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Lattice Boltzmann Simulationsmethoden fuer chemisch reaktive Systeme im Microbereich

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ZUSAMMENFASSUNG

Eine neue Annäherung für die rechenunterstützte Strömungsdynamik in einer Mikrometerskala wird hergeleitet. Diese Annäherung basiert auf den vor kurzem entwickelten so genannten minimalen entropisch-kinetischen Modellen der Boltzmann-kinetischen Gleichung. Die thermischen, sowie die isothermischen Modelle werden dargestellt, und das einfachste Entropisch-Bhatnagar-Gross-Krook Isothermalgitter (ELBGK) wird ausführlich analysiert, um seine Bedeutung für die Microflow-Simulation quantitativ zu bestimmen. ELBM wird mit Randbedingungen ergänzt, die von einem molekularen Modell abgeleitet wurden (diffusive Wandnäherungswerte). Eine Abbildung der dreidimensionalen kinetischen Gleichungen auf zweidimensionale Modelle, die zweidimensionalen Simulationen von quasi-zweidimensionalen Strömungen ermöglicht, wird hergestellt. Zwei detaillierte Studien von Microflows in konkreten Geometrien wurden durchgeführt. In der ersten dieser Studien, wird das ELBGK Modell weitgehend an Hand der Simulation des zweidimensionalen Poiseuille-Stroms untersucht. Das ELBGK stimmt quantitativ mit den analytischen Resultaten im Gebiet der schwachen Verdünnung (gekennzeichnet durch die Knudsen Zahl (Kn): das Verhältnis der mittleren freien Weglänge zur hydrodynamischen Skala), bis zu Kn=0.01 überein. Dieses ist das wichtigste Gebiet für Microflow-Simulation. Ausserdem stimmt das Resultat qualitativ über den gesamten Kn-Bereich, für kleine Kn stimmen die Resultate für das Minimum der Mengenflussrate und für grosse Kn die logarithmische Skalierung. Die gezeigten Resultate spielen auf die Möglichkeit an, dass ELBM ergänzen zu können, oder sogar kostspielige mikroskopische Simulations-Techniken wie kinetisches Monte-Carlo und/oder molekulare Dynamik für niedrige Mach- und Knudsen Zahlen zu ersetzen. Zur weiteren Entwicklung in Rahmen dieses Projektes gehört die numerische Implementierung des thermischen Modells. Bereits haben wir ein thermisches Modell (das so genannte Thermal D2Q9 Modell) entwickelt und erfolgreich getestet. Die zweite Studie befasste sich mit der Strömung in einer Mikro-Kavität. Eine detaillierte, parametrische Untersuchung von qualitativen so wie quantitativen Eigenschaften der Strömung wurde für einen umfassenden Bereich von Verdünnung durchgeführt. Zudem wurde die Stabilität dieser Strömung untersucht.

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Projektziele

The ultimate goal of this project is to develop efficient models and computational algorithms for complicated physical and chemical processes in fluid flows far from equilibrium. While such processes constitute a great challenge for both fundamental and applied sciences, our specific focus is on non-isothermal weakly compressible flows at a micrometer scale. Such flows are typical in many current problems of aerothermochemistry, and are further complicated by chemical reactions, both in the flow bulk and on the surface (homogeneous and heterogeneous catalytic reactions). Furthermore, one often deals with multi-phase flows such as liquid-vapor coexistence, and flows with solid particles. 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 (0.1-1) 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 mesoscopic *lattice Boltzmann models* which will replace both the heuristic continuous mechanic models and computationally intensive molecular models.

The goals of this year studies were the following:

1. To develop the basic computational models (lattice Boltzmann models) for microflow simulation, both isothermal and (especially) thermal cases.
2. To establish the relations between the lattice Boltzmann models and fully microscopic atomistic approaches and nonequilibrium thermodynamics.
3. To test the performance of the lattice Boltzmann models in at least two representative benchmark problems in order to access their accuracy with respect to molecular dynamics.

