Smoothed particle hydrodynamics continuous boundary force method for Navier–Stokes equations subject to a Robin boundary condition

Wenxiao Pan\textsuperscript{a,}\textsuperscript{*}, Jie Bao\textsuperscript{a}, Alexandre M. Tartakovskya\textsuperscript{a,}\textsuperscript{b}

\textsuperscript{a} Pacific Northwest National Laboratory, Richland, WA 99352, USA
\textsuperscript{b} School of Geosciences, Department of Mathematics and Statistics, University of South Florida, Tampa, FL, USA

\textbf{Article info}

\textbf{Article history:}
Received 1 August 2013
Received in revised form 2 December 2013
Accepted 5 December 2013
Available online 12 December 2013

\textbf{Keywords:}
Robin boundary condition
Smoothed particle hydrodynamics
Slip boundary condition
No-slip boundary condition
Navier–Stokes equations

\textbf{Abstract}

A Robin boundary condition for the Navier–Stokes equations is used to model slip conditions at the fluid-solid boundaries. A novel continuous boundary force (CBF) method is proposed for solving the Navier–Stokes equations subject to the Robin boundary condition. In the CBF method, the Robin boundary condition is replaced by the homogeneous Neumann boundary condition and a volumetric force term added to the momentum conservation equation.

Smoothed particle hydrodynamics (SPH) method is used to solve the resulting Navier–Stokes equations. We present solutions for two- and three-dimensional flows subject to various forms of the Robin boundary condition in domains bounded by flat and curved boundaries. The numerical accuracy and convergence are examined through comparison of the SPH–CBF results with the solutions of finite difference or finite-element method. Considering the no-slip boundary condition as a special case of the slip boundary condition, we demonstrate that the SPH–CBF method accurately describes both the no-slip and slip conditions.

© 2013 Elsevier Inc. All rights reserved.

1. Introduction

Smoothed particle hydrodynamics (SPH) is a fully Lagrangian particle method for solving partial differential equations (PDEs) describing momentum, mass and energy conservation laws [1]. In SPH, a fluid is represented by a set of particles that are used as interpolation points to numerically solve the governing PDEs. SPH discretization of PDEs is based on a meshless interpolation scheme, which allows the PDEs to be written in the form of a system of ordinary differential equations (ODEs). Due to its Lagrangian nature, SPH has several advantages for modeling physical phenomena involving multiphase flows, flows with free surfaces, highly compressible flows, advection-dominated flows, and fragmentation of materials: 1) in the Lagrangian coordinate system there is no non-linear advection term in the momentum conservation equation; 2) SPH models advection exactly; 3) free surfaces and interfaces between fluids move with particles, and hence there is no need for front tracking schemes; 4) mass, momentum, and energy are explicitly conserved; 5) SPH discretization schemes are Galilean invariant; 6) and complex physics can be included via simple molecular-like interactions. As a result, SPH has been used to model various physical problems including ice sheet flows [2,3], friction stir welding [4], wave breaking [5], multiphase flows, reactive transport and mineral precipitation in porous media [6,7], emulsions [8], and moulding flows [9].

* Corresponding author. Tel.: +1 509 375 6686; fax: +1 509 372 4720.
E-mail address: wenxiao.pan@pnnl.gov (W. Pan).
Despite significant progress in the theory of SPH, an accurate implementation of boundary conditions in SPH remains to be an open question, especially for the no-slip or partial-slip boundary condition for the Navier–Stokes equations [10]. The main challenge is due to the fact that kernels used in SPH interpolation are incomplete near boundaries. A number of methods have been proposed for imposing the no-slip boundary condition for the Navier–Stokes equations. Some of them involve placing mirror or ghost particles across the boundary from the fluid particles [11]. These methods have proved to be accurate but difficult to implement in three-dimensional domains bounded by complex boundaries with sharp corners. Another popular approach is to place one or several layers of stationary particles and let fluid particles interact with those stationary particles through a combination of viscous forces with either repulsive forces [12] or bounced-back reflections [13]. Although the latter approach is easy to implement in three-dimensional domains with arbitrary complex boundaries, it has a lower accuracy than the other methods. However, to the best of our knowledge, no methods currently exist for implementing the partial-slip boundary condition in SPH.

In the present manuscript we aim to develop a new method for solving the Navier–Stokes (NS) equations

\[ \frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v} \]

and

\[ \frac{d\mathbf{v}}{dt} = -\nabla P + \nabla \cdot \mathbf{\tau} + \rho \mathbf{g} \quad \text{in } \Omega, \]

subject to the Robin boundary condition (BC)

\[ \mathbf{\tau} \cdot \mathbf{n} = f \quad \text{on } \Gamma. \]

We assume that the solid boundary \( \Gamma \) is impermeable and set the normal velocity at \( \Gamma \) to zero:

\[ \mathbf{v} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma. \]

Here, \( \rho(\mathbf{x}, t) \) is the fluid density; \( P(\mathbf{x}, t) \) is the pressure; \( \mathbf{v}(\mathbf{x}, t) \) is the fluid velocity; \( \mathbf{g} \) is the gravitational acceleration; \( \mathbf{\tau}(\mathbf{x}, t) = \mu (\nabla \mathbf{v}(\mathbf{x}, t) + (\nabla \mathbf{v}(\mathbf{x}, t))^\top) \) is the deviatoric stress tensor; and \( \mathbf{n}(\mathbf{x}_i) \) denotes the outer unit normal vector on \( \Gamma \).

