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Projekt Nr. 100862

Lattice Boltzmann Simulationsmethoden für chemisch reaktive Systeme im Microbereich

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ZUSAMMENFASSUNG

Eine neue Annäherung fuer die rechnenunterstuetzte Stroemungsdynamik an einer Mikrometerskala wird hergeleitet. Diese Annäherung basiert auf die Entwicklung sogenannten Boltzmann Gitter-Modellen (Lattice Boltzmann Method) der Boltzmann kinetischen Gleichung. Sowohl die thermischen, als auch die isothermischen Modellen wedren dargestellt. Die Fortsetzung der Arbeit in dieser Richtung im Jahr 2005 hat die folgenden Ergebnisse gebracht:

1. Das Modell für mehr-phasige Strömungen wurde entwickelt, und für die zwei-komponenten Mischungen von Gasen implementiert und getestet.
2. Ein rechnerisch effizientes drei-dimensionales Modell für isotherme Strömungen wurde entwickelt und an mehreren „benchmark"-Problemen getestet. Dieses Modell zeigt numerische Stabilität und ist deshalb sehr wichtig bei hohen Reynoldsche Zahl Simulationen. Durch die speziellen Modifikationen (zum Beispiel, Rand Bedingungen) ist es gelungen, effiziente Simulationen in Angriff zu nehmen (siehe Publikationsliste).
3. Ein drei-dimenzionales thermishes Modell wurde entwickelt und realisiert in einigen benchmark Strömungen.

Theoretischen Fragen sind dabei vollständig geklärt, wie der Herleitung von Lattice Boltzmann Methode aus den molekularen Theorien (Boltzmann kinetischen Gleichung), so wie die praktischen Fragen der effektiven Anwendung. Das mikroskopisch abgeleitetes thermisches Modell verbessert im Wesentlichen die frühere Ergebnisse der isothermalen Modelle. Diese Modellen ersetzen kostspielige mikroskopische Simulationtechniken wie kinetisches Monte-Carlo und/oder molekulare Dynamik für niedrige Mach-Zahl und moderate Knudsen-Zahl zu ersetzen. Die Ergebnisse wurden in zwölf Publikationen und Preprints dargestellt.
Es eröffnen sich die 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.

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Projektziele

The ultimate goal of this project is 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 weakly compressible flows at a micrometer scale. Such flows are typical in many current problems of aero-thermo-chemistry at a micron scale, and are further complicated by chemical reactions, both in the flow bulk and on the surface (heterogeneous catalytic reactions). Rarefaction is characterized by Knudsen number Kn, ratio of the mean free path of molecules to a characteristic variation of hydrodynamic fields (density, momentum, temperature). Moderate values of Kn (0.01-0.1) are most important for applications and at the same time too difficult for both continuous hydrodynamic models and the purely molecular-dynamics approaches. Within this project, we aim at developing the so-called *Entropic Lattice Boltzmann Models* which are capable to replace both the heuristic continuous mechanic models and computationally intensive molecular models.

The goals of this year studies were the following:

1. To give a consistent microscopic derivation of the lattice Boltzmann method and establish a model for simulation of thermal cases in the micro-flow domain.
2. To massively increase the efficiency of three-dimensional simulations.
3. To develop and test the performance of the lattice Boltzmann models for mixtures.

Durchgeführte Arbeiten und erreichte Ergebnisse

Thermal Entropic Lattice Boltzmann model for micro-flows. A link between the Lattice Boltzmann models and the kinetic theory was established (Ref. 1, 2, 3). For the first time, Lattice Boltzmann models were derived consistently from the Boltzmann kinetic equation in Ref. 2. These models enable efficient non-isothermal simulations of the micro-flow systems (Fig. 1).