Durchgeführte Arbeiten und erreichte Ergebnisse

Our work on the development of the lattice Boltzmann models for microflows is based on our previous experience in developing such models for incompressible hydrodynamic simulations, such as the one used in Ref [1] for a simulation of turbulence past a square cylinder. For the microflows, we have developed more advanced lattice Boltzmann models which include energy conservation and/or use more discrete velocities. This enormously extended the domain of validity of the lattice Boltzmann method which becomes competitive in terms of accuracy to molecular dynamics. In a benchmark problem of a microflow in a pressure driven Poiseuille flow, for example, a molecular dynamics approach takes several months to compute the mass flow rate through the channel. In Fig. 1, the performance of the isothermal and the newly developed thermal lattice Boltzmann method are presented. It is clear that both models are able to predict quantitatively the flow rate in a wide range of Knudsen number while the computation time reduces dramatically (hours instead of months).

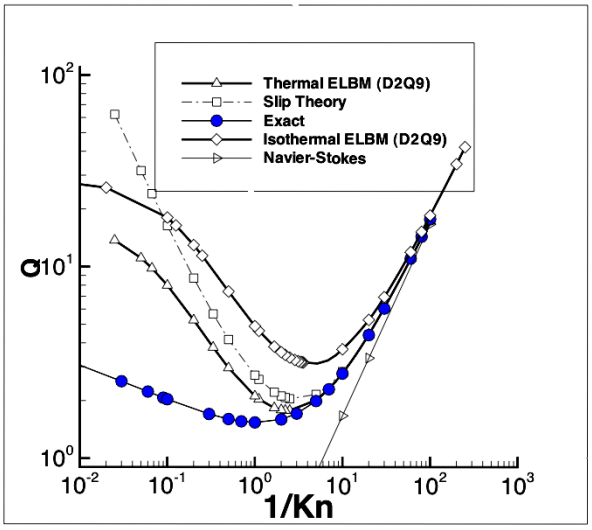

Fig. 1 Mass flow rate through a micro-channel Q versus rarefaction 1/Kn. Continuous (hydrodynamic) limit corresponds to 1/Kn>1000, while the free-molecular flow corresponds to 1/Kn<0.01. Performance of the two lattice Boltzmann models (lines “Isothermal ELBM” and “Thermal ELBM”) is compared with the molecular dynamics (line “Exact”), as well as with continuous theory (line “Navier-Stokes”) and the asymptotic solution of the kinetic theory (line “Slip theory”). Quantitative comparison of the lattice Boltzmann model to the exact result is visible in the micrometer range (Kn<1). The Figure is taken from Ref. [2].

Relations between the lattice Boltzmann models and the rigorous nonequilibrium thermodynamics are fully clarified. This work is summarized in the monograph [3] and the papers [4,5]. The establishing of the lattice Boltzmann method as a simple and robust simulation method for microflows enabled for the first time to perform a parametric study of the interplay between gas rarefaction and boundary conditions in a realistically complex flow in a lid driven microcavity. This work is summarised in Ref. [6]. A comparison of Direct Simulation Monte Carlo (DSMC) with the lattice Boltzmann method is shown in Fig. 2.