A special case of the linear Robin BC is the Navier slip boundary condition [14]:

\[ \mathbf{\tau} \cdot \mathbf{n} = \beta \mathbf{v} \quad \text{on } \Gamma. \]

When multiplied by tangent and bi-tangent unit vectors to the boundary, it specifies the slip velocity on the plane tangent to the boundary. For simple fluids and shear rates smaller than \( 10^8 \text{ s}^{-1} \), the Navier boundary condition has been experimentally shown to be accurate [15], while for larger shear rates a non-linear behavior of \( f \) has been observed in molecular dynamics simulations [16]. In Eq. (5), \( \beta \) is the friction coefficient, a property of the fluid-solid interface. The slip length, the outer normal distance from the boundary to where the fluid velocity is extrapolated to become zero, is hence defined by \( \beta \) as \( b = \mu / \beta \). For wetting fluids, \( b \) is on the order of molecular size. For non-wetting fluids, \( b \) can be in the range of 10–15 nanometers [17]. In some complex flows, a relatively large slip length can be due to the presence of a third phase separating fluid and solid. For example, in ice sheet flows subject to a basal sliding on the bedrock, the slip length in the order of 100 meters [18]. The relationship between \( \beta \) and the slip length implies two special cases of the Navier slip boundary condition: 1) \( \beta = 0 \), corresponding to a full-slip boundary; 2) and \( \beta = \infty \), corresponding to a no-slip boundary (i.e., \( \mathbf{v} = 0 \) on \( \Gamma \)).

In this work, we propose a method for implementing the Robin boundary condition in SPH, which we call the continuous boundary force (CBF) method. We demonstrate that the CBF method can be used to model boundary conditions ranging from no slip to full slip. The continuum surface reaction method [19–21] was previously developed for an SPH discretization of the diffusion equation subject to Robin boundary conditions. In the same spirit, the CBF method is formulated to solve the Navier–Stokes equations subject to Robin boundary conditions. In our method, the Robin boundary condition is replaced by a homogeneous Neumann boundary condition and a source term added into the momentum equation. The derivation is based on the approximation of the sharp boundary with a diffuse interface of finite thickness by means of a color function. In this, the CBF method is similar to the continuum surface force (CSF) method introduced by Brackbill et al. [22] where the Young–Laplace boundary condition is replaced with a volumetric force acting on a diffuse interface separating two fluids. In the past, various CSF formulations were implemented in SPH models for multiphase flow with surface tension [23–25]. Another approach, the immersed boundary (IB) method, has been integrated into finite-element and finite-difference methods to investigate flows around no-slip elastic boundaries [26,27]. Like the CSF model, the IB method replaces boundary conditions at the interface with volumetric forces defined in a small volume around the interface. The advantage of the CSF model is that it uses a simple color function to calculate the volumetric forces over the diffuse interface, whereas the IB method relies on the level set function that may be difficult and computationally costly to calculate for complex and dynamically changing boundaries [27].

In the present work, we demonstrate that the SPH discretization of the equations and boundary condition resulting from the CBF method provides a computationally efficient way for modeling flows subject to either no-slip or slip boundary condition. We present the CBF formulation and its SPH implementation along with numerical solutions of the Navier–Stokes...
equations subject to different slip boundary conditions. The test cases include a two-dimensional (2-D) plane shear flow with the Navier slip condition (i.e., Eq. (5)) at the lower boundary, a flow through a periodic lattice of cylinders with the Navier slip condition at the surface of each cylinder, and a 2-D plane shear flow with a space-dependent \( f_R \) at the lower boundary. To demonstrate computational capabilities of the model, the last case is further extended to three spatial dimensions. The space-dependent Robin boundary condition is commonly used in ice sheet models [18,28].

Comparison of the SPH–CBF solutions, obtained with different spatial resolutions, with analytical and grid-based solutions are used to demonstrate the accuracy and convergence of the SPH–CBF method. Finally, we conduct simulations with the slip length \( b \ll 1 \) to approximate the no-slip boundary condition. Good agreement of the SPH–CBF solution with the finite element solution of the Navier–Stokes equation subject to the (exact) no-slip boundary condition demonstrates that the SPH–CBF method with the appropriately chosen slip length accurately simulates no-slip flows.

This paper is organized as follows. Section 2 describes the CBF method. In Section 3 we lay out SPH discretization of the modified Navier–Stokes equations and boundary condition resulting from the CBF method. Numerical results are given in Section 4 and Section 5 summarizes our findings.

2. Continuum boundary force method

Here we consider a physical space \( \Omega = \Omega_F \cup \Omega_S \), where fluid occupies the sub-domain \( \Omega_F \) and \( \Omega_S \) is occupied by a solid phase. The fluid flow is governed by the Navier–Stokes equations (1) and (2), subject to the Robin boundary condition, Eq. (3), on the boundary \( \Gamma \) separating \( \Omega_F \) and \( \Omega_S \). The main idea of the CBF method is to replace the Robin boundary condition with the homogeneous Neumann boundary condition and a corresponding volumetric source term, \( f_\Omega(x,v) \), added into the momentum equation (Eq. (2)).

