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LATTICE BOLTZMANN SIMULATIONSMETHODEN FÜR CHEMISCH REAKTIVE SYSTEME IM MICROBEREICH

Schlussbericht

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Zusammenfassung

In Rahmen dieses gerade abgeschlossenen Projektes, wird eine neue Annäherung für die rechenunterstützte Strömungsdynamik an einer Mikrometerskala entwickelt. Diese Annäherung basiert auf den sogenannten Boltzmann Gitter-Modellen (Lattice Boltzmann Method) der Boltzmann-kinetischen Gleichung. Als Ergebnisse des Projektes, sind folgende Ziele erreicht worden:

1. Die komplette Klasse von neuen und numerisch stabilen Lattice Boltzmann Modellen mit mehreren Geschwindigkeiten der Teilchen ist hergeleitet und mathematisch bewiesen.
2. Rechnerisch effiziente drei-dimensionale Modelle für isotherme Strömungen wurden entwickelt und dazugehörige effiziente parallele Computerprogramme an mehreren Problemen getestet. Diese Modelle zeigten numerische Stabilität und sind deshalb sehr wichtig für die Simulation bei höheren Reynolds-Zahlen, wie sie in turbulenten Strömungen vorherrschen. Durch die speziellen Modifikationen (zum Beispiel Outflow Randbedingungen) ist es gelungen, effiziente Simulationen in Angriff zu nehmen.
3. Ein drei-dimensionales thermisches Modell wurde weiter entwickelt und realisiert in einigen „benchmark“ Strömungen (zum Beispiel die Rayleigh-Benard Strömung). Es ist auch gelungen die Strömungen mit erheblichen Temperatur- und Dichteschwankungen mit diesem Modell zu beschreiben.
4. Das Modell für Strömungen mit mehreren Komponenten wurde entwickelt, implementiert und getestet.
5. Die neuen Modelle wurden auch zur Beschreibung von Strömungen von verdünnten Gasen angewendet.
6. Eine Methode zur Reduktion komplexer Reaktionsmechanismen wurde entwickelt und getestet für zukünftige Verbrennungsanwendungen.

Theoretische Fragen sind dabei vollständig geklärt, wie die längst nötige stabile Lattice Boltzmann Modellen auf grössere Gittern, und die praktischen Fragen der effektiven Anwendung. Das mikroskopisch abgeleitete thermische Modell verbessert im Wesentlichen die früheren Ergebnisse der isothermalen Modelle, was unter anderem mit einer neuen Klasse der exakten Lösungen bewiesen wurde. Diese sehr effizienten Modelle ersetzen kostspielige mikroskopische Simulationstechniken wie kinetisches Monte-Carlo und/oder molekulare Dynamik für niedrige Mach-Zahl und moderate Knudsen-Zahl. Die Ergebnisse wurden in insgesamt 30 Publikationen und Pre-prints dargestellt.
Durch diese Ergebnisse eröffnen sich neue Möglichkeiten, Strömungen in Mikrokanälen und poröse Medien effizient zu rechnen, was für zukünftige Komponenten von Energiewandlern (Reformer, Katalysatoren, Mikrobrenner, Brennstoffzellen usw.) von grosser Bedeutung ist. Die damit entstandenen neuen Simulationsmöglichkeiten sind bereits weiter ausgebaut in Rahmen unseren CCEM-CH Projekten „CEMTEC“.

1. Ausgangslage

Meeting modern challenges in engineering require an understanding of the flow phenomena in complex, multicomponent fluids in a wide range of scales, starting from turbulent flows to flows at a micron scale where the traditional continuum mechanics approach becomes invalid. These challenges

are mirrored in the development of modern computational approaches which have to tackle multi-scale physics in simulation. This is important in the case of reactive thermo-fluidics where efficient computational models are sought. In recent years, much attention was given on development new computational approaches such as lattice gas automata, lattice Boltzmann models, dissipative particles dynamics etc. In spite of a rapid progress over the last decade, these methods still require a further development before becoming a tool for engineering applications. The goal of this project was to significantly advance the development of a particularly promising approach – the Lattice Boltzmann Method – and to bring it to a ready-to-use state for engineering applications.

