast chemical reactions occur on time scales ten orders of magnitudes below. Likewise, there are many orders of magnitudes separating the total dimensions of the combustion device and the smallest time scales in the turbulent flow field. Because of this, direct numerical simulation (DNS) of turbulent flames is only possible on today's largest supercomputers.

To address these problems, a reacting flow solver has been implemented in the open-source CFD framework OpenFOAM [1]. Compared to OpenFOAM's standard solvers, which do not support the calculation of detailed diffusion coefficients, the new solver is coupled to the open-source library Cantera [2]. This makes it possible to compute transport coefficients (heat conductivity, diffusion coefficients and viscosity) for each chemical species from kinetic gas theory.

Because the solver is mainly used for large-scale parallel simulations, a number of performance optimizations have been implemented. By using detailed chemical mechanisms, the combustion process is described by a large number of chemical species and chemical reactions. Computing the chemical reaction rates for each species therefore requires a large percentage of the total simulation time. To overcome this, three important optimizations have been realized: First, a special open-source tool for integrating stiff ordinary differential equations, Sundials [3] is used to decouple the computation of chemical reaction rates from the calculation of the flow field (operator splitting). Secondly, a converter tool has been developed which automatically generates highly optimized C++ source code to compute chemical reaction rates. Lastly, a load balancing approach is implemented which specifically targets the computation of chemical reaction rates by forming pairs of processes that share their workload. These three optimizations lead to significant savings in computing time and help to better utilize the hardware of modern supercomputers.

The work concludes by presenting two validation cases, a canonical one-dimensional flame and the classical three-dimensional Taylor-Green vortex, and an application of the solver to a laboratory-scale turbulent flame.

2 NUMERICAL IMPLEMENTATION

The solver is implemented in the OpenFOAM framework. OpenFOAM is used to solve the governing equations while Cantera is used to compute detailed transport properties. The details are given below and further information can be found in [4, 5, 6, 7, 8, 9]. The solver has thus far been validated and used in a number of works [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27].

2.1 Governing Equations

The governing equations (assuming ideal gases and perfect mixtures) are implemented as follows:

- Conservation of total mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad (1)$$

ρ is the density, t time and \vec{u} the fluid velocity.

- Conservation of momentum:

$$\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \vec{g} \quad (2)$$

p is the pressure, \vec{g} the gravitational acceleration. The viscous stress tensor $\boldsymbol{\tau}$ is computed for a Newtonian fluid using the Stokes assumption:

$$\boldsymbol{\tau} = \mu \left(\nabla \vec{u} + (\nabla \vec{u})^T - \frac{2}{3} I \nabla \cdot \vec{u} \right) \quad (3)$$

where I is the identity tensor and μ the dynamic viscosity.

- Conservation of species mass:

$$\frac{\partial (\rho Y_k)}{\partial t} + \nabla \cdot (\rho (\vec{u} + \vec{u}_c) Y_k) = \dot{\omega}_k - \nabla \cdot \vec{j}_k, \quad k = 1 \dots N-1 \quad (4)$$

Y_k is the mass fraction of species k and $\dot{\omega}_k$ its reaction rate. N is the number of species. The correction velocity \vec{u}_c forces the sum of all diffusive fluxes \vec{j}_k to be zero:

$$\vec{u}_c = -\frac{1}{\rho} \sum_k \vec{j}_k \quad (5)$$

- Conservation of energy: The transport of energy is formulated in terms of the total sensible enthalpy $h_s + \frac{1}{2} \vec{u} \cdot \vec{u}$:

$$\frac{\partial (\rho (h_s + \frac{1}{2} \vec{u} \cdot \vec{u}))}{\partial t} + \nabla \cdot \left(\rho \vec{u} (h_s + \frac{1}{2} \vec{u} \cdot \vec{u}) \right) = -\nabla \cdot \vec{q} + \frac{\partial p}{\partial t} - \sum_k h_k^\circ \dot{\omega}_k \quad (6)$$

with

$$-\nabla \cdot \vec{q} = \underbrace{\nabla \cdot \left(\frac{\lambda}{c_p} \nabla h_s \right) - \sum_k \nabla \cdot \left(\frac{\lambda}{c_p} h_{s,k} \nabla Y_k \right)}_{=\nabla \cdot (\lambda \nabla T)} - \sum_k \nabla \cdot (h_{s,k} \hat{j}_k) \quad (7)$$

