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Direkte Numerische Simulation der Verbrennung bei höheren Reynoldszahlen

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ZUSAMMENFASSUNG

Die direkte numerische Simulation (DNS) ist ein potentes Werkzeug bei der detaillierten Analyse von Verbrennungsphänomenen. Das diesem zugrundeliegende Gleichungssystem wird mit einer hohen räumlichen und zeitlichen Auflösung gelöst und liefert dadurch Informationen, zu welchen man auf andere Art keinen Zugang hat. Da DNS mit sehr grossem Rechenaufwand verbunden ist, sind effiziente numerische Algorithmen und Parallelisierung grundlegende Voraussetzungen für die Simulation von komplexen Phänomenen/Geometrien oder praktischen Anwendungen. In den letzten Jahren haben wir mit unserem zweidimensionalen DNS Code grundlegende Phänomene in der Verbrennung mit detaillierter Chemie und Transporteigenschaften untersucht. Dieselben Algorithmen werden jetzt in einen parallelen dreidimensionalen Code für nicht reaktive Strömungen implementiert, welcher mit effizienten Lösungsalgorithmen versehen ist und dessen Rechenzeit gut mit der Anzahl der verwendeten Prozessoren skaliert. Dieser erweiterte Code wird die Basis für die Untersuchung von laminaren und transienten Verbrennungsphänomenen bilden. Zudem wird auf der Basis dieses Codes die Implementierung des Grobstruktur Simulation (LES) Ansatzes zur Simulation der turbulenten Verbrennung implementiert. Während des Berichtjahres 2003, wurde ein Einschritmechanismus für die chemische Reaktion und ein vereinfachter Transportmechanismus in den dreidimensionalen Code implementiert und auf dem vom LAV/ETHZ kürzlich erworbenen 64–CPU Cluster validiert. Die perfekte Skalierbarkeit des parallelen Codes erlaubte es Instabilitäten in Diffusionsflammen nahe der Auslöschung in einem dreidimensionalen Jet zu untersuchen. Ähnlich wie in Experimenten welche an der EPFL durchgeführt wurden, zeigten die Simulationen eine zellenförmige Struktur in der Flamme, die aus zwei bis sechs Zellen besteht. Für ein und dasselbe Parameterset wurden koexistierende, zellenförmige Strukturen entdeckt was auf das experimentell beobachtete Hystereseverhalten hindeutet. Im nächsten Jahr wird der Code noch durch detaillierte Beschreibung der Chemie und Transportprozesse erweitert. Gleichzeitig wollen wir uns schon mit der bestehenden 1-Schritt-Reaktionskinetik Problemen an generischen Geometrien bei transitionellen Reynoldszahlen (um 10^3) widmen.

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1 Project description

Direct Numerical Simulation (DNS) is a powerful tool for the detailed study of combustion phenomena. It solves the system of governing equations with high spatial and temporal accuracy and can provide information that cannot be obtained by other means. Unfortunately, it also carries a very high computational cost. Efficient numerical algorithms and parallelization are essential for simulating complex phenomena or problems of practical interest. During the last few years, our two-dimensional DNS code was used to study phenomena of fundamental interest in combustion with detailed chemistry and transport properties. The same algorithms are now being implemented in a parallel, non-reactive, three dimensional code with efficient solvers and very good scalability on a number of parallel architectures. The extended code will be the main tool for the study of laminar and transitional combustion phenomena. It will also be the basis for the implementation of Large Eddy Simulation (LES) approaches for the simulation of turbulent combustion. First results have been obtained on the 64-CPU Linux cluster of LAV/ETHZ for jet diffusion flame instabilities close to extinction that have been observed experimentally at EPFL.

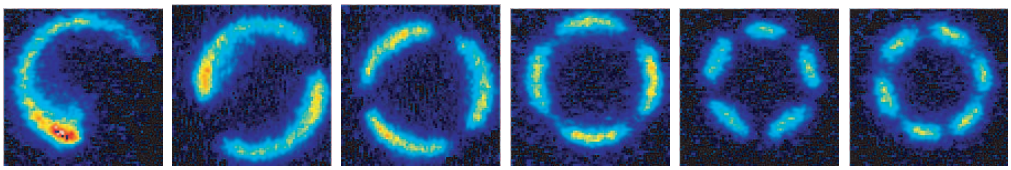
2 Numerical approach

Our simulation tool is based on the spectral element discretization of the partial differential equations describing the conservation equation of mass, momentum, species, and energy for three-dimensional chemically reacting system at the low Mach number limit. The spectral element method combines the flexibility of the finite element method to discretize complex geometries with the accuracy of spectral methods. Locally, the mesh is structured, with the data and geometry expressed as sums of N^{th}-order tensor product polynomials [4]. Globally, the mesh is an unstructured array of deformed hexahedral elements. Temporal discretization is based on a high-order, operator-splitting formulation for low speed compressible reacting flow that permits large time steps. More information about the numerical algorithm can be found in [1, 2, 3, 4].

