Computational Solution of the Extended Navier–Stokes PDE’s: Incorporating Nonlinear Fluid-Solid Boundary Conditions for Microfluidic Simulations

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Abstract
Traditionally no-slip and temperature-jump conditions in fluid mechanics are modelled using a linear first order mathematical model to incorporate the tangential momentum accommodation coefficient (TMAC) at a fluid-solid interface, however this formulation is only generally accurate at macroscopic length scales and pressures for Knudsen numbers in which the dominant flow regime is such that the continuum assumption is valid. In this paper we consider the application of a nonlinear slip model for the specification of the boundary conditions in the extended Navier-Stokes system of PDE’s. A numerical discretization scheme is developed for a 2D Couette-Poiseuille problem to simulate microfluidic flow in the interface gap of a piston-cylinder pressure balance with application to an absolute pressure primary scientific standard.

Keywords: Navier-Stokes, microfluidic simulation, no-slip, fluid-solid interface, pressure metrology

Résumé
Traditionnellement les conditions de non glissement et la température de saut en mécanique des fluides sont modélisés en utilisant un modèle mathématique premier ordre linéaire pour intégrer le coefficient dynamique tangentielle hébergement (TMAC) à une interface fluide-solide, mais cette formulation est que généralement précisées à des échelles de longueur macroscopique et pressions pour des nombres de Knudsen dans laquelle le régime d'écoulement dominante est telle que l'hypothèse est valide continuum. Dans ce document, nous considérons l'application d'un modèle non linéaire de glissement pour la spécification des conditions aux limites dans l'étendue de Navier-Stokes système d'EDP. Un schéma de discrétisation numérique est développé pour une 2D de Couette-Poiseuille problème pour simuler l'écoulement microfluidique de l'écart de l'interface d'un équilibre de pression piston-cylindre avec application à une pression primaire norme absolue scientifiques

Mots clés: Navier-Stokes, simulation microfluidique, aucun glissement, l'interface fluide-solide, à la métrologie de pression

1. Introduction
Fluid mechanics plays a compelling role in many areas both at an applied and pure level encompassing problems in both traditional engineering such as gas dynamics analysis in the aerospace sector, magnetohydrodynamics in plasma physics, as well as ongoing research in mathematics [12]. In the majority of cases the underlying physico-mathematical models are based on continuum PDE’s which are either developed directly from the Boltzmann equation [8] or further macroscopic extensions which are derived from the Boltzmann equation [16].

In order to solve this system of equations boundary conditions are required and the two aspects of slip-velocity and temperature-jump must be considered. For real gases at a fluid/solid interface gas molecules will impinge at an angle of incidence to the solid surface and a combination of specular and diffuse reflection will occur at a localized microscopic scale such that the angle of reflectance will be different and uncorrelated with the entry angle due to local surface roughness and imperfections [29].

2. Physical Basis of Velocity-Slip and Temperature-Jump Phenomena
A consequence of the localized physical microscopic imperfections exhibited through surface irregularities and roughness effects at a fluid/solid interface is the macroscopic experimentally observable effect of velocity-slip originally studied by Maxwell where a localized deficit of tangential momentum at the point of impact parallel to the surface occurs and consequently in order to preserve conservation of momentum a non-zero slip velocity \( u_s \) must be introduced of the form \( u_s = u - u_w = \left( \frac{2}{\gamma} - 1 \right) \frac{\partial p}{\partial n} |_w \) where \( l \) is the mean free path of the gas, \( u \) is the tangential gas velocity in contact at the wall, \( u_w \) is the all tangential velocity and the subscript \( w \) indicates evaluation at the wall surface as discussed in [29]. Local thermodynamic equilibrium will also fail to hold if \( l \) is large compared to the flow dimensions resulting in an analogous temperature-jump phenomenon studied by Smoluchowski that is modelled in the form \( T - T_w = \left( \frac{2}{\alpha} - 1 \right) \frac{\gamma + 1}{\gamma + 1} \frac{\partial p}{\partial n} |_w \) in which a
thermal-accomodation coefficient $\alpha$ is utilized in analogous manner to the diffuse-reflection coefficient $f$ in the Maxwell first order no-slip model.

The slip velocity

$$u_s = u_t - u_w$$  \hspace{1cm} (1)$$

is a measure of the difference between the actual fluid velocity adjacent to a wall boundary i.e. tangential to the wall and the wall tangential velocity and in linear slip theories the slip velocity $u_s$ is expressed in terms of the mean free path $\lambda$ of fluid molecules and tangential momentum accommodation coefficient (TMAC) $\sigma_t$ with the assumption that the slip velocity is proportional to $\lambda$ and the normal velocity gradient term $\frac{\partial u_n}{\partial n}$.

The TMAC is expressed as

$$\sigma_t = \frac{\left| p_t^{(i)} - p_t^{(r)} \right|}{\left| p_t^{(i)} - p_t^{(w)} \right|}$$

which is the ratio of the difference in incident and reflected tangential momentum transfer from the fluid molecule striking the surface to that of fluid molecules striking the surface’s temperature, and where for a wall moving at velocity $u_w$ the momentum is expressed as $p_t^{(w)} = m_g \dot{u}_w$ where $m_g$ is the mass of the fluid molecule.