λ is the heat conductivity of the mixture, c_p the isobaric heat capacity and T the temperature. Viscous work $\nabla \cdot (\boldsymbol{\tau} \cdot \vec{u})$, potential energy $\rho \vec{g} \cdot \vec{u}$, radiation and the Dufour effect are neglected. The sensible enthalpy $h_{s,k}$ of species k and the sensible enthalpy of the mixture h_s for ideal gases is

$$h_{s,k} = h_k - h_k^\circ, \quad h_s = \sum_k Y_k h_{s,k} \quad (8)$$

and $h_k^\circ \equiv h_k(298 \text{ K})$ is the enthalpy of formation of species k . The corrected diffusive mass flux \hat{j}_k is

$$\hat{j}_k = \vec{j}_k - Y_k \sum_k \vec{j}_k \quad (9)$$

and Fourier’s second law $\nabla \cdot (\lambda \nabla T)$ is rewritten (assuming ideal gases and that all species have the same temperature) in order to obtain the first term on the r.h.s. of Eq. 7, which can be discretized implicitly.

2.2 Coupling with Cantera

The computation of the transport coefficients (diffusion coefficients, heat conductivities and viscosities for each species) is done with Cantera, while OpenFOAM solves the governing equations above, according to Fig. 1. In this way, mixture-averaged diffusion based on the Curtiss-Hirschfelder approximation as well as full multi-component diffusion can be used in the simulations.

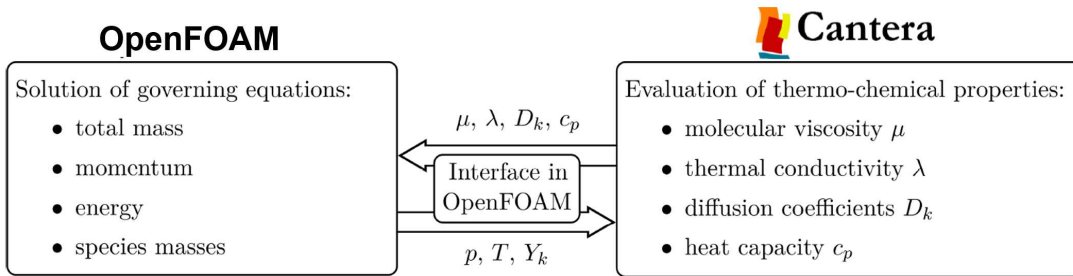


Figure 1: Coupling of OpenFOAM with Cantera. OpenFOAM solves the governing equations while Cantera computes detailed transport coefficients for molecular diffusion.

3 OPTIMIZATION OF REACTION RATE COMPUTATION

Because combustion is described by a large number of chemical species and reactions, the computation of chemical reaction rates can make up a large portion of the total simulation times.

3.1 Operator Splitting

In order to decouple the small time scales of the chemical reactions from the large time scales of the flow, chemical reaction rates are integrated over the simulation time step assuming that each cell in the computational domain is a perfectly stirred reactor. The integration is performed with the open-source tool Sundials, which is specifically optimized for this kind of integration. Compared to OpenFOAM’s built-in integrators, this can reduce computing times by several orders of magnitudes. For more information, see [8, 22].

3.2 Automated Code Generation

The information about chemical reactions is usually given to the simulation software in form of a text file. This file contains the parameters, like Arrhenius constants A , b , E_a , for each chemical reaction:

$$k_r = AT^b \exp\left(\frac{-E_a}{RT}\right) \quad (10)$$

k_r is the rate constant of reaction r , T the temperature, R the universal gas constant, A the pre-exponential frequency factor, b the temperature exponent and E_a the activation energy. At

the start of the simulation, this text file is read and the chemical reaction rates are computed based on the data. However, in many detailed reaction mechanisms, many of the computations can be avoided. For example, in the popular GRI 3.0 [28] reaction mechanism, more than one hundred reactions have zero activation energy, meaning that the computation of exponential term in Eq. 10 can be omitted.

Therefore, a converter tool has been developed that reads in the text file containing the information about the chemical reactions, deletes unnecessary computations like the one described above, reorders species and reactions to create easily vectorizable loops and lays out all data linearly in memory to avoid cache misses. Using these optimized chemistry routines together with the Sundials integrator CVODE leads to large savings in computing time, compared to the default methods implemented in OpenFOAM's standard solver reactingFoam, as shown in Fig. 2. For more information about this topic, see [7, 9, 29].

