ANALYSIS OF BOUNDARY CONDITIONS PROPERTIES IN THE SPH METHOD

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Abstract
This article deals with analysis of boundary conditions for meshfree Smoothed particle hydrodynamics method (SPH). Two variants of boundary condition were analyzed, Dynamic boundary condition (DBC) and Boundary integral (BI), on one simple case. Furthermore we introduce a possible shape of an additional term for BI formulation, which models the tangential interaction of the fluid with boundary. A comparison between BI with additional term and DBC is made using the example of horizontal motion of fluid particle over an infinite wall.

Keywords: SPH, boundary conditions, DBC, BI.

1 Introduction
Smoothed particle hydrodynamics is a relatively new numerical method used for modeling of cases of fluid mechanics and astrophysics. SPH is a meshfree particle method based on Lagrangian description of continuum. This fact makes SPH ideal numerical method for solving problems with free surface, multiphase problems and other problems challenging for mesh based methods. However, as well as other methods, SPH has its problems, formulated and described as so called Grand Challenges of SPH. [1]. The one we address in this work is related to formulation of boundary conditions.

In SPH, there are three common formulations of boundary condition for solid walls. The first one is called Dynamic boundary condition [2] which is widely used approach for all sort of problems, based on several layers of virtual particles, placed beyond boundary. The second one is modification of DBC, called Modified Boundary Condition (MDBC). For MDBC, the particles are ordered in the same way as for DBC, but the difference is in computation of variables on boundary particles which provides some improvement over DBC [3]. The third one is completely different from both previous formulations. It is based on boundary integrals (BI) [4, 5]. We distinguish BI in two forms, purely numerical and semi-analytical form which differs in evaluation of the boundary integral. We will focus on the purely numerical variant. In this work we will focus only on DBC and BI variants. Analysis of particle interactions with DBC was made in [2], we are expanding this work by adding analysis of interaction with BI boundary condition and analysis of a case of horizontal motion of fluid particle above wall.

A serious problem is hidden in BI formulation, its natural form doesn’t allow capturing of tangential interaction between fluid and wall (i.e. boundary layer). Attempts to solve this problem can be found in work [6]. In [6] problem is solved by application of Taylor expansion to SPH approximation of differential operators and further adjustment of the approximation of differential operators. In this article we propose another possible solution of this problem by introducing additional term based on Newton’s law of viscosity.

2 SPH method
SPH is based on convolution integral

\[ f(x) = \int_{\Omega} f(x') \delta(x - x') dx', \]

where \( \delta(x - x') \) is Dirac delta distribution. We can approximate this \( \delta \)-distribution by suitable function which we call weight function. This function has compact support, is normalized, radial and positive and is denoted as \( W(x - x', h) \). The first parameter of \( W \) is distance between two
points and second parameter, $h$, is the smoothing length, responsible for shape of and size of the support of $W$. This gives us approximation of identity 1:

$$f(x) \simeq \langle f(x) \rangle = \int_{\Omega} f(x') W(x - x', h) dx'.$$

The most used kernels are Cubic spline and C2 Wendland kernel. Due to properties of weight function, we can approximate function derivatives as well, transforming the derivative from the function to the weight function using Green-Gauss formula [7]. Basic idea behind SPH is that we discretize continuous domain $\Omega$ by finite number of particles. Every particle represents material particle and bears kinematic and thermodynamic variables. During the particle discretization, the total measure of the domain needs to be preserved and values of the continuous fields are assigned to the particles based on their positions. Every particle has constant mass which together with its density $\rho_i$ gives a volume $V_i = m_i / \rho_i$. Taking this into account, we can rewrite 2 like

$$\langle f(x_i) \rangle_i = \sum_{j=1}^{N} f(x_j) W(x - x_j, h) V_j.$$  \hspace{1cm} (3)

Lets assume that particle is located near the boundary $\partial \Omega$. There are no particles behind the boundary, and thus the support of particle kernel is not filled behind the boundary. We analyze two variants of boundary condition, DBC and BI. DBC formulation of boundary condition solves this problem by defining additional particles (called ghost particles) beyond the boundary. Ghost particles are arranged into an equidistant grid that fill the kernel support for particles near the boundary (Figure 1 left). This particles obey the same equation as standard particle but their positions remain fixed in time. This formulation is quite simple to implement for simpler geometries and moreover robust. Disadvantages are that DBC formulations are difficult to implement for more complex geometry and produce more viscous behaviour [7, 8]. In BI formulation, we determine contribution of part of the kernel support behind wall by using integral identities, together with the solution of the boundary integral at the intersection of the kernel with the boundary of the domain. The boundary is discretized using only one layer of boundary particles (Fig. 1 right). BI formulation of boundary condition is simple to implement even for complex geometry but the main disadvantage is that it cannot simulate tangential interaction of fluid with wall by definition [7]. Moreover, BI conditions are not suitable for stationary cases [8].