For many microfluidic studies involving Navier-Stokes equations these Maxwell-Smoluchowski effects are usually specified with first order modifications as

$$u_s = \frac{2 - \alpha}{\sigma_u} \left( \frac{\partial u}{\partial n} \right)_w + \frac{3}{4} \frac{\mu}{\rho u_w} \frac{\partial T}{\partial x} \left|_w \right. \hspace{1cm} (2)$$

$$T - T_w = \frac{2 - \alpha}{\sigma_T} \frac{2 \gamma}{\rho r^{(y+1)}} \lambda \left( \frac{\partial T}{\partial x} \right)_w \hspace{1cm} (3)$$

following the approach in [9] in which it is assumed that the slip coefficient is independant of the Knudsen number, however recent studies performed by [1] indicate that this assumption may be incorrect. Classification of slip models can be broadly defined as linear or nonlinear [5] and for linear slip models an extension to the Maxwell-Smoluchowski first order system is to consider a slip model in terms of two slip constants $C_1$ and $C_2$ in the form

$$u_s = C_1 \lambda \left( \frac{\partial u}{\partial n} \right)_w - C_2 \lambda^2 \left( \frac{\partial^2 u}{\partial n^2} \right)_w \hspace{1cm} (4)$$

The limitation of linear first order slip models is that they only produce accurate results for Knudsen numbers of $Kn < 0.1$ as discussed by [5] and as a result will introduce errors. Based on results cited within the review article of [5] the errors in velocity within the Knudsen layer can be as large as $u_s = \sqrt{2} u_{KE}$ where $u_s$ is the slip velocity obtained with a linear slip model and $u_{KE}$ represents the actual velocity at the wall as obtained with a kinetic energy solution approach to the Boltzmann transport equation. The issue with the use of linear slip models is that if the first order parameters are modified to produce accurate velocities within the Knudsen layer then there is a large change in inaccurate velocity profiles outside the Knudsen layer, and as a result a first order slip model is only beneficial at small Knudsen numbers when either the Knudsen layer is thin or when the flow exhibits weak slip. Hence significant restrictions apply on the flow conditions and ranges that can be simulated with linear and first order slip models.

Detailed experimental measurements of the slip coefficient terms $C_1$ and $C_2$ for a combination of experiments of flat plates and rotating cylinders when compared with kinetic energy based simulations using the Boltzmann equation and direct numerical Monte Carlo numerical studies reveal inconsistencies which can not be adequately accounted for within a linear slip model framework.

For this reason nonlinear slip models present an alternative for more accurate results and the general approach adopted is to instead of attempting refinement of only the velocity slip parameters $C_1$ and $C_2$ to consider further refinements on the fluid’s tangential shear stress $\tau$ and mean free path $\lambda$ which on rearranging the classical Maxwell slip model with the temperature jump i.e. Smoluchowski condition may be written as $u_s = \frac{2 - \alpha}{\sigma_\tau} \lambda^2 \frac{\mu}{\rho}$ Different approaches in terms of modelling the stress and mean free path have been reported in the literature [5] and research is ongoing however a majority of the studies utilize a generalized viscosity $\mu_{eff}$ and generalized mean free path $\lambda_{eff}$ terms in conjunction with slips coefficients that are expressed on a fundamental level in terms of the TMAC $\sigma_t$. Studies performed by [30] where the TMAC $\alpha$ was varied over the range from $\alpha = 0.1$ to $\alpha = 1.0$ and an effective viscosity of form

$$\mu_{eff} = \frac{\mu}{1 + 9.638 \cdot Kn^{1.135}}$$

using results originally performed by [15] based on the solution of the Boltzmann equation was considered.

At present the TMAC is determined by experimental measurements supplemented by DSMC numerical studies as existing theoretical results are inconclusive due to the presence of gas-solid adsorption and surface roughness effects. Representative values for the TMAC discussed in [5] for nitrogen gas on steel for Knudsen number range of 0.01 to 1.00 at a temperature of 293 K yielded a values as

$$0.83 \leq \sigma_t \leq 1.01 \hspace{1cm} (5)$$

which is representative to the case for a piston-cylinder manufactured of steel when calibrated in absolute mode.
using dry nitrogen as the fluid medium.

Existing approaches reported in the literature [4] for hydrodynamics problems i.e. incompressible flows cannot be directly implemented for modifications to the traditional Dirichlet and Neumann type boundary conditions of form

\[ u = g \quad \forall \quad x \in \partial \Omega \]  \hspace{1cm} (6)

\[ n \cdot \sigma = h \quad \forall \quad x \in \partial \Omega \]  \hspace{1cm} (7)

where \( \sigma \) is the fluid stress tensor \( \sigma(u,p) = -pI + 2\mu \varepsilon(u) \) and \( \varepsilon(u) = \frac{1}{2} [\nabla u + (\nabla u)^T] \) which are usually represented in the form, for 2D geometries ignoring an additional specification for a bi-tangent vector in 3D,

\[ n \cdot u = 0 \]  \hspace{1cm} (8)

\[ t \cdot \sigma(u,p) \cdot n = \beta t \cdot u \]  \hspace{1cm} (9)