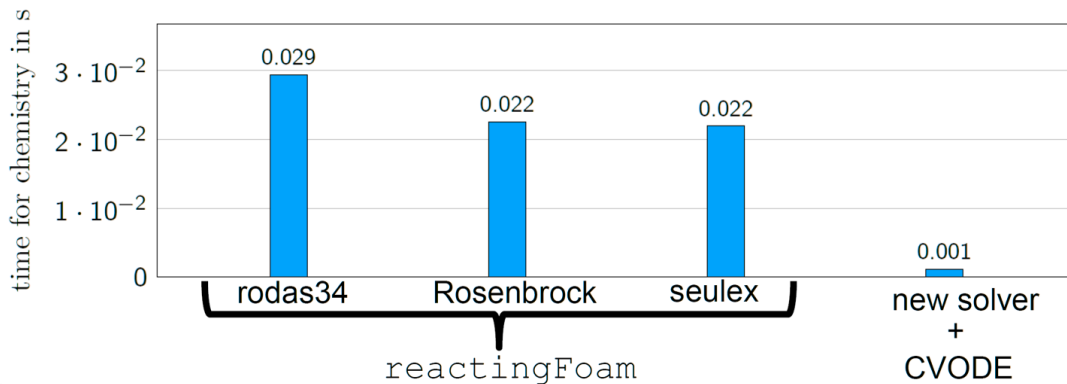


Figure 2: Time required to compute chemical reaction rates. Three cases on the left are OpenFOAM's default methods, case on the right is the automatically generated chemistry code together with Sundials CVODE solver [9, 29].

3.3 Load Balancing

Because the chemical reaction rates are computed decoupled from the flow using iterative ODE solvers, a load-imbalance can be created. When the computational domain is decomposed into sub-domains for parallel computation, there may be some processes that have to simulate large parts of the flame, while other processes might have sub-domains which contain no part of the flame at all. Because of this, a special load balancing implementation has been devised which communicates the workload of processes to form pairs of processes. One process in the pair has a low workload while the other has high workload. The workload is then shared between the processes. Even though the theoretical speedup is limited by a factor of two, the implementation creates a low number of additional MPI connections, which is beneficial for large-scale parallel simulations. For more information about the load balancing, see [6]. Together with the aforementioned optimizations, simulation times can be reduced with the new solver by 70%.

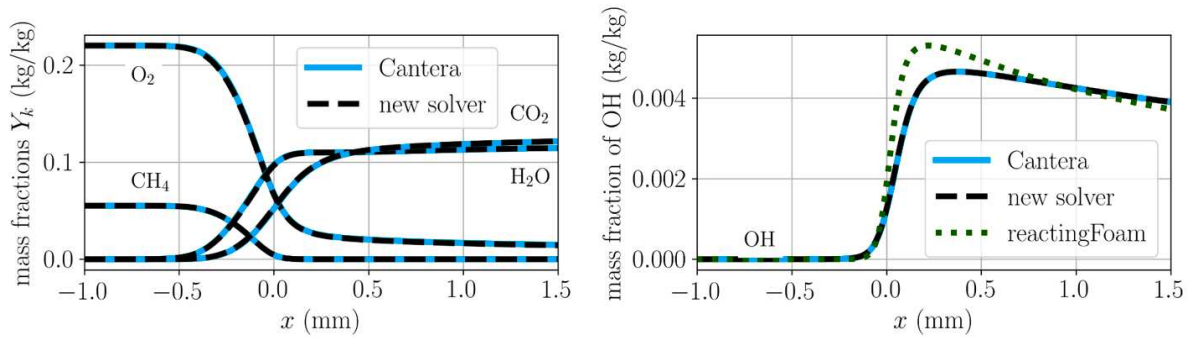


Figure 3: One-dimensional flame results compared to a reference solution computed with Cantera [5].

4 VALIDATION

4.1 1D Model Flame

A canonical validation case for flames is the one-dimensional, steady-state premixed flame. The computational setup consists of an inlet with the premixed fuel/air mixture and an outlet for the burnt gases. In the middle of the domain, a flame burns. Figure 3 compares the profiles of selected species from the results of the optimized solver with a reference solution by Cantera for a methane/air flame. For more information about this setup, see [5].