We first consider a two-sided problem, i.e. the velocity field \( v \) is approximated with \( v' \) defined on \( \Omega \). In the two-sided formulations of the CBF method we approximate Eqs. (1)-(3) as:

\[
\frac{d\rho}{dt} = -\rho \nabla \cdot v',
\]

\[
\rho(x,t) \frac{d\tilde{v}'(x,t)}{dt} = -\nabla P(x,t) + \nabla \cdot \tau(x,t) + \rho(x,t)g - f_\Omega(x,v'), \quad x \in \Omega_F \cup \Omega_S,
\]

\[
[S\tau(x,t)|_{x \in \Gamma_F} - \tau(x,t)|_{x \in \Gamma_S}] \cdot n(x) = 0, \quad x \in \Gamma,
\]

where \( \Gamma_F \) and \( \Gamma_S \) are the fluid and solid sides of \( \Gamma \), respectively. The boundary condition (Eq. (8)) emphasizes that the extended velocity field is continuous across \( \Gamma \). Comparing the weak formulations of Eqs. (2)-(3) with the CBF formulations (Eqs. (7)-(8)), it yields the relation between \( f_\Omega \) and \( f_R \) as:

\[
\int_{\Omega_F \cup \Omega_S} f_\Omega(x,v') \, dx = \int_{\Gamma} f_R(x',v) \, dx'.
\]

Here the weak formulations are derived by integrating the momentum equations over their respected domains and then applying Gauss theorem with the corresponding boundary conditions. To express \( f_\Omega \) as a function of \( f_R \), we define a sharp characteristic function as:

\[
\phi(x) = \begin{cases} \phi_F = 0, & x \in \Omega_F, \\ \phi_S = 1, & x \in \Omega_S, \end{cases}
\]

and its smooth counterpart as:

\[
\tilde{\phi}(x) = \int_{\Omega_F \cup \Omega_S} \phi(x') W(x-x', h) \, dx'.
\]

The normalized kernel function, \( W \), is a positive bell-shaped function with a compact support \( h \) and satisfying the following conditions:

\[
\int_{\Omega_F \cup \Omega_S} W(x-x', h) \, dx' = 1
\]

and

\[
\lim_{h \to 0} W(x-x', h) = \delta(x-x').
\]

From Eq. (11), the gradient of \( \tilde{\phi} \) can be found as:

\[
\nabla \tilde{\phi}(x) = \int_{\Omega_F \cup \Omega_S} \phi(x') \nabla_x W(x-x', h) \, dx'.
\]
Using the definition of the surface delta function [29]:
\[
\delta [n(x_e) \cdot (x_e - x)] = n(x) \cdot \nabla \phi(x), \quad x \in \Omega_F \cup \Omega_S, \quad x_e \in \Gamma,
\]
and noting that
\[
\lim_{h_r \to 0} \phi = \phi,
\]
we express the surface delta function in terms of \( \phi \) as:
\[
\delta [n(x_e) \cdot (x_e - x)] = n(x) \cdot \lim_{h_r \to 0} \nabla \phi(x), \quad x \in \Omega_F \cup \Omega_S, \quad x_e \in \Gamma.
\]
The normal vector within the diffuse interface region can be calculated as:
\[
n(x) = \frac{\nabla \phi(x)}{|\nabla \phi(x)|}, \quad x \in \Omega_F \cup \Omega_S.
\]
The surface delta function is then used to rewrite the surface integral of \( f_r \) as the volume integral
\[
\iint_{\Gamma} f_r(x',v) \, dx' = \iiint_{\Omega_F \cup \Omega_S} f_r(x,v) \delta [n(x_e) \cdot (x_e - x)] \, dx, \quad x_e \in \Gamma,
\]
where \( f_r(x,v) \) is now defined in the domain \( \Omega_F \cup \Omega_S \). Substituting Eq. (17) for the surface delta function gives
\[
\iint_{\Gamma} f_r(x',v) \, dx' = \lim_{h_r \to 0} \iiint_{\Omega_F \cup \Omega_S} f_r(x,v') \, n(x) \cdot \nabla \phi(x) \, dx.
\]
Next, we require \( f_\Omega(x,v') \) to vanish at a normal distance greater than \( h_r \) from \( \Gamma \) and
\[
\lim_{h_r \to 0} f_\Omega(x,v') \, dx = f_r(x_e,v) \delta [n(x_e) \cdot (x_e - x)],
\]
so that \( \lim_{h_r \to 0} v' = v \). Comparing Eqs. (20) and (21) yields the expression for the volumetric term \( f_\Omega(x,v') \) as:
\[
f_\Omega(x,v') = f_r(x,v') n(x) \cdot \nabla \phi(x), \quad x \in \Omega_F \cup \Omega_S.
\]
Combining Eqs. (22) and (14) we rewrite the momentum equation (7) as
\[
\rho(x,t) \frac{d\v(x,t)}{dt} = -\nabla P(x,t) + \nabla \cdot \tau(x,t) + \rho(x,t)g - f_r(x,v') \iiint_{\Omega_F \cup \Omega_S} \n(x) \cdot \left[ \phi(x') \nabla x \cdot W(x - x', h_r) \right] \, dx',
\]
\[
\quad x \in \Omega_F \cup \Omega_S.
\]
To avoid solving the NS equations for \( \v \) on \( \Omega_S \), we introduce a one-sided CBF formulation by approximating Eq. (23) as:
\[
\rho(x,t) \frac{d\v(x,t)}{dt} = -\nabla P(x,t) + \nabla \cdot \tau(x,t) + \rho(x,t)g - f_r(x,v') \iiint_{\Omega_F \cup \Omega_S} \n(x) \cdot \left[ \phi(x') \nabla x \cdot W(x - x', h_r) \right] \, dx',
\]
subject to the homogeneous Neumann boundary condition
\[
\tau(x_e,t) \cdot \n(x_e) = 0, \quad x_e \in \Gamma.
\]
Here
\[
\iiint_{\Omega_F} f_r(x,v') \, \iiint_{\Omega_F \cup \Omega_S} [\n(x) + \n(x')] \cdot \left[ \phi(x') \nabla x \cdot W(x - x', h_r) \right] \, dx' \, dx \approx \iiint_{\Gamma} f_r(x_e,v) \, dx'.
\]
Note that \( \phi \) has a non-zero value only in \( \Omega_S \), which is equal to 1 as defined in Eq. (10). Thus, the momentum equation takes its final form as:
\[
\rho(x,t) \frac{d\v(x,t)}{dt} = -\nabla P(x,t) + \nabla \cdot \tau(x,t) + \rho(x,t)g - f_r(x,v') \iiint_{\Omega_S} [\n(x) + \n(x')] \cdot \nabla x \cdot W(x - x', h_r) \, dx',
\]
\[
\quad x \in \Omega_F.
\]
**Fig. 1.** Comparison of SPH–CBF and FD velocity profiles of the 2-D plane shear flow with $f_r = \beta v$ at $t = 55.3$ s for $\beta = 0.01, 0.1, 1.0, 10.0$, and $dp = 5.0 \times 10^{-4}$ m. Here, $Re = 1$.

