Simulations of micro channel gas flows with domain decomposition technique for kinetic and fluid dynamics equations

Sudarshan Tiwari[1], Axel Klar[1] and Steffen Hardt[2]

Key words: Domain decomposition, Particle methods, Boltzmann equation, Navier-Stokes equations

1 Introduction

In the last 20 years many research papers have been reported about the development of domain decompositions for the kinetic and the fluid dynamic equations, see for example [7, 8, 10, 14, 11, 12, 15, 16]. From large to small scale geometries one may experience different degrees of rarefaction of a gas. The degrees of rarefaction of a gas can be measured by the Knudsen number $Kn = \lambda/L$, where λ is the mean free path and L is the characteristic length, for example the channel width. For $Kn < 0.001$, the flow is in the continuum regime, the compressible Navier-Stokes equations with no-slip boundary conditions are solved. For $0.001 < Kn < 0.1$, the flow is in the slip regime, where the Navier-Stokes equations with velocity-slip and temperature jump conditions are solved [1]. For $Kn > 0.1$ a kinetic type approach, based on the Boltzmann equation is required. We note that the kinetic approach is valid in the whole range of rarefaction of a gas. At standard conditions the mean free path of a gas in a micro- or nano channel is of the order L or larger, so the Knudsen number is no longer small. Therefore, the fluid dynamic equations, the compressible Euler or Navier-Stokes equations, cannot predict the flows correctly in a small scale geometry [9].

In this paper we present stationary solutions of a Poiseuille flow in a micro channel. We have considered the large range of Knudsen numbers. We use the domain decomposition of the Boltzmann and the compressible Navier-Stokes equations. We have coupled a meshfree particle method for the compressible Navier-Stokes equations and a DSMC type of particle method for the Boltzmann equation. We have first observed the discrepancy in the Boltzmann and Navier-Stokes solutions. Then we have defined boundary layers and solved the Boltzmann equations in the boundary layers and the Navier-Stokes equations in the rest of the channel. We have used the standard interface boundary conditions between both domains, see [16, 15]. Alternatively, we have solved the Navier-Stokes equations until steady state has been

Department of Mathematics, TU Kaiserslautern, Erwin-Schroendinger Strasse, 67663 Kaiserslautern, Germany tiwari@mathematik.uni-kl.de, klar@mathematik.uni-kl.de · Center of Smart Interfaces, TU Darmstadt, Petersenstr. 32, 64287 Darmstadt, Germany hardt@csi.tu-darmstadt.de

reached. It gives quite diffusive solutions, however, this is the good candidate to initialize the Boltzmann solver. One can apply a breakdown criterion to the stationary Navier-Stokes equations and then decompose the Boltzmann and Navier-Stokes domains.

The paper is organized as follows. In section 2 we present the mathematical models and numerical methods. In section 3 we discuss the numerical solutions and the domain decompositions.

2 Governing equations and numerical methods

In this section we introduce the Boltzmann equation, the Navier-Stokes equations as its hydrodynamic limit, numerical methods and domain decomposition strategies.

2.1 The Boltzmann equation and its hydrodynamic limits

The Boltzmann equation describes the time evolution of a distribution function $f(t,x,v)$ for particles of velocity $v \in \Re^3$ at $x \in D \subset \Re^s (s = 1,2,3)$ and time $t \in \Re_+$. It is given by

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = Q(f,f), \tag{1}$$

where

$$Q(f,f) = \int_{\Re^3} \int_{S^2} \beta(|v-w|,\eta)[f(v')f(w') - f(v)f(w)]d\omega(\eta)dw$$

with

$$v' = T_{v,w}(\eta) = v - \eta < \eta, v-w >,\ w' = T_{w,v}(\eta).$$

Here, β denotes the collision cross section, η is the unit normal vector on the sphere, $d\omega(\eta)$ is the solid-angle element in the direction of η and $<,>$ is the scalar product. For the sake of simplicity, we have not used any bold letters for vector quantities, like x, v, w, etc. Writing the equations in dimensionless form one observes that Q is of the order $\mathcal{O}(\frac{1}{Kn})$. The local mean free path $\lambda = \lambda(x,t)$ is given by

$$\lambda = \frac{kT}{\sqrt{2}\pi p d^2}, \tag{2}$$

where k is the Boltzmann constant, $T = T(x,t)$ the temperature, $p = p(x,t)$ the pressure and d is the diameter of molecules. For more details we refer to [6]. For Kn tending to zero one can show that the Boltzmann distribution function f tends to the local Maxwellian [5]