which are generally aligned with either the assumption of a no-slip condition or a modification which assumes an empirical coefficient \( \beta \) which prescribes a tangent stress proportional to the tangent velocity component. Noting that the gradient of a vector field is a tensor where

\[
\nabla u = \begin{bmatrix}
\frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} & \frac{\partial u_1}{\partial x_3} \\
\frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} & \frac{\partial u_2}{\partial x_3} \\
\frac{\partial u_3}{\partial x_1} & \frac{\partial u_3}{\partial x_2} & \frac{\partial u_3}{\partial x_3} \\
\end{bmatrix}
\]

is the matrix representation of the tensor using the indicial notation for convenience it is seen that the existing approach for velocity slip with \( t_j \sigma_{ij} n_i = \beta t_j u_k \) in tensor form with the Einstein summation convention for convenience effectively amounts to a type of mixed linear slip velocity model in terms of the velocity \( u_i \) with \( i \in \{1,2\} \), the velocity gradients \( \frac{\partial u_i}{\partial x_j} \) with \( i,j \in \{1,2\} \), pressure, and the experimental parameter \( \beta \) for known tangent and normal unit vectors. Applications for this approach to compressible flows similarly utilize linear velocity slip models of form \( u \cdot n = 0 \) and \( u \cdot t \propto \frac{\lambda}{\rho} \) as per the Smoluchowski condition as previously discussed. As a result modifications to existing computational fluid dynamics codes which incorporate linear first order velocity slip models with for example FVM or FEM discretizations to higher order linear slip models and nonlinear slip models can prove difficult.

Due to the wide variety of nonlinear slip models reported in the literature we will consider the physical experimental problem as illustrated in figure 1 with the following slip model

\[ u_s = \frac{z_s - u_l}{\sigma_l} \lambda \left( \frac{\partial u_l}{\partial n} + \frac{\partial u_s}{\partial t} \right) \]  \hspace{1cm} (10)

where \( u_e \) and \( u_n \) are the gas velocities in the tangential and normal directions to the surface boundary as reported in [5] and which is based on a simplification by setting the temperature gradient term in the full expression of \( u_s \) in [26] to zero, by assuming an isothermal temperature distribution although ideally a full solution would require the simultaneous solution of the mass, momentum and energy conservation equations.

\[ \lambda = \frac{\mu}{\rho} \sqrt{\frac{RT}{2}} \]  \hspace{1cm} (11)

3. Derivation of Numerical Scheme for Nonlinear Boundary Conditions

For many solid and fluid mechanics problems the three general numerical techniques of the finite difference method (FDM), finite volume method (FVM) and finite element method (FEM) discretization for the numerical solution of PDE’s are commonly utilized, of which the FVM enjoys favour for fluid mechanics problems whilst the FEM is commonly applied for both linear and nonlinear elasticity simulations in solid and composite mechanics.

Although both the FVM and FEM techniques may be utilized in a variety of problems the application of these methods for nonlinear boundary conditions can present considerable difficulty since in the majority of cases for the mathematical analysis of PDE’s boundary conditions are generally expressed in terms of either first-type or Dirichlet type i.e. specified value, second-type or Neumann type i.e. specified gradient value or third-type i.e. Robin type which is a linear combination of Dirichlet and Neumann BC’s on a part of the domain’s boundary. Other categories of BC’s such as the Cauchy BC i.e.

Figure 1 Schematic illustration of piston-cylinder operated pressure balance

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simultaneous Dirichlet and Neumann specification, other forms such as nonlinear oblique derivative BC's or oblique boundary value problem also exist but require further mathematical investigation in terms of existence and uniqueness of results [7].

Due to the complexities in applying the FVM and FEM for nonlinear boundary conditions the FDM continues to find wide application in the numerical solution of nonlinear boundary value problems both in terms of ODE's [25] and via. coordinate mapping in PDE's as well [19].

Utilizing a cartesian coordinate system for the physical domain and fluid velocity field \( \mathbf{u} \) as illustrated in figure 2 it follows that the normal and tangential unit vectors are

\[
\hat{t} = [\cos \theta, \sin \theta]^T \\
\hat{n} = [-\sin \theta, \cos \theta]^T
\]  

(12) (13)

Figure 2 Illustration of orientation of coordinate system and fluid velocity components

using the relation \( \frac{dy}{dx} = \tan \theta \) where \( \theta \) is the angle between the tangent at a point along the curve and the horizontal axis from vector analysis, and where the cartesian orthogonal components are related to tangential and normal components using the symbols \( t \) and \( n \) to represent the tangent and normal according to the transformation mapping for a rotation as

\[
\begin{bmatrix}
\hat{u}_x \\
\hat{u}_y \\
\hat{u}_n
\end{bmatrix} =
\begin{bmatrix}
\cos \theta & \cos \left( \frac{\pi}{2} + \theta \right) & 0 \\
\sin \theta & \sin \left( \frac{\pi}{2} + \theta \right) & 0 \\
0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
\hat{u}_t \\
\hat{u}_n
\end{bmatrix}
\]  