2. Ziel der Arbeit

The goal of this project was to develop novel efficient models and computational algorithms for complicated physical and chemical processes in fluid flows far from equilibrium. Our specific focus is on non-isothermal compressible flows at a micrometer scale. Such flows are typical in many current problems of aero-thermo-chemistry at a micron scale, and further complications arise due to chemical reactions, both in the bulk flow and on the surface (heterogeneous catalytic reactions). Rarefaction is characterized by Knudsen number, Kn, the ratio of the mean free path of molecules to a characteristic variation of hydrodynamic fields (density, momentum, temperature). Moderate values of Kn (up to 1) are most important for industrial applications and at the same time too difficult for both continuous hydrodynamic models and the purely molecular-dynamics approaches. Within this project, we aimed at developing the *Entropic Lattice Boltzmann Models* which are capable of replacing both the heuristic continuous mechanic models and computationally intensive molecular models.

The goals of the project were the following:

1. To give a derivation of the multi-speed lattice Boltzmann models which would enhance accuracy of the present standard models and allow for a novel class of simulations of thermal and multiphase flows.
2. To massively increase the efficiency of three-dimensional simulations.
3. To develop the lattice Boltzmann models for multi-component mixtures.

3. Methode

The Lattice Boltzmann method (LBM) is a mesoscopic approach in modeling and simulation of fluid dynamics. These methods occupy an intermediate place between the purely continuum mechanics on the one hand and the molecular dynamics on the other (see Fig. 1). It can be considered as a kinetic equation for fictitious particles which have only a small number of allowed velocities (typically, from a dozen to several dozens), constructed in such a way that their dynamics recovers the equations of hydrodynamics in a long-time large-scale limit. Lattice Boltzmann models allow an extremely simple and efficient realization on parallel computer architectures.

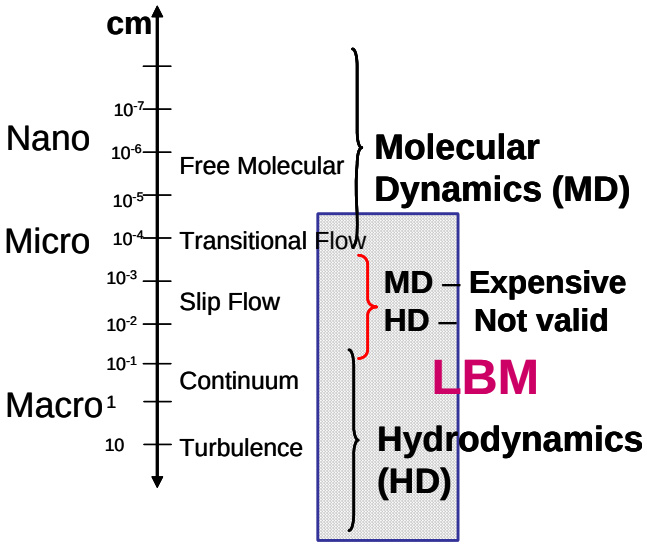

Fig.1: A schematic diagram indicating the domain of validity of the Lattice Boltzmann Method for various system sizes.

4. Ergebnisse

4.1: State-of-the art Lattice Boltzmann computing.

We have described all Lattice Boltzmann models for arbitrary number of speeds which essentially conclude the theoretical development of the Lattice Boltzmann method, and open a new perspective on numerically stable thermal and multiphase flow simulations (S.S. Chikatamarla, I.V. Karlin, **Entropy and Galilean invariance of lattice Boltzmann theories,** Physical Review Letters, **97**, 190601 (2006)). This new class of multispeed models (termed the Lattice Boltzmann Hierarchy) systematically corrects the inherent errors of the standard, low-order accurate Lattice Boltzmann models (incomplete Galilean invariance, isotropy etc.). These models are thermodynamically consistent (all the models are supported by pertinent entropy functions) and result in numerically stable and computationally efficient algorithms.

We have developed new three-dimensional Entropic Lattice Boltzmann model for hydrodynamic simulation (S.S. Chikatamarla, S. Ansumali, I.V. Karlin, **Entropic lattice Boltzmann models for hydrodynamics in three dimensions**, Physical Review Letters, **97**, 010201 (2006)). A well optimized parallel code has been developed and tested on several cluster architectures. The new multi-speed Lattice Boltzmann models were implemented and tested in a number of benchmark flows. In Fig. 1, a test of a fully resolved three-dimensional simulation of the Kida-vortex flow with the new code is presented.