$$f_M(t,x,v) = \frac{\rho}{(2\pi RT)^{3/2}}\, e^{-\frac{|v-U|^2}{2RT}}, \tag{3}$$

where $\rho = \rho(x,t)$ is the density, $U = U(x,t)$ the mean velocity and R is the gas constant. The parameters of the Maxwellian ρ, U, T solve the compressible Euler equations. This can be verified from the asymptotic expansion of f in Kn, where the zeroth order approximation gives the local Maxwellian distribution and the first order approximation [3] gives the Chapman-Enskog distribution

$$f_{CE}(t,x,v) = f_M(t,x,v)\,[1+\phi(t,x,v)], \tag{4}$$

with

$$\phi(t,x,v) = \frac{2}{5}\frac{q\cdot c}{\rho(RT)^2}\left(\frac{|c|^2}{2RT} - \frac{5}{2}\right) - \frac{1}{2}\frac{\tau : c\otimes c}{\rho(RT)^2}, \tag{5}$$

where $c = v - U$. Here, $\phi = \mathscr{O}(Kn)$ and the parameters ρ, U, T, q, τ satisfy the compressible Navier-Stokes equations

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla\cdot(\rho U) &= 0 \\ \frac{\partial(\rho U)}{\partial t} + \nabla\cdot(\rho U\otimes U + pI - \tau) &= 0 \\ \frac{\partial(\rho E)}{\partial t} + \nabla\cdot[(\rho E + p)U - \tau\cdot U - q] &= 0, \end{aligned} \tag{6}$$

where $E = |U|^2/2 + e$ is the total energy and e is the internal energy. The stress tensor τ and heat flux vector q are of order Kn and given by

$$\tau_{ij} = \mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\nabla\cdot U\ \delta_{ij}\right), \qquad q = -\kappa\nabla T. \tag{7}$$

The dynamic viscosity $\mu = \mu(x,t)$ and the heat conductivity $\kappa = \kappa(x,t)$ for a monatomic gas of hard sphere molecules are of order Kn. They are given, see [4], by

$$\mu = \frac{5}{16d^2}\sqrt{\frac{mkT}{\pi}}, \qquad \kappa = \frac{15k}{4m}\mu, \tag{8}$$

where m is the molecular mass. In this paper we have considered a monatomic gas of hard spheres.

2.2 Numerical methods

We apply Lagrangian particle methods of different characters for both types of equations. The Boltzmann equation is solved by a DSMC type Monte Carlo method,

whereas the Navier-Stokes equations are treated with a meshfree particle method, which is called the Finite Pointset Method (FPM).

2.2.1 Particle Method for the Boltzmann equation

For solving the Boltzmann equation we have used a variant of the DSMC method [4], developed in [13, 2]. The method is based on the time splitting of the Boltzmann equation. Introducing fractional steps one solves first the free transport equation (the collisionless Boltzmann equation) for one time step. During the free flow, boundary and interface conditions are taken into account. In a second step (the collision step) the spatially homogeneous Boltzmann equation without the transport term is solved. To simulate this equation by a particle method an explicit Euler step is performed. The result is then used in the next time step as the new initial condition for the free flow. To solve the homogeneous Boltzmann equation the key point is to find an efficient particle approximation of the product distribution functions in the Boltzmann collision operator given only an approximation of the distribution function itself. To guarantee positivity of the distribution function during the collision step a restriction of the time step proportional to the Knudsen number is needed. That means that the method becomes exceedingly expensive for small Knudsen numbers.

2.2.2 Meshfree particle method for the Navier-Stokes equations

We solve the Navier-Stokes equations by a meshfree Lagrangian particle method. We approximate the spatial derivatives at an arbitrary particle from its surrounding clouds of points with the help of the least squares method. We express the compressible Navier-Stokes equations in primitive variables according to the Lagrangian form. We first fill a computational domain by a finite number of particles and assign all fluid quantities to them. Then we approximate the spatial derivatives at every particle position. The resulting equations reduce to a time dependent system of ordinary differential equations. This system can be solved by a simple integration scheme. One can use the explicit Euler scheme, but this requires a very small time step. Here a two step Runge-Kutta method is used which is sufficient for the test cases considered in this paper. Due to space limitations, we do not present the meshfree method, we refer to our earlier reports, see [17, 16].