**Fig. 2.** The velocity profiles of the 2-D plane shear flow with $f_r = \beta v$ at different times for $\beta = 0.1$ (top), and the calculated relative $L_2$ errors ($|\varepsilon|_2$) (bottom) assuming the FD solution is the “exact” solution.
3. SPH discretization of governing equations

In the following, we present the SPH discretization of Eqs. (1) and (27) subject to the boundary condition (25). To simplify notation, we omit superscript $r$ for the variables in the CBF formulation in subsequent derivations.

In the proposed SPH–CBF method, the domains $\Omega_F$ and $\Omega_S$ are discretized with a set of $N$ points with positions denoted by a vector $\mathbf{r}_i = [r_{i,1}, r_{i,2}, r_{i,3}]^T$ and mass $m_i$ ($i = 1, \ldots, N$). Initially, the points are distributed uniformly (e.g. placed on a regular cubic lattice) and the mass of each particle is calculated as $m_i = V \rho_0^i$, where $V$ is the lattice cell volume and $\rho_0^i$ is the prescribed initial density at $\mathbf{r}_i$. In the absence of molecular diffusion, the mass $m_i$ is conserved over time. The points (which are also referred to as particles) serve as discretization points for solving the Navier–Stokes equations. In the following, we refer to the points within $\Omega_F$ as fluid particles and the points within $\Omega_S$ as solid particles. Positions of fluid particles are evolved over time according to the ODEs:

$$\frac{d\mathbf{r}_i}{dt} = \mathbf{v}_i, \quad \mathbf{r}_i(t = 0) = \mathbf{r}_i^0,$$

(28)

where $\mathbf{r}_i^0$ are the initial positions of the particles, and $\mathbf{v}_i$ denote the velocities of particles governed by the ODEs obtained from an SPH discretization of the momentum equation (Eq. (27)).

The SPH discretization is based on the meshless interpolation scheme:

$$A_i \approx \sum_j m_j \frac{A_j}{\rho_j} W(\mathbf{r}_{ij}, h),$$

(29)
Fig. 4. The velocity profiles of the 2-D plane shear flow with $f_r = \beta v$ at different times for $\beta = 1.0, 5.0, 10.0$ (top), and the calculated relative $L_2$ errors ($||e||_2$) (bottom) given the analytical solution of the no-slip flow as the exact solution. Here, $Re = 100$.

Fig. 5. Single cylinder within a periodic lattice.
Fig. 6. Comparison of SPH–CBF and FEM velocity profiles of flow around a cylinder, along lines 1 (top) and 2 (bottom) for $\beta = 0.0, 0.01, 0.1, 1.0, 10.0$ with a spatial resolution of $dp = 5.0 \times 10^{-4}$ m. Here, $Re = 0.1–0.2$.

where $A_i = A(r_i)$ is a function defined at point $i$, $r_{ij} = r_i - r_j$ and $W$ is a bell-shaped SPH weighting function with at least a first continuous derivative and compact support $kh$ ($W(|r| > kh) = 0$), where the value of $k$ depends on the specific functional form of $W$. The interpolation scheme assumes a summation over all SPH particles, but due to the compact support of $W$ only particles within a distance of $kh$ from $r$ have a non-zero contribution and are actually included in the summation. Spatial derivatives of $A$ can then be calculated as

$$\nabla_i A_i \approx \sum_j m_j \frac{A_j}{\rho_j} \nabla_i W(r_{ij}, h),$$

where $\nabla_i = [\partial / \partial r_{i,1}, \partial / \partial r_{i,2}, \partial / \partial r_{i,3}]^T$.

The SPH approximations of functions and their spatial derivatives allow the mass and momentum conservation equations (1) and (27) to be written as a system of ODEs for the density and velocity of fluid particles [1]:

$$\frac{d\rho_i}{dt} = \rho_i \sum_{j \in \text{fluid+solid}} \frac{m_j}{\rho_j} \nabla_i W(r_{ij}, h),$$

$$\frac{dv_i}{dt} = -\sum_{j \in \text{fluid+solid}} m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W(r_{ij}, h) - \sum_{j \in \text{fluid}} m_j \Pi_{ij} \nabla_i W(r_{ij}, h) + g + \sum_{k \in \text{solid}} F_{ik},$$

where the viscous term $\Pi_{ij}$ is given by [1],
Fig. 7. Comparison of SPH-CBF and FEM velocity profiles of flow around a cylinder along lines 1 (top) and 2 (bottom) at varying spatial resolutions for \( \beta = 0.1 \).