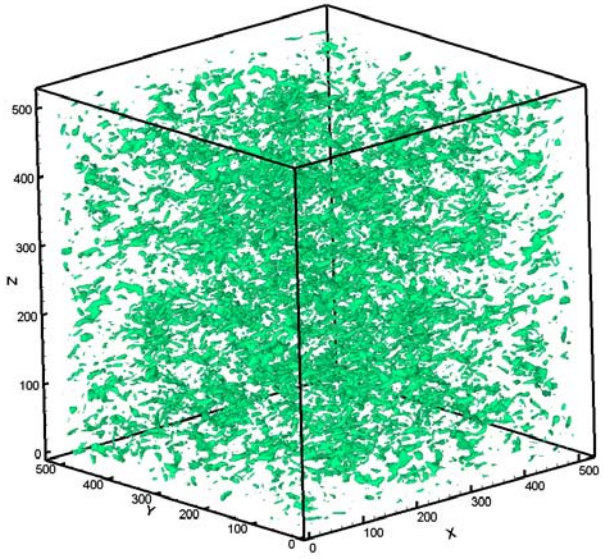

Fig.1: Entropic Lattice Boltzmann simulation of the three-dimensional Kida-vortex flow at Re=20000. Iso-vorticity surfaces at the peak of enstrophy are presented on a 512x512x512 grid.

4.2: Thermal Lattice Boltzmann model at variable Prandtl number. In the beginning of this project, we have introduced a novel Lattice Boltzmann model with energy conservation (S. Ansumali, I.V. Karlin, **Consistent lattice Boltzmann method**, Physical Review Letters, **95**, 260605 (2005)). This model overcomes some inherent limitations of the standard isothermal Lattice Boltzmann equation (in particular, the presence of spurious bulk viscosity). In the sequel, the consistent Lattice Boltzmann model was substantially modified, and a novel algorithm for thermal flow simulation has been established (N.I. Prasianakis, I.V. Karlin, **Lattice Boltzmann method for thermal flow simulation on standard lattices**, Phys. Rev. E **76**, 016702 (2007)). The novel thermal Lattice Boltzmann model can simulate flows with tailored Prandtl number and large temperature and density variations, which are pertinent to combustion problems. In Fig. 2, a shock tube benchmark simulation with the new thermal Lattice Boltzmann model is presented. In Fig. 3, a three-dimensional simulation of the fluid enclosed between two walls at different temperatures and subject to gravitational force is presented (Rayleigh-Benard convection problem).