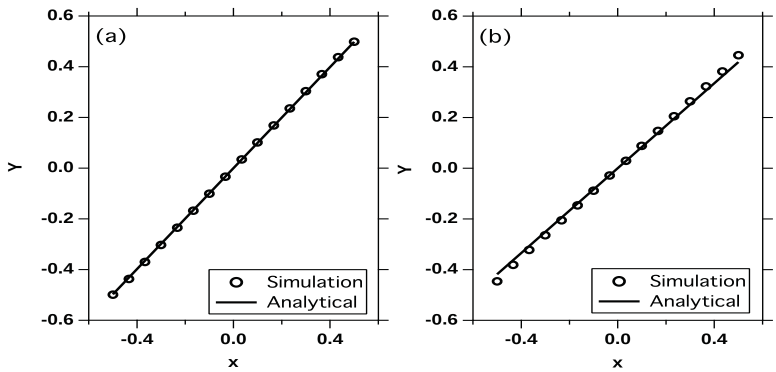

Fig.1. **Steady-state temperature variation between parallel walls**; Reduced temperature Y is shown as the function of the reduced distance at two different degrees of rarefaction Kn (Knudsen number): (a) Kn=0.001 and (b) Kn=0.05. Symbols: Lattice Boltzmann simulation; Line: Analytical solution of Boltzmann equation (From Ref. 2).

Efficient Lattice Boltzmann models for three-dimensional simulation. Nonlinearly stable Entropic Lattice Boltzmann for small velocity sets was derived for three-dimensional simulations (Ref. 11). Several important issues for practical applications were resolved, such as the in- and outlet

the stability condition (Ref. 8, 9), and fast
ws were studied (Fig. 2).

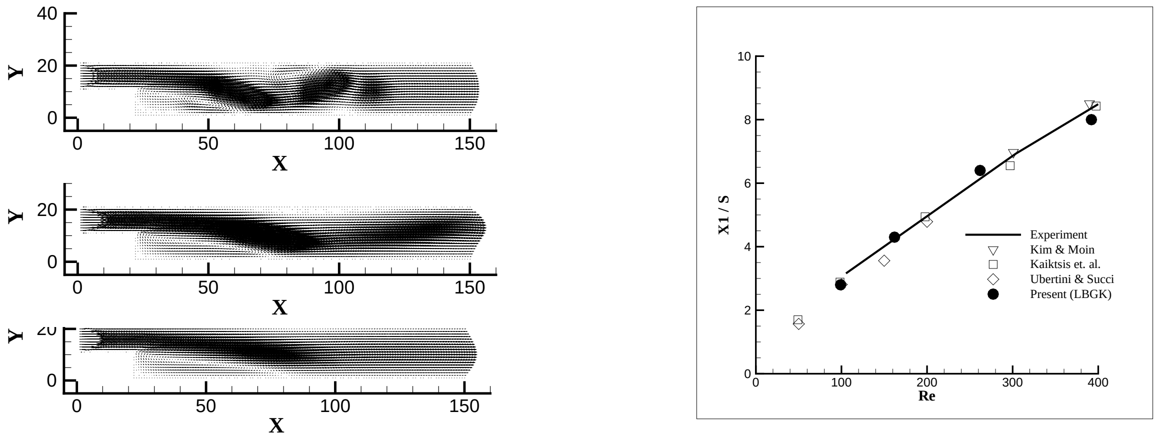

Fig. 2. **Three-Dimensional Entropic Lattice Boltzmann simulation of backward facing step flow**. Left: Snapshots of the velocity field on the mid-plane at Re=270 at $9\text{x}10^3$, $18\text{x}10^3$, and $40\text{x}10^3$ time steps in lattice units (from top to bottom). **Right:** Primary reattachment length X_1 normalized by the step height S. Comparison of the present simulation with the experiment and reference simulation data (From Ref. 4).

Entropic Lattice Boltzmann models for mixtures. A new class of Lattice Boltzmann models was constructed for simulation of complex fluids (Ref. 12). Specific cases included a thermodynamically consistent model for simulation of fluids with a variable Prandtl number (Ref. 12), and a model for mixtures of fluids (Ref. 6, 12). The mixture model demonstrated possibility to simulate fluids with large mass disparity (Fig.3).