2.2.3 Coupling particle methods for the Boltzmann and the compressible Navier-Stokes equations

The DSMC method is a mesh-based method since gas molecules have to be sorted into cells for the intermolecular collisions. As already described, the compressible Navier-Stokes equations are solved by a meshfree method. Therefore, we need to couple the mesh-based and the meshfree particle methods. We decompose a domain

into Boltzmann and Navier-Stokes domains, then we have to prescribe the interface boundary conditions from one domain into another domain.

In order to apply the interface boundary conditions for the Boltzmann equation, we have to define the boundary cells (or interface cells) in the Navier-Stokes domain. On these buffer cells we generate gas molecules according to a Maxwellian distribution, where the parameters are approximated from the Navier-Stokes equations. If the gas molecules leave the Boltzmann domain and enter to Navier-Stokes one, we delete them.

The interface boundary conditions for the Navier-Stokes equations are applied as follows. In the Boltzmann domain we sample and store the macroscopic quantities at the cell centers. Near the interface there may be several Boltzmann cell centers, which are the neighbor of a Navier-Stokes particle. In this case we consider all neighboring Boltzmann cells and approximate the spatial derivatives from the least squares method. Instead of using the Dirichlet boundary condition at the Boltzmann interface cell, we find this approach is sufficient. When the Navier-Stokes particles leave the Navier-Stokes domain, we delete them. If they thinned out the domain, we add new particles and interpolate the data from its neighboring particle values.

It is well known that in all DSMC type solvers there are some statistical fluctuations in the solutions of the Boltzmann equation. These fluctuating data destabilize the Navier-Stokes solver. Therefore, we need a smoothing operator, see [16, 15] for details.

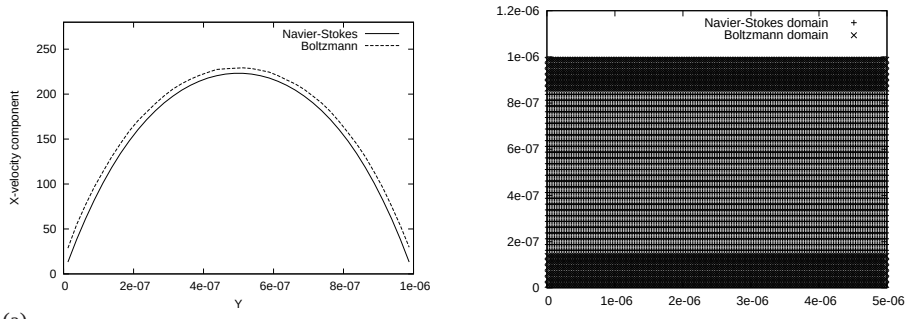
3 Numerical results

We consider a micro channel of size $[0,\ 5\cdot H]\times[0,\ H]$ with $H = 1\cdot 10^{-6}m$ as shown in Fig. 1(b). The left and right walls are inflow and outflow boundaries, respectively and the upper and lower are solid wall boundaries. While solving the Navier-Stokes equations, we prescribe a temperature T_{in} and a pressure p_{in} on the inflow boundary. Similarly, we prescribe a pressure p_{out} on the outflow boundary. We use the Neumann boundary conditions for the velocity and temperature, on the in- and outflow boundaries. Furthermore, zero velocity and $T = T_0$ are considered on the upper and lower boundaries, where T_0 is the initial temperature of the gas. We choose Argon as a gas with a molecular mass $m = 6.63\cdot 10^{-26}kg$. The Boltzmann constant $k = 1.38\cdot 10^{-23}JK^{-1}$, the molecular diameter $d = 3.68\cdot 10^{-10}m$, the ratio of specific heats $\gamma = 5/3$ enter as parameters. These parameters give the gas constant $R = 208JkgK^{-1}$. The dynamic viscosity and thermal conductivity in the compressible Navier-Stokes equations are assumed to be constant and are evaluated with the initial temperature according to eq. (8). The initial velocity is zero. The initial pressure is $(p_{in}+p_{out})/2$ and the initial density is determined from the ideal gas law.