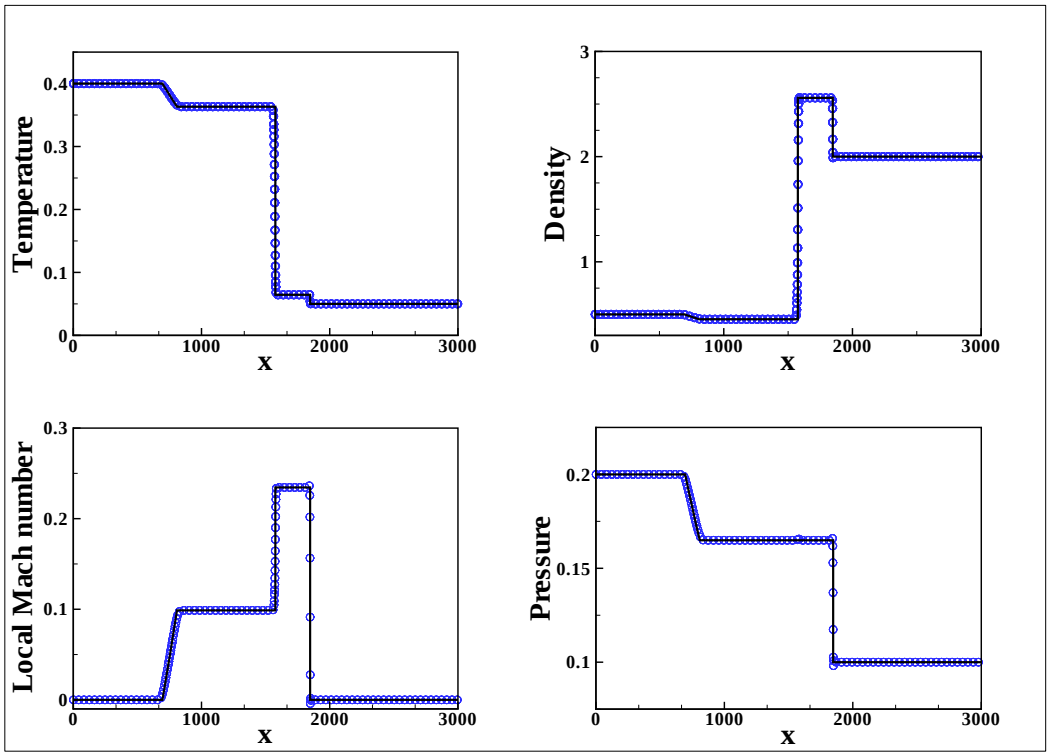

Fig. 2: Shock tube simulation using the thermal Lattice Boltzmann model; a comparison with the analytical solution for density, temperature, pressure and local Mach number of the flow. Solid line represents the analytical solution, while the symbol represents the forced thermal D2Q9 model (t=900 time steps).

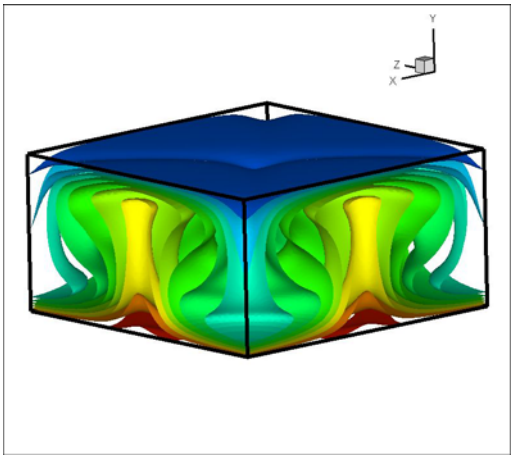

Fig. 3: Contours of the temperature field at Rayleigh number Ra=50000 in the Rayleigh-Benard convective flow using three-dimensional thermal Lattice Boltzmann method.

4.3: Lattice Boltzmann models for microflow simulations. The special focus in the development of the Lattice Boltzmann models is application to gas flows under moderate rarefaction i.e., in the regime where the continuum fluid dynamics is no more applicable. We have demonstrated that the higher-order Lattice Boltzmann models developed within this project are capable of describing microflow physics in a computationally efficient way. In particular, we have found analytical solutions to the standard and novel multi-speed Lattice Boltzmann equations in some standard flows (S. Ansumali, I. V. Karlin, S. Arcidiacono, A. Abbas, N. I. Prasianakis, **Hydrodynamics beyond Navier-Stokes: Exact**

Solution to the Lattice Boltzmann Hierarchy, Physical Review Letters **98**, 124502 (2007)). Such solutions are indispensable for accessing the physics of the new models in a way which is free of numerical errors. In Fig. 4, the mass flow rate in the two-dimensional micro-Poiseuille flow for the lowest-order Lattice Boltzmann model with only nine particle velocities is compared with the classical slip-flow theory based on the solution to the Boltzmann equation (infinite number of particles' velocities). Thus, the lowest-order (standard) Lattice Boltzmann models are quantified as physically relevant slip-velocity models. The higher-order multi-speed Lattice Boltzmann models significantly improve the standard ones. In Fig. 5, the slip velocity at the walls and the slope of the velocity profile at the centerline in a micro-Coquette flow for two models (with nine and sixteen velocities [19], respectively) are compared to the Direct Simulation Monte Carlo (DSMC) method and the Boltzmann kinetic equation. The quality of comparison dramatically improves with increasing number of speeds.

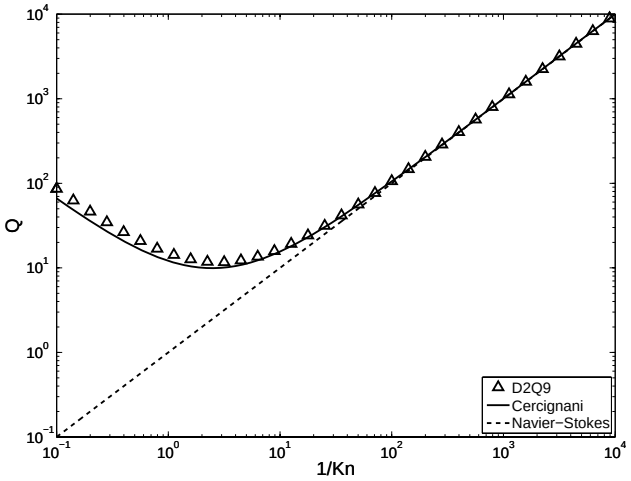

Fig. 4: Flow rate as the function of rarefaction in the Poiseuille flow (Knudsen minimum problem). Symbol: Exact solution to the standard Lattice Boltzmann model; Line: Slip theory from the Boltzmann kinetic equation; Dash: Navier-Stokes equation with no-slip boundary conditions; from Ref. 30.