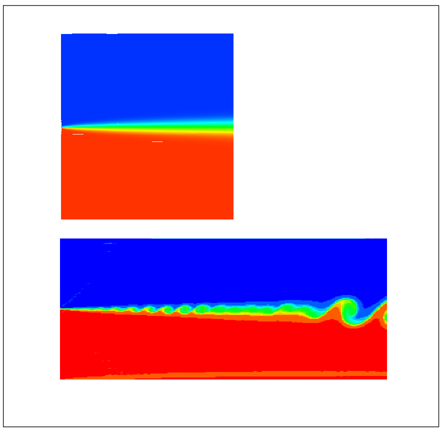

Fig.3. Development of a laminar and of a turbulent diffusive mixing layer computation with the Entropic Lattice Boltzmann model for mixtures (Ref. 6). Red: fast fluid; Blue: slow fluid.

Nationale Zusammenarbeit

Collaboration was continued with Dr. **I. Mantzaras** and Dr. **S. Arcidiacono** (PSI) on the mixture model. Collaboration was initiated with Dr. **A. Gusev** and Dr. **A. Bardow** (ETH) on a finite-elements formulation of the Lattice Boltzmann Method. Collaboration was continued with Prof. **M. Deville** (EPFL) on establishing a network of groups working on Lattice Boltzmann Methods.

Internationale Zusammenarbeit

International collaboration on the Entropic Lattice Boltzmann Method was continued with the groups of Prof. **G. Vahala** (William & Mary) and Prof. **J. Yepez** (Air Force Research Laboratory, Hanscom Field). Three-dimensional Entropic Lattice Boltzmann model was run on massively parallel supercomputers such as *Earth Simulator* (Yokohama) for classical turbulent flows. Results strongly favour the Entropic Lattice Boltzmann Method in terms of stability in large Reynolds number simulations. Further perspective is focused on reduction of computational effort.

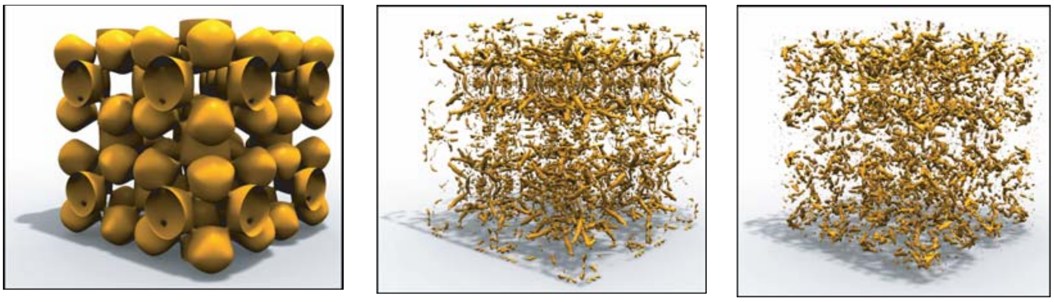

FIG. 5: Turbulent flow visualization at t = 0, 1200, 3600 ray tracing of the vorticity isosurface in a 512^3 grid. Simulations of the three-dimensional Entropic Lattice Boltzmann Model were carried out on the DoD supercomputer Kraken (IBM-P4) at NAVO Major Shared Resource Centre. The flow is initialized with the Kida profile. **Figure courtesy of G. Vahala**

Collaboration with the group of Prof. **S. Succi** (Institute of Applied Computations, CNR, Rom) was continued on the subject of increasing efficiency of Entropic Lattice Boltzmann schemes (Ref. 10). Collaboration with Prof**. A. Gorban** (University of Leicester, UK) on model reduction and kinetic theory was continued (Ref. 7). Prof. **S. Ansumali** (Nanjang University of Technology, Singapore) contributed to model developments.

Bewertung 2005 und Ausblick 2006

The most important progress of this year is the three results described above: Derivation of the Entropic Lattice Boltzmann from microscopic theory which made possible to develop a **thermal model** for micro-flows in a natural way; Development of new **three-dimensional Entropic Lattice Boltzmann models** with enhanced numerical performance; Development of the Entropic Lattice Boltzmann model for **mixtures**. This progress is crucial for the problems we will address in the next year: Inclusion of chemical reactions and effective implementation of a complex geometry.

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