(14)

using standard vector analysis for a flat \( \mathbb{R}^2 \) metric space from which it easily follows that

\[
\begin{bmatrix}
\hat{u}_t \\
\hat{u}_n
\end{bmatrix} =
\begin{bmatrix}
\cos \theta & \sin \theta & 0 \\
-\sin \theta & \cos \theta & 0
\end{bmatrix}
\begin{bmatrix}
\hat{u}_x \\
\hat{u}_y
\end{bmatrix}
\]  

(15)

using the notation that \( \hat{u}_t \) and \( \hat{u}_n \) are positive for positive \( u_x \) and \( u_y \). It is seen that \( \frac{\partial u_x}{\partial n} \) and \( \frac{\partial^2 u_x}{\partial n^2} \) are required for a linear slip model, and \( \frac{\partial u_x}{\partial t} \) and \( \frac{\partial^2 u_x}{\partial t^2} \) are required for a nonlinear slip model. As a result by application of the standard application of vector analysis for the directional derivitative it follows that for a vector field \( \mathbf{u} = [u_x, u_y]^T \) in a cartesian coordinate system that the directional derivatives for a linear slip model are

\[
\frac{\partial u_x}{\partial n} = \frac{\partial u_x}{\partial x} \sin \theta + \frac{\partial u_y}{\partial x} \cos \theta \quad \frac{\partial^2 u_x}{\partial n^2} = \left[ \frac{\partial}{\partial x} \left( \frac{\partial u_x}{\partial x} \right) \right] \sin \theta + \left[ \frac{\partial}{\partial y} \left( \frac{\partial u_y}{\partial y} \right) \right] \cos \theta
\]  

(16) (17)

whilst for the nonlinear slip model in the case that the tangential temperature gradient term is negligible it follows using standard vector analysis and vector calculus that

\[
\frac{\partial u_x}{\partial n} = (\nabla u_x) \cdot \hat{n} \\
\frac{\partial u_y}{\partial n} = (\nabla u_y) \cdot \hat{n}
\]  

(18) (19)

so that

\[
\frac{\partial u_x}{\partial t} + \frac{\partial u_y}{\partial y} = \left[ \frac{\partial}{\partial x} \left( u_x \cos \theta + u_y \sin \theta \right) + \frac{\partial}{\partial y} \left( -u_x \sin \theta + \cos \theta u_y \right) \right] \sin \theta + \left[ \frac{\partial}{\partial x} \left( u_x \cos \theta + u_y \sin \theta \right) + \frac{\partial}{\partial y} \left( -u_x \sin \theta + \cos \theta u_y \right) \right] \cos \theta
\]  

(20)

In the above system for both linear and nonlinear velocity models we consider the unknowns to solve for as the two components \( u_x \) and \( u_y \) of the velocity field \( \mathbf{u} \) as \( u_x = u_x \cos \theta \) and \( u_y = u_y \sin \theta \) where \( \theta(x,y) = \arctan \left( \frac{dy}{dx} \right) \) is known since the curve corresponding to the piston/cylinder boundary may with finite differences or a spline curve fit be differentiated.

4. Application of Nonlinear Velocity-Slip to an Industrial Microfluidics Problem

The above scheme may be implemented to study the effect of microfluidic flow in the interface gap of a precision piston-cylinder operated pressure balance as illustrated in figure 1 and figure 2 by utilizing an algebraic grid transformation as discussed in [28] which maps the physical domain into a rectangular domain as illustrated in figure 3.

In the case of steady state flow the mass and momentum equations setting \( u_x = u \) and \( u_y = v \) for brevity read as
Figure 3 Illustration of an algebraic grid generation mapping from a physical to computational domain

\[ \frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}(\rho u) - \frac{\partial}{\partial y}(\rho v) \]  
(21)

\[ \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left[ \rho \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] - \rho \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} \left( \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right) \right) \]  
(22)

\[ \frac{\partial v}{\partial t} = \frac{\partial}{\partial y} \left[ \rho \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) \right] - \rho \frac{\partial}{\partial y} (\rho v) + \frac{\partial}{\partial x} \left( \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right) \right) \]  
(23)

following [29] and the density is defined in terms of the ideal gas equation of state

\[ p = \rho RT \]  
(24)

where \( R \) is the universal gas constant divided by the gas molecular mass i.e. the gas constant for the particular gas species and \( T \) is the thermodynamic temperature. The pressure-velocity coupling in fluid systems governed by traditional no-slip boundary conditions i.e. \( u = u_{\Omega} \) may be considered in terms of the semi-implicit pressure linked equation (SIMPLE) algorithm [29] however the difficulty with this well known algorithm in the recovery of the pressure for a nonlinear velocity slip is that both the pressure and velocity are unknowns on the solid boundary.