4.2 Numerical Accuracy

Another test case for a non-reacting flow is the classical Taylor-Green vortex. It can be used to assess the numerical accuracy of solvers. An initial velocity field places vortices in a three-dimensional box, which then decay into a pseudo-turbulent flow. Figure 4 shows the dissipation rate over time inside that box. The black dashed line is a reference solution from a spectral DNS code. Using OpenFOAM’s cubic discretization yields comparable results to the spectral DNS solution on the same mesh, while the central difference (CD) and first order upwind schemes

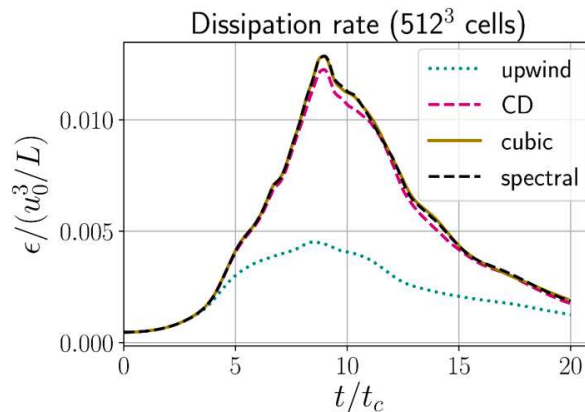


Figure 4: Dissipation rate over time inside the computational domain. Compared are OpenFOAM simulations with different discretization schemes with a spectral DNS [5].

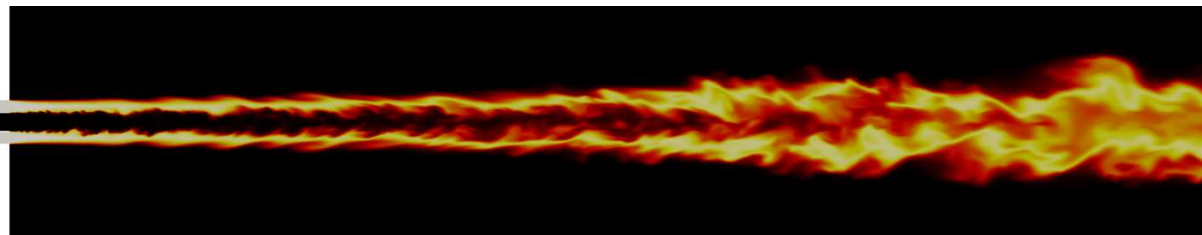


Figure 5: Snapshot of the temperature field on a 2D cutting plane from the simulation of the Sydney/Sandia flame [5].

would result in less accurate solutions. It is therefore highly recommended to use OpenFOAM's cubic scheme for simulations with a need for high accuracy. For more information about the Taylor-Green case, see [5].

5 APPLICATION: SYDNEY/SANDIA FLAME

A well documented and experimentally investigated turbulent flame of laboratory scale is the Sydney/Sandia flame [30, 31, 32]. Using the new solver, a quasi-DNS of this flame has been conducted and a database consisting of 10 TB of data has been created. Figure 5 shows a snapshot of the temperature field on a two-dimensional cutting plane.

5.1 Numerical Setup

The numerical domain contains of 150 000 000 cells. The mesh is locally refined and the smallest resolution is $10\ \mu\text{m}$. A reaction mechanism with 19 chemical species and 200 chemical reactions is

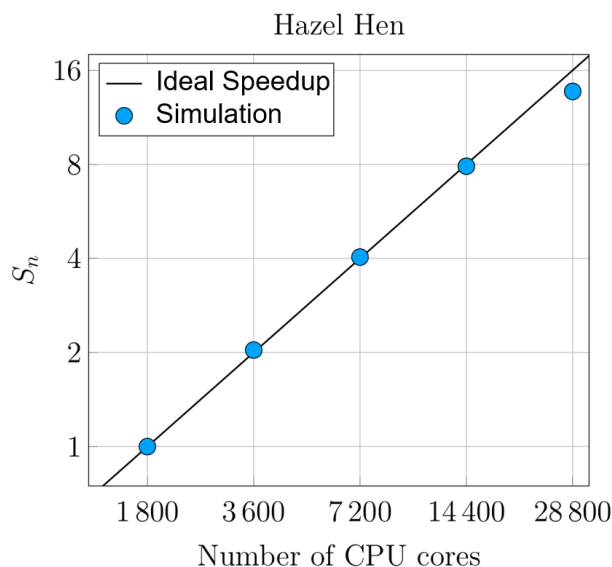


Figure 6: Parallel scaling efficiency of the simulation of the Sydney/Sandia flame on one of Germany's fastest supercomputers with the OpenFOAM based DNS solver [9, 29, 23].

employed to model the combustion process. Spatial gradients are discretized with OpenFOAM’s fourth order interpolation scheme cubic and for the temporal discretization, a second order implicit Euler method is used. For more details about the setup, see [5, 14, 10].