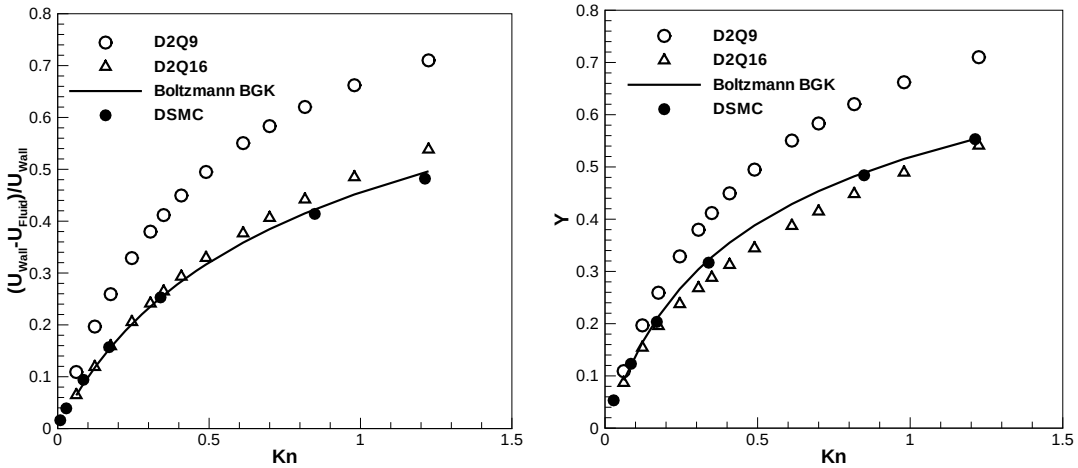

Fig. 5: Left: Slip velocity at the wall as a function of Knudsen number. Right: Slope of the velocity profile at the centerline; from Ref. 19.

4.4: Multicomponent reactive mixture Lattice Boltzmann models. The previously developed Lattice Boltzmann model for binary mixtures (S. Arcidiacono, J. Mantzaras, S. Ansumali, I.V. Karlin, C. Frouzakis, K. Boulouchos, **Simulation of binary mixtures with the lattice Boltzmann method,** Physical Review E, **74(5)** 056707 (2006)) has been extended to simulate multi-component mixtures S. Arcidiacono, I. V. Karlin, J. Mantzaras, C. E. Frouzakis, **Lattice Boltzmann model for the simulation of multicomponent mixtures**, Phys. Rev. E **76**, 016702 (2007)). The multi-component Lattice Boltzmann model recovers the Navier-Stokes equations and the Stefan-Maxwell multi-component diffusion in the continuum limit. These can also be used in the micro-flow simulation of mixtures in the

slip-flow regime. In Fig. 6, the slip coefficient in the micro-Coquette flow at Knudsen number Kn=0.2 is presented as a function of the light gas component fraction.