An alternative to such iterative pressure-velocity algorithms is to directly solve a ‘Poisson’ type pressure equation by taking the divergence of the momentum equations and utilizing the continuity equation so that in cartesian coordinates the following pressure defining equation for steady state flows results

\[ \frac{\partial}{\partial x_i} \left( \frac{\partial p}{\partial x_i} \right) = -\frac{\partial}{\partial x_i} \left[ \rho u_i u_j - \tau_{ij} \right] \]  
(25)

where the Einstein convention of summation of terms for repeated indices is used, subscripts \( i \) and \( j \) for indices 1 and 2 correspond to the \( x \) and \( y \) cartesian components, and \( \tau_{ij} \) represents the shear stress term

\[ \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \delta_{ij} \nabla \cdot \mathbf{V} \]  
(26)

where \( \delta_{ij} \) is the Kronecker delta function as per the previous notation in the Navier–Stokes equation formulation. Regardless of the mechanism to address the uncoupling of the velocity/pressure fields the underlying equations to solve are the continuity and \( x \)- and \( y \)-components of the momentum equation which when expanded for a homogeneous system are for the continuity, \( x \)-momentum and \( y \)-momentum:

\[ 0 = -\frac{\partial p}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) \]  
(27)

\[ 0 = -\rho \left( \frac{\partial u}{\partial t} + \left( u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) \right) + \rho g_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial y} \left( \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right) \right) \]  
(28)

\[ 0 = -\rho \left( \frac{\partial v}{\partial t} + \left( u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) \right) + \rho g_y - \frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left( \mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial x} \right) \right) \]  
(29)

To numerically solve the underlying PDE’s one may utilize the finite difference method for simplicity following the approach in [28] using a computational molecule scheme as illustrated in figure 4.
curvilinear mapping transformations, and are according to [21] either clumsy, of low-order accuracy, or burdened with a high computational overhead. The finite difference approximation for a Robin type boundary condition i.e. a linear combination of Dirichlet and Neumann boundary conditions on $\partial\Omega$ for a dependant variable $\varphi$ of form

$$a\frac{\partial\varphi}{\partial n} + \beta\varphi = F$$  

(30)

where $a$, $\beta$ and $F$ are piecewise continuous functions along the boundary by [20] utilized a truncated Taylor series expansion

$$\varphi = \varphi_0 + \frac{\partial\varphi_0}{\partial x}(x - x_0) + \frac{\partial\varphi_0}{\partial y}(y - y_0) + \frac{1}{2}\frac{\partial^2\varphi_0}{\partial x^2}(x - x_0)^2 + \frac{\partial^2\varphi_0}{\partial xy}(x - x_0)(y - y_0) + \frac{1}{2}\frac{\partial^2\varphi_0}{\partial y^2}(y - y_0)^2 + O(\Delta^2)$$  

(31)

where $\Delta$ is the spacing in both the $x$- and $y$- directions assumed equal for simplicity and the derivatives of the dependant variable $\varphi$ are evaluated at the center of the computational molecule using discrete finite difference approximations for the spatial derivatives based on local nodal points adjacent and within the neighbourhood of the center but not necessarily coincident to the underlying mesh. This approach was developed to estimate the value of $\varphi_P$ and $\frac{\partial\varphi}{\partial n}$ and a point $P$ that occurred on the boundary $\partial\Omega$ not coincident with the underlying mesh. Whilst linear slip models require tangential directional derivatives from a generalized linear slip model $u_x = C_1\frac{\partial\varphi}{\partial n} + C_2\frac{\partial u_y}{\partial n} + \cdots$ in order to apply a nonlinear velocity slip model both first order tangential as well as normal directional derivatives of both the tangential and normal velocity components expressed in terms of the $x$- and $y$- partial derivatives of the velocity components $u_x$ and $u_y$ are required, as well as possibly higher order directional derivatives for certain nonlinear velocity slip models.

To accommodate such a wide range of possible directional derivative specifications solely from a finite difference discretization is unwieldy and restricted to low order approximations near the boundary due to the limited number of adjacent nodes along the boundary.

Extensions to higher order approximations by utilizing additional nodes within the domain are possible but may be further complicated due to the shape of the boundary at which the discretization is attempted and may not be fully generalized throughout the domain.

As an example of the difficulties encountered in the application of a common finite difference discretization throughout the domain in figure 5 it is seen that the directional derivatives on the boundary $\partial\Omega$ marked by squares near the inlet is feasible to construct as there is sufficient nodal points to build an approximation to the dependant variable $\varphi$ in terms of the interior nodal points marked by circles whilst this is not the case as the fluid progresses further along into the domain as there is then a need for both interior nodal points (marked as circles) within the domain as well as ‘ghost’ nodal points exterior to the domain (marked with stars).

A potential alternative for the implementation for nonlinear boundary conditions is the use of power series approximations as discussed by [23] and [24] who developed the method based on generalized Taylor series expansions for a multivariable function $f(x_1, \ldots, x_d)$ of form

$$T(x_1, \ldots, x_d) = \sum_{n_1=0}^{n} \cdots \sum_{n_d=0}^{n} \frac{(x_1-a_1)^{n_1}(x_d-a_d)^{n_d}}{n_1! \cdots n_d!} \times \left(\frac{\partial^{n_1+\cdots+n_d}}{\partial x_1^{n_1} \cdots x_d^{n_d}}\right)(a_1, \ldots, a_d)$$  

(32)

In the case for two dimensions the truncated Taylor series reduces to

$$\varphi(x, y) = \sum_{r=0}^{N} \sum_{s=0}^{N} \frac{1}{r! s!} \varphi^{(r,s)}(c_0, c_1)(x - c_0)^r(y - c_1)^s$$  

(33)

and when applied to linear partial differential equations with variable coefficients results in a system of simultaneous algebraic equations to be solved for.