In collaboration with Dr. Paul Fischer (Argonne National Laboratories), we implemented the algorithms for reactive flow species and energy equations in a parallel, non-reactive, three dimensional, spectral element base code. The code uses scalable domain-decomposition-based iterative solvers with efficient preconditioners. The parallel implementation is based on the standard message-passing Single Program Multiple Data (SPMD) mode, where contiguous groups of elements are distributed to processors and the computation proceeds in a loosely synchronous manner; communication is based on the MPI standard. The code exhibits very good parallel efficiency and scalability properties, sustaining high MFLOPS, on a number of distributed-memory platforms.

Currently, single-step chemistry and simple transport have been implemented. The code is already used on the LAV 64-CPU Linux cluster for the simulation of jet diffusion flame instabilities close to extinction observed experimentally at EPFL.

3 Main results



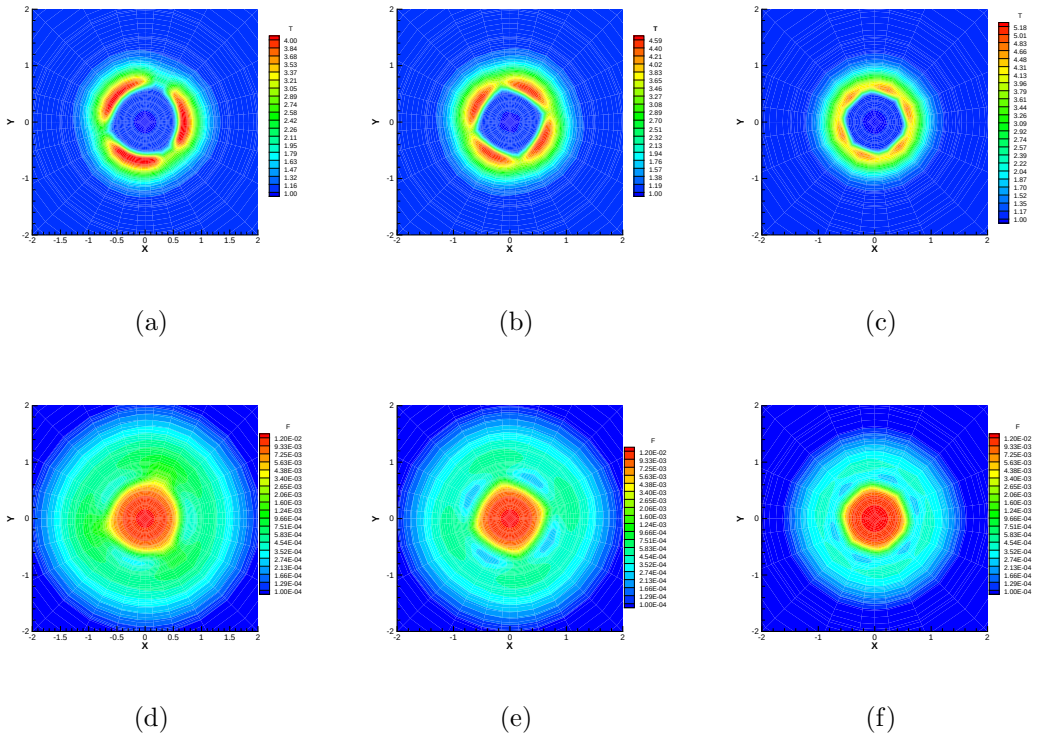
(a) 1R-cell (b) 2R-cell (c) 3R-cell (d) 4S-cell (e) 5S-cell (f) 6S-cell

Figure 1: Streamwise integrated chemiluminescence images taken from the downstream jet axis of a 22.5% H_2 (78.5% CO_2) jet flame burning in (a) 24.6% O_2 (75.4% CO_2) co-flow; (b) 26.0% O_2 co-flow; (c) 27.5% O_2 co-flow; (d) 31.0% O_2 co-flow, (e) 40.0% O_2 co-flow, and (f) 21.5% H_2 (79.5% CO_2) jet flame burning in 70.0% O_2 co-flow. "R" designates rotating and "S" stationary cell patterns.

The EPLF jet flame facility consists of a free jet apparatus, oriented vertically up and mounted on a precision traverse, together with PC-based data acquisition and control systems. An intensified CCD camera (LaVision, Flamestar II) with 384×576 pixels and 14-bit resolution was used to record images of the streamwise integrated chemiluminescence emission from above the flame tip. The flow rates of the hydrogen, oxygen, and carbon dioxide (used as diluent) gases to the jet apparatus were set with fully automated flow controllers (Teledyne-Hastings, HFC 202) with a nominal accuracy of 1% (Full Scale). Flow rate calibrations were verified with a flow calibrator (Bios, DC-2M). The gaseous fuel passed through a muffler, settling chamber with honeycomb straighteners and screens, and finally through a contoured axisymmetric contraction with an area ratio of 100:1. The diameter of the circular fuel nozzle is $D = 0.75$ cm. In order to control the oxidizer characteristics, a uniform co-flow of the oxygen-carbon dioxide mixture could be introduced through a porous plate of 7.5 cm diameter surrounding the fuel nozzle.