Fig. 8. The calculated relative \( L_2 \) errors (\( ||e||_2 \)) of the velocity profiles along lines 1 and 2 at varying spatial resolutions for \( \beta = 0.1 \), assuming the FEM solution is the “exact” solution.
Fig. 9. The velocity profiles of flow around a cylinder along lines 1 (top) and 2 (bottom) for $\beta = 1.0, 5.0, 10.0$, compared to the FEM solution with the no-slip boundary condition obtained with $dp = 5.0 \times 10^{-4}$ m.

Fig. 10. The calculated relative $L_2$ errors ($\|e\|_2$) of the velocity profiles along lines 1 and 2 for $\beta = 1.0, 5.0, 10.0$, assuming the FEM solution with the no-slip boundary condition is the “exact” solution.
Fig. 11. A snapshot of SPH particles of both fluid and solid (gray) after the flow reaches its steady state for $\beta = 10.0$. Here, the fluid particles are colored by the contour of velocity magnitude.

$$
\Pi_{ij} = -\frac{\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}}{|\mathbf{r}_{ij}|} \frac{2\mu_i \mu_j}{\gamma (\mu_i + \mu_j) h \rho_i \rho_j}.
$$

(33)

Here $\mathbf{g}$ is the body force, $\mathbf{v}_i = \mathbf{v}_i - \mathbf{v}_j$, $\mathbf{v}_i$ is the velocity of particle $i$, $P_i$ is the fluid pressure, and $\mu_i$ is the fluid viscosity. The parameter $\gamma$ is taken to be $15/112$ in two-dimensional problems and $1/8$ in three-dimensional problems [1]. In the present work, we use the quintic Wendland kernel, which has continuous and smooth first and second derivatives. The quintic Wendland kernel is defined as

$$
W(\mathbf{r}, h) = \frac{\alpha_D}{h^D} (1 - 0.5q)^4(2q + 1), \quad 0 \leq q \leq 2,
$$

(34)

where $q = |\mathbf{r}|/h$ and $|\mathbf{r}|$ is the magnitude of the vector $\mathbf{r}$. $D$ is the number of spatial dimensions ($D = 2, 3$) and $\alpha_D$ is a normalization constant ($\alpha_D = 7/4\pi$ for $D = 2$ and $21/16\pi$ for $D = 3$). With this form of $W$, only particles within the $2h$ distance from particle $i$ contribute to the summations in the SPH equations. Following [1], we set $h = 1.5dp$, where $dp$ is the size of the cubic lattice.

The equation of state $P_i = P_0[\rho_i/\rho_0]^7 - 1)$ is used to close the system of Eqs. (31) and (32). In the equation of state, $\rho_0$ is the reference density and $P_0$ is the magnitude of pressure given by $\frac{P_0}{\rho_0} = c^2$. Here, $c$ is the speed of sound of the fluid. This equation of state limits the relative density fluctuation to $V_{max}/c^2 < 1/100$. Under such conditions, a slightly compressible fluid behaves like an incompressible fluid.

The derivations of Eq. (31), as well as the first and second terms on the right-hand side of Eq. (32), representing forces due to pressure gradient and divergence of the viscous stress, have been given in [1]. In Eqs. (31) and (32), $\sum_{j, \text{solid}}$ indicates summation over all neighboring particles of fluid particle $i$, including both fluid and boundary particles. Pressure and density of the boundary particles are assumed to be equal to $P_0$ and $\rho_0$, respectively.

The homogeneous Neumann boundary condition (25) is enforced by including only the fluid particles in the summation, $\sum_{j, \text{fluid}}$, in the viscous force in Eq. (32), as is commonly employed in SPH models for free-surface flow [30].

The last term in Eq. (32) is obtained by discretizing the integral in Eq. (27) as a Riemann sum:

$$
f_r(\mathbf{x}, \mathbf{v}) \frac{|\mathbf{n}|}{\rho(\mathbf{x}, t)} \int_{\Omega_S} [\mathbf{n}(\mathbf{x}) + \mathbf{n}(\mathbf{x}')] \cdot \nabla_{\mathbf{x}} W(\mathbf{x} - \mathbf{x}', h_r) \, dx' = f_r(\mathbf{x}, \mathbf{v}) \frac{|\mathbf{n}|}{\rho(\mathbf{x}, t)} \sum_{k, \text{solid}} \Delta V_k \nabla_{\mathbf{x}} W(\mathbf{x} - \mathbf{r}_k, h_r),
$$

(35)

where $\Delta V_k = \frac{m_k}{\rho_k}$ is the volume of particle $k$ and $\sum_{k, \text{solid}}$ is the summation over solid particles. Estimating this integral at $\mathbf{x} = \mathbf{r}_i$ yields the expression for $f_{ik}^s$:

$$
f_{ik}^s = f_r(\mathbf{r}_i, \mathbf{v}_i) \frac{m_k}{\rho_i \rho_k} (\mathbf{n}_i + \mathbf{n}_k) \cdot \nabla_{\mathbf{x}} W(\mathbf{r}_{ik}, h_r).
$$

(36)

The normal $\mathbf{n}_i$ is calculated from Eq. (18), in which $\nabla \phi$ can be found from the discrete form of Eq. (11), i.e., $\nabla \phi_i = \sum_{j, \text{fluid-solid}} m_j \frac{m_j}{\rho_j} \nabla_{\mathbf{x}} W(\mathbf{r}_{ij}, h_r)$, but this expression does not exactly vanish away from the boundary where $\phi$ is a constant. An alternative SPH discretization of $\nabla \phi$ can be obtained by using the identity.
Fig. 12. Comparison of SPH–CBF and FEM velocity profiles of flow around the “sun-flower”-shaped boundary along lines 1 (top) and 2 (bottom) for $\beta = 0.0, 1.0, 10.0$ with the spatial resolution $dp = 5.0 \times 10^{-4}$ m. Here, $Re = 0.1–0.2$.