Another potential approach is a polynomial based shape function representation on an arbitrary unstructured grid as proposed by [13] that has not to date been implemented and reported in the literature. Whilst this method holds
and approach for radial basis functions. We assume \( \sin{\theta} \) and our implementation extends \( t \) and similarly \( \theta \) as previously discussed.

The implementation that we follow is this paper for demonstration purposes only is that of the well known [22] approach for radial basis functions. We assume approximations for the underlying unknown fields i.e. for \( u(x, y), v(x, y) \) and \( \rho(x, y) \) using

\[
\begin{align*}
u &= \sum_{j=1}^{N} b_j \varphi(r_j) \\
\rho &= \sum_{j=1}^{N} c_j \varphi(r_j)
\end{align*}
\]

where \( r_j = \|x - x_j\| \) with a Euclidean norm i.e.

\[
r_j = \sqrt{(x - x_j)^2 + (y - y_j)^2}
\]

with a thin-plate spline (TPS)

\[
\varphi(r) = r^{2\eta} \log r, \eta \in \mathbb{N}
\]

as the selection of radial basis function form following [11] with a choice of \( \eta = 2 \) since the Navier-Stokes equations are a second order approximation to the Boltzmann equation [8] and our implementation extends the applicability to the extended form of the Navier-Stokes equations for microfluidic gas simulations.

These equations when substituted into the continuity and momentum equations i.e. the Navier-Stokes equations (21) – (23) form the underlying homogeneous system of simultaneous equations within the interior of the domain \( \Omega \) and involve both unknown velocities and pressures within the interior.

On the boundary of the domain \( \partial \Omega_I \) for a flow inlet the inlet pressure \( p_{\text{in}} \) and the outlet pressure \( p_{\text{out}} \) can be used with the equation of state \( p = \rho RT \) to provide equations for the density specification at a known pressure on the boundary as

\[
p_{\text{in}} = \frac{\sum_{j=0}^{N} c_j \varphi(r_j)}{RT} \forall [x, y]^T \in \partial \Omega_I
\]

and similarly

\[
p_{\text{out}} = \frac{\sum_{j=0}^{N} c_j \varphi(r_j)}{RT} \forall [x, y]^T \in \partial \Omega_O
\]

for nodal points on the outlet flow boundary \( \partial \Omega_O \) and thus involve the specification for known densities i.e. pressures and unknown velocities.

Along the walls in contact with the domain the application of the nonlinear velocity slip model is applied for the specification of the fluid tangential velocity on the boundaries \( \partial \Omega_T \) on the “top” and \( \partial \Omega_B \) on the “bottom”. In two dimensions for specification of the vector of fluid velocity \( \mathbf{u} \) either the horizontal \( u_x \) and vertical \( u_y \) components are required or alternately the tangential velocity \( u_t \) and normal velocity \( u_n \) components along the “top” and “bottom” boundaries since the mapping between the two sets of components are known via the matrix transformations in equations (12) and (13). It is necessary to consider the tangential and normal velocity components where for normal velocity component at a wall boundary

\[
-\sin \theta u + \cos \theta v = -\sin \theta u_w + \cos \theta v_w \forall [x, y]^T \in \partial \Omega_T \cup \partial \Omega_B
\]

which physically means that the fluid does not flow into an impermeable or porous wall but is at the same wall velocity the fluid is in contact with (we assume that the horizontal and vertical velocity components of the wall are known), whilst for the tangential velocity component the nonlinear velocity slip model is applied by recalling that from the velocity slip definition \( u_{s} = u_t - u_w \) where \( u_{s} \) is the wall tangential velocity so that on rearrangement

\[
0 = u_w - u_t + \frac{2 - \alpha}{\alpha} \lambda (\frac{\partial u_t}{\partial n} + \frac{\partial u_n}{\partial t})
\]

For the nonlinear velocity slip the above specifications involve both unknown velocities \( u_x, u_y \) as well as densities in terms of the unknown pressures in a cartesian coordinate system, which in Cartesian coordinates may be expressed as

\[
\{ \cos \theta u + \sin \theta v \} - \{ \cos \theta u_w + \sin \theta v_w \} = \frac{2 - \alpha}{\alpha} \lambda \left[ \sin \theta \left( -\frac{\partial}{\partial x} (\cos \theta u + \sin \theta v) + \frac{\partial}{\partial y} \left( -\sin \theta u + \cos \theta v \right) \right) + \cos \theta \frac{\partial}{\partial y} (\cos \theta u + \sin \theta v) \right]
\]