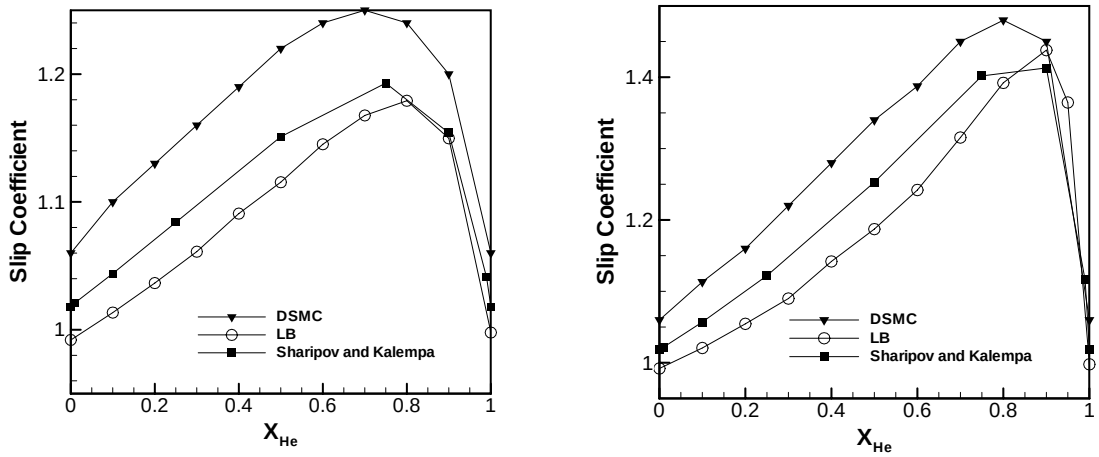

Fig. 6: Slip coefficient versus Helium molar fraction He in a micro-Couette flow of a binary mixture. Left: Helium-Argon mixture. Right: Helium-Xenon mixture. Squares: Kinetic theory results; Triangles: DSMC results; Circles: Lattice Boltzmann simulation, from Ref. 23.

The above results enabled extension of the mixture models to include surface-based chemical reactions. In Fig. 7, simulation of the surface-based one-step Methane oxidation reaction in a channel flow is presented.

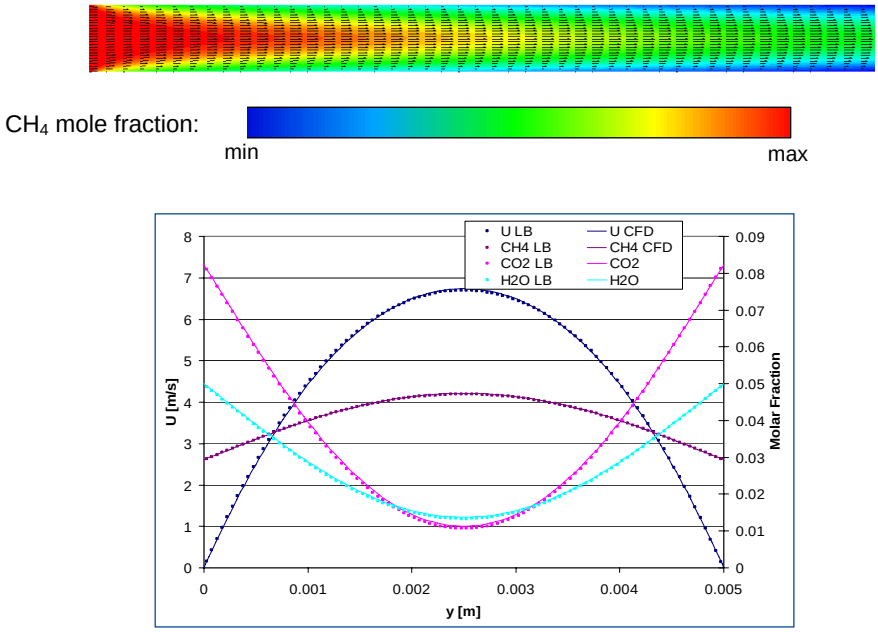

Fig. 7: Lattice Boltzmann simulation of a one-step Methane oxidation reaction in a channel. Simulation corresponds to 90/10 Oxygen/Methane mixture at the left inlet, at velocity 4 m/sec. Top: Methane concentration profile. Bottom: Comparison of species concentrations and of the velocity profile at a fixed axial position. Symbol: Lattice Boltzmann simulation; Lines: CFD solver (S. Arcidiacono, J. Mantzaras, I.V. Karlin, preprint in preparation).

4.5: Model reduction methods for complex reactions. We have developed and implemented a method to reduce the number of species in simulations of complex reactions. A grid-based realization

seeks a slow manifold (surface) in the reaction space, to which all reaction trajectories are attracted. This drastically reduces computational effort when reaction systems are integrated in time. In Fig. 7, a slow two-dimensional surface in the composition space is shown for Hydrogen combustion. In Fig. 8, time evolution of species and of the temperature of the reduced system is compared to the detailed mechanism.