$$\nabla \phi = \frac{1}{\Phi} \left[ \nabla (\Phi \phi) - \phi \nabla \Phi \right],$$

(37)

where $\Phi$ is any differentiable function. The SPH discretization of Eq. (37) with $\Phi = 1$ is

$$\nabla \hat{\phi} = \sum_{j \in \text{fluid+solid}} \frac{m_j}{\rho_j} (\phi_i - \phi_j) \nabla_i W(r_{ij}, h_r),$$

(38)

which vanishes exactly away from the boundary where $\phi$ is a constant. The final expression for calculating the normal unit vector is thus obtained as

$$n_i = \frac{\sum_{j \in \text{fluid+solid}} \frac{m_j}{\rho_j} (\phi_i - \phi_j) \nabla_i W(r_{ij}, h_r)}{|\sum_{j \in \text{fluid+solid}} \frac{m_j}{\rho_j} (\phi_i - \phi_j) \nabla_i W(r_{ij}, h_r)|}.$$  

(39)

In the simulations presented below we set $h_r = h$, but in general they can be different.

To integrate the SPH equations explicitly in time we use the second-order leapfrog algorithm [3]. The time step satisfies constraints common to other explicit SPH schemes including the Courant–Friedrichs–Lewy (CFL) condition [11],

$$\Delta t \leq \frac{c}{\epsilon},$$

(40)

and the viscosity condition [1,31].
Fig. 13. The 2-D contour plots of velocity profile $v_x$ of the 2-D plane shear flow with $f_G = \beta [1 + \sin(\omega x)]v$ at different times for $\beta = 0.1$, calculated by both SPH–CBF and FEM at $dp = 5.0 \times 10^{-4}$ m. Here, $Re = 1$.

The Robin boundary condition imposes an additional constraint as:

$$\Delta t \leq \varepsilon \min_{ij} \frac{h^2 (\rho_i + \rho_j)(\mu_i + \mu_j)}{4\mu_i \mu_j}. \quad (41)$$

The Robin boundary condition imposes an additional constraint as:

$$\Delta t \leq \varepsilon \min_{ij} \frac{h(\rho_i + \rho_j)}{2\beta}. \quad (42)$$

Here, $\varepsilon$ is a constant smaller than one. In this work, we use $\varepsilon = 0.1$.

4. Method verification for various slip boundary conditions

To illustrate the numerical accuracy of the proposed SPH–CBF method, the Navier–Stokes equations are solved in two and three spatial dimensions subject to different slip boundary conditions. The resulting velocity fields are compared with those obtained from finite difference (FD) or finite element method (FEM). In all cases, the fluid is assumed to be water with density $\rho = 1000$ kg/m$^3$ and viscosity $\mu = 1 \times 10^{-3}$ Pas. The simulation domain is set to be $0.1 \times 0.1$ m in the two-dimensional cases, and $0.1 \times 0.1 \times 0.1$ m in the three-dimensional case. Reynolds number in the considered problems ranges from 0.1 to 100. The fluid/solid boundaries are assumed to be impermeable, i.e. $v \cdot n = 0$ on $\Gamma$.

4.1. Two-dimensional plane shear flow with $f_G = \beta v$

First, we consider a two-dimensional flow bounded by impermeable plates at the top ($y = H = 0.1$ m) and the bottom ($y = 0$). The Navier–Stokes equations are solved subject to the following boundary conditions:

$$\begin{align*}
\tau \cdot n &= \beta v \quad \text{at} \quad y = 0, \ 0 \leq x \leq H, \ t > 0, \\
\tau \cdot n &= 0 \quad \text{at} \quad y = H, \ 0 \leq x \leq H, \ t > 0,
\end{align*} \quad (43)$$

and the periodic boundary conditions at the rest of the boundaries. The initial condition is

$$v = v_0 e_x \quad \text{at} \quad 0 \leq x, \ y \leq H, \ t = 0, \quad (44)$$

where $e_x = [1, 0]^T$ is the unit coordinate vector. In the simulations, we set $v_0 = 10^{-5}$ m/s and $\beta$ varying from 0.01 to 10.0 to cover a wide range of slip lengths. The resulting Reynolds number, $Re = \frac{\Delta v H}{\mu} = 1.0$. The velocity profiles at time $t = 55.3$ s, obtained from both the SPH–CBF method and FD, are plotted in Fig. 1. The SPH and FD solutions are obtained with the same resolution ($dp$), i.e. the size of lattice on which the SPH particles are initially placed is equal to the grid size of the FD solution. A good agreement between the SPH and FD solutions is observed for the entire studied range of the parameter $\beta$. To further demonstrate the accuracy of the SPH–CBF method, a convergence study is performed. Fig. 2
The velocity profiles of the 2-D plane shear flow with $f_{\Gamma} = \beta [1 + \sin(\omega x)]v$ along lines 1 ($x = 0.025$ m) and 2 ($x = 0.075$ m) at different times for $\beta = 0.1$, extracted from Fig. 13. shows the velocity profiles at different times (i.e., $t_1 = 55.3$ s, $t_2 = 276.6$ s, $t_3 = 548.4$ s and $t_4 = 1082.8$ s, respectively) for $\beta = 0.1$ with the spatial resolution $dp$ ranging from $5 \times 10^{-4}$ m to $2 \times 10^{-3}$ m. The velocity profiles are compared with the converged FD solution at $dp = 5 \times 10^{-4}$ m, which is assumed to be the "exact" solution. It can be seen that the SPH–CBF solution converges to the exact solution as the resolution of the SPH–CBF increases. Fig. 2 also shows that the relative $L_2$ error decreases, even though the rate of convergence decreases over time.