After all the above equations are combined a system of \( 3N \) simultaneous nonlinear equations in the unknowns \( a_i \) for \( u_x(x, y), b_j \) for \( u_y(x, y) \) and \( c_j \) for \( \rho(x, y) \) arise with \( 1 \leq j \leq N \) where \( N \) is the total number of nodal points i.e. \( N_i \) nodes within the domain and \( N_B \) nodes on the boundary of the domain so that

\[
N = N_i + N_B
\]

where \( a_i, b_j, c_j \in \mathbb{R} \). Due to the fact that the resulting system of nonlinear equations incorporates mixed products of the unknown \( a_i, b_j, c_j \) coefficients we consider the vector

\[
\begin{align*}
\{ \cos \theta u + \sin \theta v \} - \{ \cos \theta u_w + \sin \theta v_w \} = \frac{2 - \alpha}{\alpha} \lambda \left[ \sin \theta \left( -\frac{\partial}{\partial x} (\cos \theta u + \sin \theta v) + \frac{\partial}{\partial y} \left( -\sin \theta u + \cos \theta v \right) \right) + \cos \theta \frac{\partial}{\partial y} (\cos \theta u + \sin \theta v) \right]
\end{align*}
\]
of unknowns to solve for and linearize the resulting system of nonlinear equations i.e. the continuity, x-momentum, y-momentum, pressure on boundary and velocity on boundary equations in terms of $\mathbf{z}$ which results in a linear matrix equation

$$\mathbf{A}\mathbf{z} = \mathbf{b}$$

(46)

Overdetermined linear systems $\mathbf{A}\mathbf{x} = \mathbf{b}$ may be solved by a least squares approach as discussed by [14] by premultiplying both sides by the transpose of the coefficient matrix i.e. by solving the least squares solution $(\mathbf{A}^\top\mathbf{A})\mathbf{x} = (\mathbf{A}^\top\mathbf{b})$. The approximate linearized solution may then be used as a starting solution in the full system of nonlinear equations

$$\mathbf{F} (\mathbf{z}) = \mathbf{0}$$

(47)

The numerical approach that we propose in this paper follows an idea proposed by [18] for the solving of systems of nonlinear equations that views the system of nonlinear equations as an multiobjective optimization problem whose goal is to minimize the difference between the right and left terms of the corresponding equation. In our mathematical formulation of the fluid mechanics of the problem the nonlinear velocity slip boundary condition is incorporated as equality constraints for the normal and tangential velocity components at wall as per equations (41) and (43) and similarly for the pressure specifications in equations (39) and (40), which may then be solved with standard gradient constrained optimization techniques such as a sequential quadratic programming (SQP) routine.

In order to illustrate the application of the nonlinear velocity slip we consider an illustrative example in figure 6 which is comprised of two concentric cylinders where the domain is constructed as

$$\Omega = \{(r, \theta) : \theta_1 \leq \theta \leq \theta_2, r_1 \leq r \leq r_2\}$$

(48)

to model the physical domain of the interface gap between a piston and cylinder as illustrated earlier in figure 2.

In this example the top boundary $\partial \Omega_{T}$ is the cylinder wall, the bottom boundary $\partial \Omega_{B}$ is the piston wall, the inlet boundary $\partial \Omega_{I}$ on the left hand side of the inlet at the which the pressure is applied i.e. the boundary with a known inlet pressure $p_{in}$ e.g. 25 kPa and the outlet boundary $\partial \Omega_{O}$ on the right hand side is the outlet at which there is a residual pumped pressure e.g. 5 Pa which is a known outlet pressure $p_{out}$. In practise for physical piston-cylinder operated pressure balances when there is equilibrium i.e. the applied pressure at the inlet is balanced by the gravitational weight of the piston and the loaded mass pieces the piston is initially stationary and then moves at a terminal velocity or the piston natural fall rate [10]. We incorporate this physical boundary condition by setting the velocity of the bottom boundary $\Omega_{B}$ to a non-zero velocity $u_{w}$ i.e. a moving wall and the top boundary $\Omega_{T}$ to a zero velocity i.e. a fixed wall. It is the velocity slip that occurs when the piston travels at its natural fall rate that is modelled in this paper with a nonlinear velocity slip model. Typically a continuum occurs for pressures along the engagement length for the majority of the engagement length and near to the outlet as the pressure approaches a small residual pressure, which depends on the quality of the vacuum pumps used, the gas no longer exhibits a continuum structure i.e. the Navier-Stokes PDE’s become inaccurate and then either higher order Knudsen number based PDE’s e.g. the Burnett hydrodynamic equations [31] or extensions to the Navier-Stokes become necessary.

The delineation of the flow regimes for the validity testing of the various forms of fluid mechanics equations are:

- $0 \leq Kn \leq 0.001$ : continuum regime
- $0.001 \leq Kn \leq 0.1$ : slip regime
- $0.1 \leq Kn \leq 10$ : transitional regime
- $10 \leq Kn$ : rarefied gas dynamics

The Knudsen number is calculated as

$$Kn = \frac{\lambda}{\ell}$$

(49)

which is the ratio of the gas mean free path $\lambda$ which is defined by equation (11) using gas kinetic theory to that of the characteristics length $\ell$ and numerical experiments reported in the literature have successfully utilized the extended Navier-Stokes up to a Knudsen number of $Kn = 0.25$ although generally in many linear first order slip models the Knudsen number is not extended beyond 0.10. As a result the product of the pressure $p$ and characteristic length $\ell$ may be used as the defining parameter to determine the validity limits of the velocity slip condition for the application of the extended Navier-Stokes equations.
In our example since the flow regime moves from a continuum regime near the inlet to slip/transitional regime near the outlet the natural choice of characteristic length is that of the channel “height” along the engagement length and not the total piston/cylinder engagement length since the Knudsen number and flow regime will physically vary along the engagement length.