The simulation has been conducted on Germany’s fastest supercomputer at the time, HAZEL HEN at the High Performance Computing Center in Stuttgart. The simulation was run with up to 28 800 CPU cores and has shown very good parallel scaling (see Fig. 6).

5.2 Comparison with Experimental Results

Because the Sydney/Sandia flame has been experimentally investigated, the simulation results can be directly compared with the experimental data. Figure 7 shows mean and rms values of temperature, mixture fraction Z and oxygen mass fraction at different axial positions (x/D , D is the nozzle diameter). Apart from the deviation of mixture fraction near the nozzle, the simulation results are mostly within experimental uncertainties.

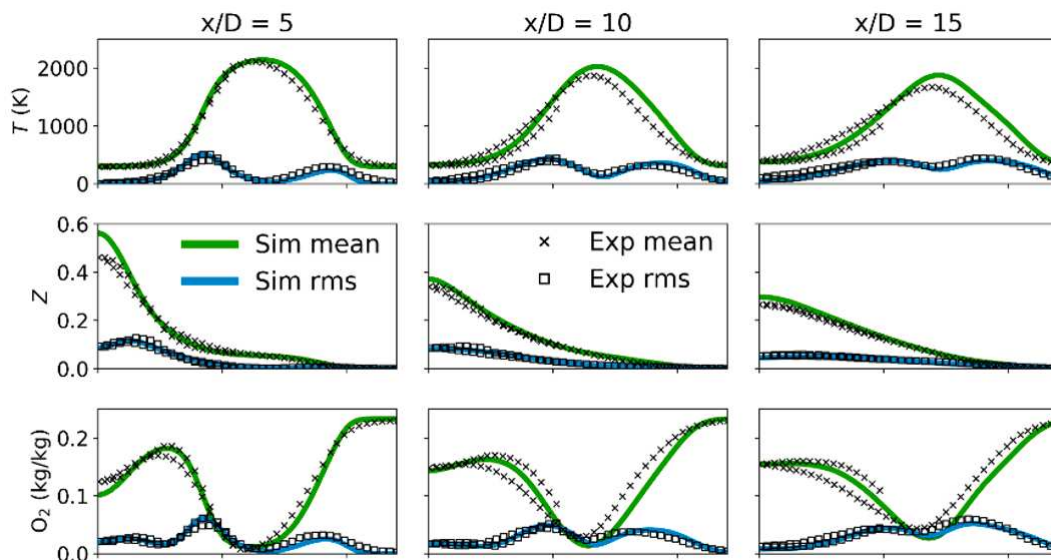


Figure 7: Comparison of experimental data and simulation results for the Sydney/Sandia flame [9, 29, 23].

6 CONCLUSIONS

An OpenFOAM based solver for the direct numerical simulation of reacting flows has been presented. The solver extends OpenFOAM’s capabilities in several aspects: First, the new solver is coupled to the open-source library Cantera to allow the computation of detailed diffusion coefficients for each chemical species. Second, the solver contains a number of performance optimizations, making it suitable to perform massively parallel simulations on today’s supercomputers.

The computation of chemical reaction rates is sped up by using a highly efficient integrator, Sundials, which outperforms OpenFOAM’s default solvers. A converter tool has been implemented

that generates highly optimized C++ code that accelerates the reaction rate computations without affecting accuracy. Lastly, a new load balancing method for chemical reaction rate computations for highly parallel applications has been introduced. In total, the new solver can save over 70% of the total simulation time this way.

The solver and its accuracy have been validated with a number of canonical test cases. From one-dimensional flames, to the three-dimensional Taylor-Green vortex case to comparison with experimental results of turbulent flames. Deviations to Cantera's reference solution for the 1D flame and to the spectral DNS code for the Taylor-Green vortex case are below 1%. In addition, the solver shows excellent parallel scaling behavior, which has been tested with up to 28 800 CPU cores.

In conclusion, the new solver has been shown to be a valuable tool for studying turbulent combustion on large parallel supercomputers.

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