The slip length is proportional to the reciprocal of $\beta$, and thus, the slip boundary condition (Eq. (43)) with sufficiently large $\beta$ can be used to approximate the no-slip boundary condition (zero slip length). Fig. 3 compares the SPH–CBF velocities obtained for $\beta = 1, 5,$ and $10$ at $Re = 1$ to the analytically calculated velocities subject to the no-slip boundary condition (i.e., $v = 0$ at $y = 0$). Fig. 3 shows that with increasing $\beta$ the velocity profiles approach that of the no-slip flow. When $\beta = 10$, the relative $L_2$ error between the SPH solution and the analytical no-slip solution is on the order of $10^{-3}$–$10^{-2}$. Similar results are obtained for $Re = 100$, as illustrated in Fig. 4. Given that the no-slip condition is difficult to directly impose in SPH, the SPH–CBF method presents an attractive alternative for solving Navier–Stokes equations subject to the no-slip boundary condition.

### 4.2. Two-dimensional flow around a cylinder with $f_{\Gamma} = \beta v$

Next, the Navier–Stokes equations are solved in the domain with a curved boundary. Specifically, a flow through a square lattice of fixed cylinders is examined. The periodic unit cell composing this domain is sketched in Fig. 5. Here, the cylinder with radius $a = 0.02$ m is centered in a square box with size $L = 0.1$ m. The flow is driven by a body force ($g = 1.5 \times 10^{-9} \text{m}^2\text{s}^{-2}\text{e}_x$), and the periodic boundary conditions are applied at the box boundaries to model an infinite periodic array of cylinders. The Robin boundary condition is assumed at the impermeable surface of the cylinder as:
Fig. 15. The velocity profiles of the 2-D plane shear flow with \( f_\Gamma = \beta(1 + \sin(\omega x)) \) along line 1 (\( x = 0.025 \) m) at varying spatial resolutions and different times for \( \beta = 0.1 \) compared to the FEM solution (top), and the calculated relative \( L_2 \) errors (\( \|e\|_2 \)) (bottom).

\[
\tau \cdot n = \beta \nu \quad \text{at} \quad \sqrt{x^2 + y^2} = a, \quad t > 0,
\]  

(45)

where the unit normal vector \( n \) is pointing to the center of the cylinder. The initial flow velocity is set to zero.

The velocity profiles along lines 1 and 2 shown in Fig. 5, are extracted and examined after the flow reaches its steady state. The resulting Reynolds number, defined as \( Re = \frac{\rho \bar{v} x a}{\mu} \), is in the range of 0.1–0.2, where \( \bar{v}_x \) is the average flow velocity.

The numerical accuracy of the SPH–CBF solutions is evaluated through a comparison with FEM solutions. Fig. 6 shows that the SPH–CBF velocity profiles are in close agreement with the FEM solutions for \( \beta \) ranging from 0 to 10. A convergence study is further performed for \( \beta = 0.1 \), as depicted in Fig. 7. The FEM solution obtained with \( dp = 5 \times 10^{-4} \) m is assumed to be the “exact” solution. It can be seen that the SPH–CBF velocity profiles converge to the FEM solution as \( dp \) decreases (i.e., the resolution of the SPH–CBF solutions increases) from \( 2 \times 10^{-3} \) m to \( 5 \times 10^{-4} \) m, which is also demonstrated by the decreasing relative \( L_2 \) errors plotted in Fig. 8.

Furthermore, we compare the SPH–CBF solutions with increasingly large \( \beta \) and the FEM solution of the NS equations subject to the no-slip boundary condition at the surface of cylinder. Fig. 9 shows that, as \( \beta \) increases, the SPH–CBF velocity profiles approach that of the no-slip flow. The \( L_2 \) relative difference between the SPH–CBF solutions and the FEM solution of the NS equations subject to no-slip BC decreases with increasing \( \beta \) and becomes approximately 0.02 for \( \beta = 10 \), as depicted in Fig. 10. These results show that solving the NS equations subject to the Robin boundary condition with a sufficiently large \( \beta \) coefficient provides a good approximation for flow with the no-slip BC.

Next, we simulate flow in a domain with a complex boundary. Specifically, we model the flow around the boundary with the “sun-flower” shape as shown in Fig. 11. The size of the computational domain, body force, and initial and boundary conditions in this case study are the same as in the case considered previously in this section. The solutions are obtained for \( \beta \) varying from 0 to 10.0. Fig. 11 shows the positions of all particles and velocities of fluid particles obtained from the simulation for \( \beta = 10.0 \) after the flow reached its steady state. It can be seen that the particles near the boundary are
regularly distributed and the velocity field is noise-free. The profiles of \( V_x \) along lines 1 \((x = 0.05 \text{ m})\) and 2 \((x = 0.1 \text{ m})\) are shown in Fig. 12 after the flow reached its steady state. The numerical accuracy of the SPH–CBF solutions is evaluated via comparison with the FEM solutions. Fig. 12 shows that the SPH–CBF velocity profiles are in close agreement with those obtained from the FEM solutions for \( \beta \) ranging from 0 to 10.0. Therefore, we demonstrate the capability of the SPH–CBF method for modeling flows with different slip lengths from no slip to full slip in such a complex geometry.