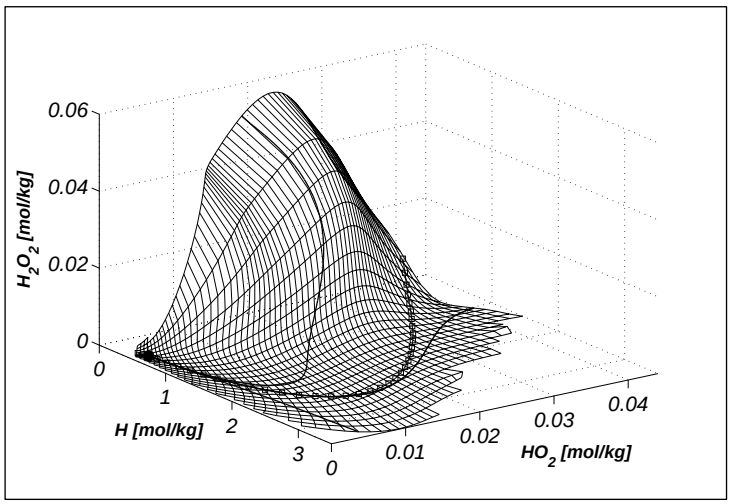

Fig. 7.The 2d invariant grid (thin lines) in Hydrogen combustion. The 1d invariant grid (squares) and solution trajectories (bold lines) are also reported.

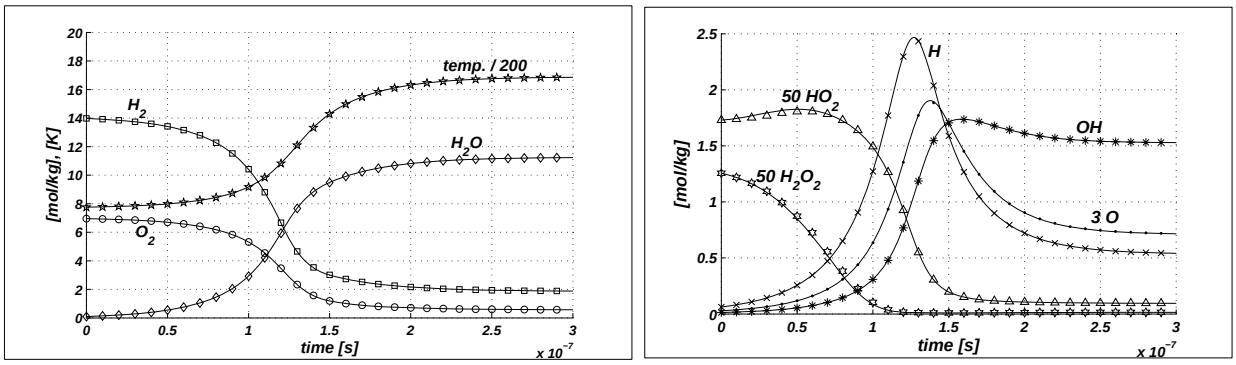

Fig. 8. Reduced model (symbols) versus detailed model (lines). Time evolution of the species concentrations and of the temperature in the Hydrogen combustion model.

5. Diskussion

In the course of this project, the framework of the Lattice Boltzmann approach to modelling of complex flows has been significantly extended in three directions: simulation of turbulent flows, simulation of thermal flows with high temperature and density variations, and multi-component mixtures, including surface-based chemical reactions. These newly developed models and state-of-the-art computational realizations enable simulation of systems with multiple scales. Some applications of this approach are currently explored within the framework of the CCEM-CH project “CEMTEC” focused on multiphase reactive flows in solid oxide fuel cells, micro-reformers and microturbines.

6. Schlussfolgerungen

Basic results obtained are:

1. A new, complete and systematic array of Lattice Boltzmann models have been constructed, implemented and tested. All admissible lattices for numerically stable implementation are described.

2. Multi-speed Lattice Boltzmann models are shown to be computationally efficient. In turbulent flow simulations, they represent a promising alternative both to direct numerical simulation and standard Lattice Boltzmann models.

3. It is demonstrated that new multi-speed Lattice Boltzmann models provide a new perspective on simulations of rarefied gas flow beyond the continuum regime.

4. Thermodynamically consistent Lattice Boltzmann models for realistic multi-component mixtures, including surface-based chemical reactions are developed.

5. Lattice Boltzmann models for compressible flows with large temperature and density variations are developed.

6. Model reduction techniques are efficiently implemented via Method of Invariant Grids which enables significant simplification of complex reaction mechanisms in combustion.

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