For practical precision manufactured piston-cylinder operated pressure balances the interface gap can typically range from 0.01 \( \mu \text{m} \) since the piston must not contact the cylinder surface to avoid “sticking” and allow a free movement to approximately 0.50 \( \mu \text{m} \) in the case of dimensionally characterized pressure balances which operate over the the pressure range up to 185 kPa [27]. As a result assuming dry nitrogen gas as the working fluid for convenience with a molecular weight of \( M = 28 \text{ g.mol}^{-1} \) it follows that with a viscosity of \( \mu = 1.663 \times 10^{-5} \text{ N.s/m}^2 \) [29] that for a flow regime to vary from the continuum into the slip/transitional flow regime for the extended Navier-Stokes equations that the corresponding Knudsen number must lie within the range

\[
0 \leq Kn \leq 0.25
\]  

or equivalently

\[
0 \leq \frac{\mu}{\pi \mu t^2} \leq 0.25
\]  

For parallel plates the conventional practice [3] based on hydraulic diameter arguments is to take the characteristic length \( L \) as twice the instantaneous channel height along the direction of flow i.e.

\[
L = 2H
\]  

and as result the extended Navier-Stokes PDE’s are found to be valid for application to microfluidic simulations of gas flow in piston-cylinder pressure balances when operated in gauge mode.

5. Discussion

In this paper we have presented the physical basis for the need of applying a nonlinear velocity-slip approach which is motivated by a practical industrial physics problem occurring in the field of microfluidics. Existing commercial CFD codes are unable to adequately solve such problems as they are reliant on a fluid continuum assumption which yields inaccurate and misleading information from the transitional to free molecular flow or rarefied gas flow regimes. As a result in order to study the fluid velocity and pressure behavior in microfluidic/nanofluidic devices and instrumentation such as microchannels recourse is necessary to research codes. Whilst many such codes generally tend to utilize the more limited form of the original Maxwell slip model the validity limits of such extensions to the Navier-Stokes equations is compromised when the fluid/solid boundaries exhibit curvature and/or rotational motion [26] with the result that the incorporation of nonlinear velocity-slip models becomes necessary in avoid to avoid excessive high performance computational (HPC) resources for direct \textit{ab initio} DSMC numerical studies.

Due to this complication it appears advantageous for future production codes to directly solve an explicit pressure equation in the primitive variables under an algebraic grid mapping with a computational domain FDM discretization, simultaneously with the momentum based velocity based equations. This approach then also presents the dual benefit of enabling the incorporation of higher order equation-of-states of the fluid medium such as the Soave-Redlich-Kwong or Peng-Robinson forms in addition to refinement of the slip coefficients as an avenue of future work in micro-electro-mechanical simulation (MEMS) study. In the present study a RBF formulation has been utilized to develop the underlying PDE’s as a system of nonlinear equations in terms of the RBF coefficients as unknowns to be solved for where the PDE boundary conditions incorporating the nonlinear velocity slip are implemented as equality constraints suitable for a laboratory research CFD code.

The limitation encountered in applying a nonlinear velocity slip condition to the extended Navier-Stokes PDE’s for simulations of pressure balances operated in absolute mode is that mean free path length will increase at the outlet which is at a residual pressure. As a result the Knudsen number will not lie within the required validity range over the full engagement length but rather remain accurate over about 90% of the engagement length. For the remaining 10% at the end of the engagement where the flow regime requires rarefied gas dynamics the “gluing” of a continuum flow solver and a molecular dynamics solver [6] is a potential area for future research work.

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References


Appendix A. Approach for Numerical Scheme Derivation

The system of equations to minimize are the continuity, x-momentum and y-momentum equations which are present at each of the nodal points for $1 \leq i \leq N$

$$f_{x,i-1} = \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v)$$

(A.1)

$$f_{x,i} = -\rho \left( u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) + \rho g_x - \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left( 2\mu \frac{\partial u}{\partial x} \right)$$

$$+ \frac{\partial}{\partial y} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right)$$

(A.2)

$$f_{y,i} = -\rho \left( u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) + \rho g_y - \frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial y} \left( 2\mu \frac{\partial v}{\partial x} + \frac{\partial u}{\partial y} \right)$$

(A.3)

which is a system of $3N$ nonlinear equations throughout the domain $\Omega$. The underlying system of equations i.e. the extended Navier-Stokes equations must be solved both in the interior as well as on the boundary of the domain. Substituting the RBF assumption into the above equations and by making use of the observation that for functions $f = \sum_{i=1}^{N} a_i \phi(r_i)$ and $g = \sum_{i=1}^{N} \phi(r_i)$ built up in terms of some choice $\phi(r)$ of RBF (not necessarily a TPS) that the product may be simply calculated as $fg = \sum_{i=1}^{N} \sum_{j=1}^{N} a_i b_j \phi(r_i) \phi(r_j)$ so that with the assumed equation of state $p = \rho RT$ it follows that for continuity

$$f_{x,i-1} = \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v)$$

(A.4)

Similar equations will result for the x- and y-momentum components, and analogous forms will occur for the boundary conditions in equations (41) and (43) as constraints.

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