4.3. Two-dimensional plane shear flow with \( f = \beta (1 + \sin(\omega x))v \)

Here, we consider a 2-D plane shear flow subject the Robin boundary condition with the space dependent slip length:

\[
\mathbf{r} \cdot \mathbf{n} = \beta \left[ 1 + \sin(\omega x) \right] v \quad \text{at} \quad y = 0, \ 0 \leq x \leq H, \ t > 0,
\]

where \( \omega = 2\pi / H \) and \( \beta = 0.1 \). This boundary condition is commonly used to verify ice sheet numerical models [18]. The rest of the boundary conditions and the initial condition are assumed to be the same as in Section 4.1. The NS equations are solved using both SPH–CBF method and FEM with the spatial resolution \( dp = 5.0 \times 10^{-4} \text{ m} \), and the results are compared at different times. Fig. 13 shows the 2-D contour plots of \( V_x \), and Fig. 14 depicts the velocity profiles along two cross-lines: line 1 at \( x = 0.025 \text{ m} \); and line 2 at \( x = 0.075 \text{ m} \). As in the previous examples, we can see a good agreement between the SPH–CBF and FEM solutions.

The convergence study of the SPH–CBF solutions is performed by repeating simulations with \( dp \) ranging from \( 5 \times 10^{-4} \text{ m} \) to \( 2 \times 10^{-3} \text{ m} \) and comparing to the FEM solution obtained with \( dp = 5 \times 10^{-4} \text{ m} \). The resolution of the FEM solution corresponds to the finest resolution considered in the SPH–CBF solutions, and the converged FEM solution at this resolution is assumed to be “exact”. The results of convergence study (the velocity profiles found with different \( dp \) and the corresponding
Fig. 17. The contour plots of velocity profile $v_x$ of the 3-D plane shear flow with $f_R = \beta[1 + \sin(\omega x) \sin(\omega z)]v$ at $t = 55.3$ s and $dp = 1.0 \times 10^{-3}$ m for $\beta = 0.1$, compared to the FEM solution. Here, $Re = 1$.

$L_2$ errors) are plotted in Fig. 15 for line 1 and Fig. 16 for line 2, respectively. We can see that the SPH–CBF velocity profiles converge to those of FEM and the relative $L_2$ error is decreasing with decreasing $dp$.

4.4. Three-dimensional plane shear flow with $f_R = \beta[1 + \sin(\omega x) \sin(\omega z)]v$

Finally, we consider a 3-D flow bounded by impermeable planes at the top ($y = H = 0.1$ m) and the bottom ($y = 0$). In this case, the NS equations are solved in a cubic domain $\Omega = [0, H] \times [0, H] \times [0, H]$, subject to the boundary conditions:

$$
\begin{align*}
\mathbf{r} \cdot \mathbf{n} &= \beta[1 + \sin(\omega x) \sin(\omega z)]v \\
&= \begin{cases} \\
\mathbf{r} \cdot \mathbf{n} = \beta[1 + \sin(\omega x) \sin(\omega z)]v & \text{at } y = 0, \ 0 \leq x, z \leq H, \ t > 0, \\
\mathbf{r} \cdot \mathbf{n} = 0 & \text{at } y = H, \ 0 \leq x, z \leq H, \ t > 0, 
\end{cases}
\end{align*}
$$

(47)

and the periodic boundary conditions at the rest of the boundaries. The initial condition is:

$$
\mathbf{v} = v_0^0 \mathbf{e}_x, \quad \mathbf{x} \in \Omega, \ t = 0,
$$

(48)

where $\mathbf{e}_x = [1, 0, 0]^T$ is the unit coordinate vector. Here, we set $v_0^0 = 10^{-5}$ m/s, $\beta = 0.1$, and $dp = 1.0 \times 10^{-3}$ m. The comparison of velocity profiles at $t = 55.3$ s, found from the SPH–CBF and FEM methods, is given in Fig. 17. Specifically, this figure shows slices of the contour of $v_x$ (right) and projection of the contour to the $x$–$z$ plane (left). A good agreement is observed between the two methods. Due to the high computational cost of the three-dimensional solution ($10^6$ particles and grid points have been used in the SPH–CBF and FEM solutions, respectively), the convergence study for this case is omitted.

5. Conclusion

The continuum boundary force method has been presented for solving the Navier–Stokes equations subject to a Robin boundary condition. In the CBF method, a Robin BC is replaced with the homogeneous Neumann BC and a force term is added into the NS equations. The CBF formulation has several advantages for solving the NS equations subject to a Robin BC with numerical methods such as smoothed particle hydrodynamics. In SPH, the homogeneous Neumann BC can be implemented very easily, and discretization of the added force term does not present a significant challenge. Conversely, a direct implementation of a Robin BC can be very challenging. In fact, no fully satisfactory implementations of the no-slip BC (taken as a special case of the slip BC) in SPH currently exist.
We used the SPH method to numerically solve the CBF formulation of the NS equations in two and three spatial dimensions subject to various forms of the Robin BC prescribing slip velocity at the boundary. The accuracy of the resulting SPH–CBF method was verified via comparison with standard FD or FEM solutions of the NS equations subject to the Robin BC.

We also demonstrated that taking a sufficiently large value of the coefficient $\beta$ in the Robin BC, the SPH–CBF solution approaches the solution of the NS equations subject to the no-slip boundary condition. In such, we demonstrated that the SPH–CBF method is an effective and accurate approach for solving NS equations subject to the both slip and no-slip boundary conditions.

Acknowledgements

The authors gratefully acknowledge the funding support by the Applied Mathematics Program within the U.S. Department of Energy Office of Advanced Scientific Computing Research as part of the Collaboration on Mathematics for Mesoscopic Modeling of Materials (CM4), under award number DE-SC0009247. The Pacific Northwest National Laboratory is operated for the U.S. Department of Energy by Battelle under Contract DE-AC06-76RL01830.

References