When we solve the Boltzmann equation we initialize the gas according to the Maxwellian distribution in each cell with the initial parameters as described for the Navier-Stokes solver. We generate the molecules according to the Maxwellian distribution at the inflow boundary, where the density is determined from the given

pressure and the temperature using the ideal gas law. The mean velocity is extrapolated from the the interior of the Boltzmann cells. Similarly, we also generate the molecules according to the Maxwellian distribution at the outflow boundary, where we extrapolate the mean velocity and the temperature from the interior cell values and the pressure is given. If the molecules leave the inflow or outflow boundary we delete them. On the upper and lower walls we use the diffuse reflection with thermal accommodation. We choose 200×40 cells for the Boltzmann solver and the mesh-free particles for the Navier-Stokes solver of the same order. For the Navier-Stokes solver we choose the time step Δt equal to $3 \cdot 10^{-11} s$ and $0.5 * \Delta x / \sqrt{(2RT0)}$, where Δx is the cell size. In all cases we compute upto the final time $t = 1 \cdot 10^{-6} s$.

In the first test case, we consider $p_{in} = 624000Pa, p_{out} = 208000Pa$ and $T_0 = 300K$. This gives the Knudsen number on the left of 0.01101 and on the right of 0.03303. We are now in the slip regime, where we expect the Navier-Stokes solutions with no slip boundary conditions do not match with the Boltzmann ones. In Fig. 1(a) the x component of velocities from both solvers at 2/3rd of the channel length along the y axis are plotted. We observe that there is a discrepancy between the solutions of both equations. It is required to use slip boundary conditions for the Navier-Stokes equations on the solid boundaries. Instead of that we define boundary layers, 5 cells adjacent to the top and bottom walls as the Boltzmann domain and the rest is the Navier-Stokes one, see Fig. 1 (b). After the domain decomposition the coupled solutions of the Boltzmann and Navier-Stokes equations match perfectly, see Fig. 2(a) for this small range of the Knudsen number.

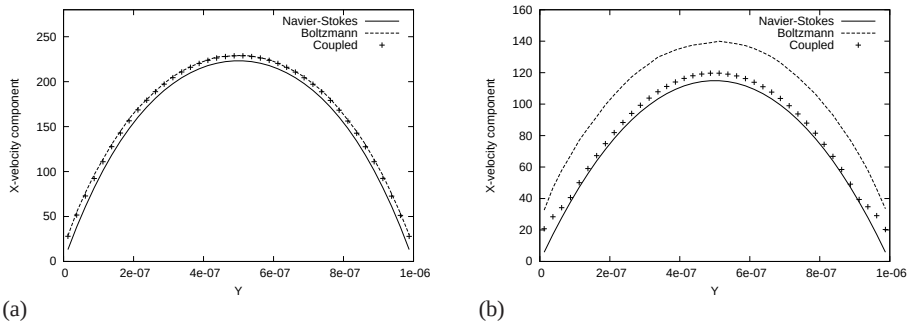


(a) (b)

Fig. 1 (a) x component of velocity along the y axis at 2/3rd of the channel length for $Kn = 0.01101$ to 0.03303 from Boltzmann and Navier-Stokes solvers (b) A priori domain decomposition: 'red' or '+' = Navier-Stokes domain, 'green' or 'x' = Boltzmann domain

In the second test case, we increase the Knudsen number by changing different inlet and outlet pressures $168480Pa$ and $56160Pa$, respectively. This corresponds the Knudsen number varying 0.0408 to 0.12 from left to right boundaries. For this range of Knudsen numbers, we decrease the time step Δt to $2 \cdot 10^{-11} s$ for the Navier-Stokes solver. We are still in the slip regime and close to it, however, for this range of Knudsen numbers defining the boundary layers like in Fig. 1(b) does not provide the

correct coupled solutions as shown in Fig. 2(b). Here, we observe that the coupled solution is close to the Navier-Stokes solution. In this case one may increase the size of boundary layers, but it is not clear how much one has to increase. So, we use the alternative strategy.



(a) (b)

Fig. 2 x component of velocity along the y axis at 2/3rd of the channel length. (a) for $Kn = 0.01101$ to 0.03303 (b) for $Kn = 0.0408$ to 0.12