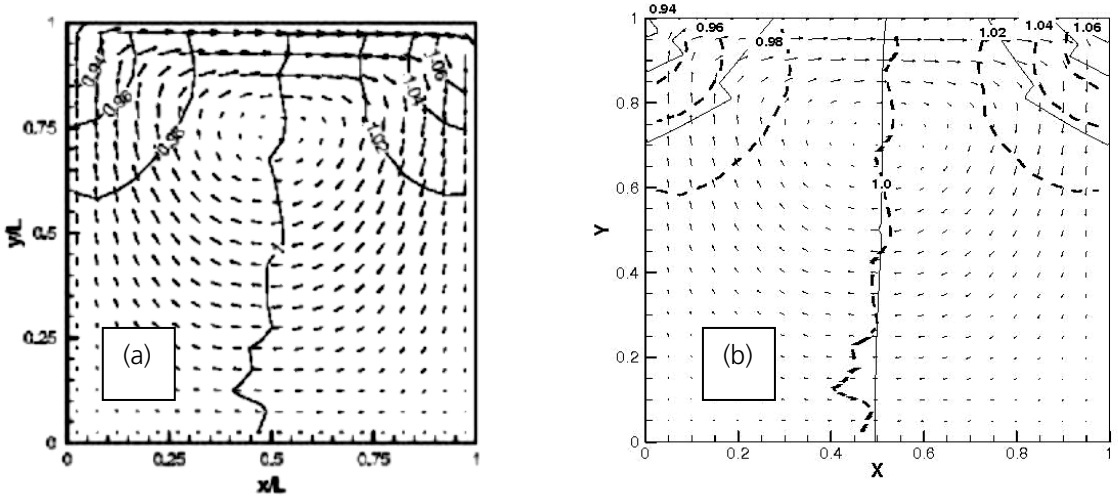

Fig. 2 Flow in a micro-cavity for Kn=0.1 and Ma=0.14: (a) DSMC simulation (from J.-Z. Jiang, J. Fang, and C. Shen, p. 784-790, 23rd Int. Symposium on Rarefied Gas Dynamics, 2003), (b) velocity vector plot and density isolines from ELBM (solid lines) with the DSMC density isolines (dashed lines) superimposed. Figure from Ref. [6].

Finally, in Ref [7], we established an effective way to reduce the dimension of the problem for chemical kinetics. This work will be crucial at further stages of the project when the chemical reactions will be coupled to the flow. An example of the invariant two-dimensional manifold for a model hydrogen burning reaction is given in Fig. 3.

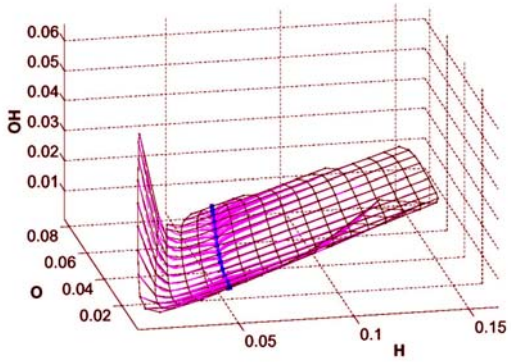

Fig.3 Two-dimensional invariant manifold (surface) in the concentrations space for a model hydrogen burning reaction. All solutions of the reaction kinetics system are rapidly attracted to this surface, and after that proceed to the equilibrium along it. The one-dimensional backbone curve (blue) is the slowest one-dimensional invariant manifold within the two-dimensional. Red curves are individual solutions of the reaction system. Figure from Ref. [7].

Nationale Zusammenarbeit

We are establishing working collaboration with the group of Dr. I. Mantzaras (PSI) on a coupling of the lattice Boltzmann method with molecular dynamics for surface reactions in microchannels.

Internationale Zusammenarbeit

International collaboration on various parts of the project are going on with Prof. Y. Kevrekidis (Princeton) (micro-cavity flow), Prof. A. Gorban (Leicester) (relations between lattice Boltzmann models and nonequilibrium thermodynamics), Dr. A. Zinovyev (IHES, Bures-sur-Yvette) (model reduction for chemical kinetics).

Bewertung 2004 und Ausblick 2005

The success of this year is, in the first line, the establishment of new lattice Boltzmann models which enable efficient simulations of microflows. Two representative benchmark simulations (Poiseuille flow and micro-cavity flow) confirmed good performance and viability of the thermal and isothermal models. In addition, relations with the nonequilibrium thermodynamics established the place of these models among other approaches, and the methods of model reduction of chemical kinetics indicate viability of the extension to chemically reactive flows.

The lines of research for the year 2005 are summarised as follows:

1. A furher increase in performance of our models requires to develop lattice-free implementations. This is needed, in particular, to simulate microflows in channels and porous media

with realistic aspect ratios (which are typically quite high). Preliminary results on lattice-free implementations are currently available.

2. To develop and implement the extension to multiple-relaxation time models. This will enable more accurate matching of transport coefficients, and is the crucial step towards implementation of models for mixtures.

Referenzen

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[4] A.N. Gorban, I.V. Karlin, A.Yu. Zinovyev, ***Constructive methods of invariant manifolds for kinetic problems***, Physics Reports **396,** pp.197-403 (2004).

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