A systematic experimental investigation of cell formation in CO_2-diluted H_2-O_2 circular jet non-premixed flames was performed on this burner. The uniform fuel velocity was $U_F = 76$ cm/s, and the co-flowing oxidizer stream velocity, U_O,

was fixed at 4 cm/s. The parameter space near the extinction limit was investigated by fixing the fuel composition (H_2-CO_2 mixture), and then systematically lowering the O_2 concentration in the co-flowing oxidizer stream (O_2-CO_2 mixture). The O_2 concentration was lowered in decrements of less than 0.1% (by volume) until first a transition to cellular flames was observed, and then further until the extinction (blow-off) limit was reached. The conditions for these near-extinction experiments covered a range of reactant Lewis numbers, *based on the overall fuel-oxygen mixture at 300 K* of [1.1-1.2] for oxygen and [0.25-0.29] for hydrogen. Figure 1 shows the various types of cellular modes observed at a fixed jet fuel composition (22.5% H_2, except for the last image (f) observed for 21.5% H_2) and various oxygen concentrations above the extinction limit of 23.2% O_2. These images were taken from above the flame, and the false-color scale is related to the intensity of the chemiluminescence, integrated in the streamwise direction over the entire length of the flame.



(a) (b) (c)

(d) (e) (f)

Figure 2: Temperature iso-contours of the (a) 3- ($A = 1.8 \cdot 10^8$, at z=0.8*D), (b) 4- ($A = 1.8 \cdot 10^8$, at z=0.8*D), and (c) 6-cell flame ($A = 2.5 \cdot 10^8$, at z=0.5*D); (d)-(f) corresponding fuel mass fraction iso-contours.

The computational domain is a cylinder with diameter equal to five times the jet-nozzle diameter, D=0.75 cm, and height equal to $10 * D$. The fuel stream is

CO_2-diluted H_2 ($X_{H_2}^{fuel} = 0.215$) and enters the domain with a top-hat velocity profile of $U_F = 76cm/s$ at T=300K. Oxidizer is a O_2/CO_2 mixture ($X_{O_2}^{ox} = 0.50$), with a uniform velocity profile of $U_O = 4cm/s$, and T=300K. Single-step chemistry was employed; $2H_2 + O_2 \rightarrow H_2$, with rate $r = A\,T^n\,\exp(-T_a/T)\,[H_2]^2\,[O_2]$ with reaction rate parameters $n = 0.91$, T_a=27.7 , and dimensionless heat of reaction ΔH_r=44.12. The starting of the non-dimensional pre-exponential factor was $A = 1.33 \cdot 10^9$, and constant but unequal Lewis numbers ($Le_{H_2} = 0.26, Le_{O_2} = 1.15, Le_{H_2O} = 1.12, Le_{CO_2} = 1.7$) were used. Two resolutions were employed with 1166 and 2376 spectral elements with interpolating polynomial orders $6 \leq N \leq 8$ and $N = 4$ in each of the three spatial directions, respectively. The largest simulation had a total of about 600,000 points, corresponding to more than 5 million unknowns.

By varying the dimensionles pre-exponential factor,A, the simulations captured many of the phenomena observed experimentally: existence of cellular structures with different number of cells close to extinction, co-existence of different cellular structures close to extinction (fig. 2), and sensitivity to (numerical) noise. More details can be found in the attached paper that was submitted to the upcoming Combustion Symposium.

4 National collaborations

In collaboration with the Fluid Mechanics Laboratory of EPFL, we are studying diffusion flame instabilities close to extinction. The work is a combination of experiments, numerical simulation and stability analysis.

5 International collaborations

The parallel, three-dimensional reactive flow DNS code is being developed in collaboration with Dr. Paul Fischer of Argonne National Laboratory, USA.

6 Conclusions and outlook

During 2003 single-step chemistry and simplified transport was implemented in the 3-D parallel code and validated on the 64-CPU Linux cluster recently acquired by LAV/ETHZ. The linear scalability of the new reacting flow code allowed us to study cellular flames instabilities in the full 3-D context. Phenomena like cellular structures with different number of cells, and co-existence of different cellular structures for the same parameter values observed experimentally at EPFL in jet diffusion flames close to extinction were captured by the simulation. In 2004, we plan to continue the study of cellular flames over extended parameter ranges. In

addition, the code will be extended for the detailed description of chemistry and transport.

7 Publications

C.E. Frouzakis, A.G. Tomboulides, P. Papas, P.F. Fischer, R.M. Rais, K. Boulouchos, and P. Monkewitz, "Three-dimensional numerical simulations of cellular jet diffusion flames", *Proc. Comb. Inst.*, **30**, (submitted).

This publication is appended at the end of the report.

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[2] A.G. Tomboulides, J. Lee, and S.A. Orszag, Numerical simulation of low Mach number reactive flows, *J. Sci. Comp.*, **12**(2) 139–167, (1997).

[3] A.G. Tomboulides, and S.A Orszag, A quasi two-dimensional benchmark problem for low Mach number compressible codes, *J. Comp. Phys.*, **146**(2), 691–706, (1998)

[4] M.O. Deville, P.F. Fischer, and E.H. Mund, *High-Order Methods for Incompressible Fluid Flow.* Cambridge University Press, (2002).