The efficient way is to use a breakdown criterion to decompose the domains as suggested in [15] for steady problems. The idea is to solve first the Navier-Stokes equations everywhere until the steady state is reached. As we have seen in Fig. 2 (b), the Navier-Stokes solutions do not match with the Boltzmann solutions in this regime, however, they are somehow near to the Boltzmann ones. Then we apply the breakdown criterion $\|\phi\|$ suggested in [14] and decompose the domain. We assume, for example, if the value of $\|\phi\|$ at a cell is less than 0.01 the cell is defined as a Navier-Stokes cell, otherwise a Boltzmann one. In Fig. 3 the time evolution of the domain decompositions for the Knudsen numbers ranging from 0.01103 to 0.03303 at time different times are plotted. One can solve the Boltzmann and the Navier-Stokes equations in the corresponding domains. However, for the stationary solutions, it is sufficient to solve the Navier-Stokes equations until they reach the steady state and then to further use the domain decomposition and coupling method. After $t = 3 \cdot 10^{-8} s$ we reach the steady state of the Navier-Stokes equations and the domain decomposition does not change. After $t = 3 \cdot 10^{-8} s$ we solve both equations in their domains of validity until the final time. When we compare the figures Fig. 1(b) and Fig. 3 at time $t = 3 \cdot 10^{-8} s$, we see the Boltzmann domain is bigger in the latter figure. There is no unique values for this breakdown quantity. It depends upon the problem considered.

Now, for higher Knudsen numbers ranging from 0.0408 to 0.12 we observed that in the steady state the Navier-Stokes domain becomes smaller for the same criterion, see Fig. 4. Here the above coupling algorithm will not be the optimal one since we have a very small Navier-Stokes domain and we need additional effort to use the interface boundary conditions. Therefore, it is convenient to consider the entire domain as Boltzmann one with the initial conditions as stationary solutions

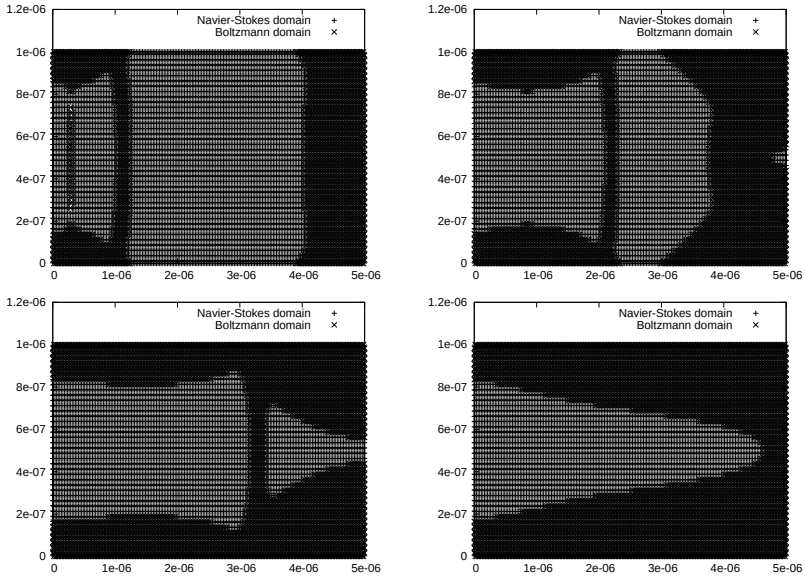


Fig. 3 Domain decomposition: 'red' or '+' = Navier-Stokes domain and 'green' or 'x' = Boltzmann domain after application of the breakdown criterion to solutions of the Navier-Stokes equations for the range $Kn = 0.01101$ to 0.03303 . Top rows are for $t = 3 \cdot 10^{-9} s$ and $t = 6 \cdot 10^{-9} s$ and the bottom rows are for $t = 9 \cdot 10^{-9} s$ and $t = 3 \cdot 10^{-8} s$.

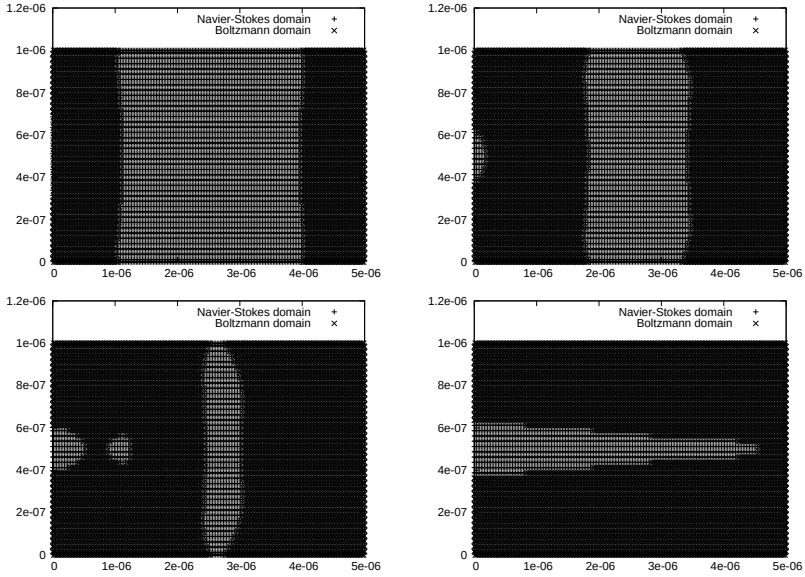


Fig. 4 Domain decomposition: 'red' or '+' = Navier-Stokes domain and 'green' or 'x' = Boltzmann domain after application of the breakdown criterion to stationary solutions of the Navier-Stokes equations for the range $Kn = 0.0408$ to 0.12. Top rows are for $t = 2 \cdot 10^{-9} s$ an $t = 4 \cdot 10^{-9} s$ and the bottom rows are for $t = 6 \cdot 10^{-9} s$ and $t = 2 \cdot 10^{-8} s$.

of the Navier-Stokes equations. Then, we run for few more iterations and then start sampling the data.

The above results show that the coupling method may be relevant for regimes where the Knudsen number is less than 0.03.

Acknowledgements This work was partially supported by the German Research Foundation (DFG), grant number KL1105/17-1.

References

1. Aktas, O., Aluru, N.R.: A combined continuum/dsmc technuque for multiscale analysis of microfluidic filters. J. Comput. Phys. **178**, 342–372 (2002)
2. Babovsky, H., Illner, R.: A convergence proof for nanbu's simulation method for the full boltzmann equation. SIAM J. Numer. Anal. **26**, 45–64 (1989)
3. Bardos, C., Golse, F., Levermore, D.: Fluid dynamic limits of kinetic equations. J. Stat. Phys. **63**, 323–344 (1991)
4. Bird, G.A.: Molecular Gas Dynamics and Direct Simulation of Gas Flows. Oxford University Press, New York (1994)
5. Caflish, R.: The fluid dynamical limit of the nonlinear boltzmann equation. Commun. Pure Appl. Math. **33**, 651–666 (1980)
6. Cercignani, C., Illner, R., Pulvirenti, M.: The Mathematical Theory of Dilute Gases. Springer-Verlag, Berlin (1994)
7. Chen S.and Weinan, E., Y., L., Shu, C.W.: A discontinuous galerkin implementation of a domain decomposition method for kinetic hydrodynamic coupling multiscale problems in gas dynamics and device simulations. J. Comput. Phys. **225**, 1314–1330 (2007)
8. Degond, P., Dimarco, G., Mieussens, L.: A moving interface method for dynamic kinetic-fluid coupling. J. Comput. Phys. **227**, 1176–1208 (2007)
9. Gad-el Hak, M.: The fluid mechanics of microdevices - the freeman scholar lecture. ASME J. Fluids Enggs. **121(403)**, 5–33 (1999)
10. Klar, A.: Domain decomposition for kinetic problems with nonequilibrium states. Eur. J. Mech., B/Fluids **15,2**, 203–216 (1996)
11. Le Tallec, P., Mallinger, F.: Coupling boltzmann and navier-stokes equations by half fluxes. J. Comput. Phys. **136**, 51–67 (1997)
12. Levermore, D., Morokoff, W.J., Nadiga, B.T.: Moment realizability and the validity of the navier-stokes equations for rarefied gas dynamics. Phys. Fluids **10(12)** (1998)
13. Neunzert, H., Struckmeier, J.: Particle methods for boltzmann equation. Acta Numer. **4**, 417–457 (1995)
14. Tiwari, S.: Coupling of the boltzmann and euler equations with automatic domain decomposition. J. Comput. Phys. **144**, 710–726 (1998)
15. Tiwari, S., Klar, A.: Coupling of the navier-stokes and the boltzmann equations with a meshfree particle and kinetic particle methods for a micro cavity. In: M. Griebel, M.A. Schweitzer (eds.) Meshfree Methods for Partial Differential Equations V, LNCSE 79, Berlin/Heidelberg, pp. 155–171. Springer (2011)
16. Tiwari, S., Klar, A., Hardt, S.: A particle-particle hybrid method for kinetic and continuum equations. J. Comput. Phys. **228**, 7109–7124 (2009)
17. Tiwari, S., Kuhnert, J.: Modeling of two phase flows with surface tension by finite pointset method (fpm). J. Comput. Appl. Math. **203**, 376–386 (2007)