![Figure 1: Realization of boundary conditions using additional particles located beyond the boundary (left) and using a single layer of particles, usually supplemented by a renormalization procedure (right). Initial distance between particles is marked $d_p$.](image)

3 System of equations and its SPH discretization

In this article we will work with weakly compressible model of Newtonian fluid closed by Cole equation of state [9]. This model is described by following set of equations

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v},$$  \hspace{1cm} (4)

$$\frac{D\mathbf{x}}{Dt} = \mathbf{v}.$$  \hspace{1cm} (5)
\[
\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho} \nabla p + \nu \Delta \mathbf{v} + \mathbf{f},
\]
where \(D/\!\!Dt\) denotes material derivative, \(\rho\), \(\mathbf{v}\), \(t\) and \(\mathbf{x}\) represent the density of material particle, velocity, time and position of material particle respectively. Further we have \(p\), \(\nu\), \(\mathbf{f}\), \(c\), \(\rho_0\) and \(p_0\) which represent the pressure, kinematic viscosity, external forces, numerical speed of sound, referential density of the fluid and background pressure respectively [7].

### 3.1 SPH discretization

The previous system of equations together with DBC variant for boundary conditions is discretized as follows [2]

\[
\rho_i = \sum_{j \in F \cup B} m_j W_{ij}, \quad i \in F,
\]
\[
\rho_i = \sum_{j \in F} m_j W_{ij} + m_i W_{ii}, \quad i \in B,
\]
\[
\frac{D\mathbf{x}_i}{Dt} = \mathbf{v}_i,
\]
\[
\frac{D\mathbf{v}_i}{Dt} = -\sum_{F,j \in B} \left( \frac{\rho_i}{\rho_j} + \frac{\rho_j}{\rho_i} + \Pi_{ij} \right) \nabla_j W_{ij} m_j + f_i,
\]
\[
\Pi_{ij} = \begin{cases} 
-\alpha c_{ij} \mu_{ij} + \beta \mu_{ij}^2, & \mathbf{v}_i \cdot \mathbf{x}_j < 0, \\
0, & \mathbf{v}_i \cdot \mathbf{x}_j > 0 
\end{cases},
\]
\[
\mu_{ij} = \frac{h \mathbf{v}_i \cdot \mathbf{x}_j}{|\mathbf{x}_j|^2 + \epsilon h^2}
\]
\[
p_i = c_h^2 (\rho_i - \rho_0),
\]
where \(\mathbf{v}_i = \mathbf{v}_i - \mathbf{v}_j\), \(\mathbf{x}_i = \mathbf{x}_i - \mathbf{x}_j\), \(W_{ij} = W(\mathbf{x}_i - \mathbf{x}_j, h)\), \(\bar{\rho}_i = 0.5(\rho_i + \rho_j)\), \(c_{ij} = 0.5(c_i + c_j)\) and \(m_j\) is weight which is constant for each particle. \(F\) is used to denote set of fluid particle and \(B\) mean set of boundary particle. For BI formulation, previous system of equations is discretized as follows [7]

\[
\rho_i = \sum_{j \in F \cup B} m_j W_{ij}, \quad i \in F,
\]
\[
\frac{D\mathbf{x}_i}{Dt} = \mathbf{v}_i,
\]
\[
\frac{D\mathbf{v}_i}{Dt} = -\frac{1}{\gamma_i} \left( \sum_{j \in F} (\Lambda_{ij} + \Pi_{ij}) \nabla_j W_{ij} m_j + \sum_{k \in B} \rho_k (\Lambda_{ik} + \Pi_{ik}) n_k W_{ik} s_k \right) - \mathbf{f}_i,
\]
\[
\Lambda_{ij} = \frac{\rho_i}{\rho_j^2} + \frac{\rho_j}{\rho_i^2},
\]
\[
p_i = c_h^2 (\rho_i - \rho_0),
\]
\[
\gamma_i = \begin{cases} 
\frac{1}{2} \left( \frac{|\mathbf{x}_j - \mathbf{n}_k|}{kh} + 1 \right), & |\mathbf{x}_i \cdot \mathbf{n}_k| \leq \kappa h, \\
1, & |\mathbf{x}_i \cdot \mathbf{n}_k| > \kappa h 
\end{cases},
\]
\[
f(x_k) = \frac{\sum_{j \in F} f_j W(\mathbf{x}_k - \mathbf{x}_j)}{\sum_{j \in F} W(\mathbf{x}_k - \mathbf{x}_j)}
\]
where \(\gamma_i\) is called Shephard renormalization factor and \(\mathbf{n}_k = (n_{x_k}; n_{y_k})\) is outer normal vector of boundary on \(k\)-th boundary particle. The constant \(\kappa\) denotes the size of kernel support with respect to \(h\).
4 Case of horizontal motion of fluid particle above wall

In this section, we will focus on simple model case of horizontal motion of single fluid particle above wall (figure 2). Using this case we will introduce main differences between DBC and BI formulation of boundary conditions and we will demonstrate their properties.

![Diagram of case (left BI, right DBC)]

Interaction between particle of fluid and particles of boundary condition will be examined. We will focus on viscosity of both formulations and interaction in tangential direction. In both cases we assume following settings: smoothing length \( h = 0.5 \text{ m} \), distance between boundary particles \( dp = h / 2.5 \), weight of each particle \( m = 0.1 \text{ kg} \), referential density \( \rho_0 = mW(0,h) \), numerical speed of sound \( c_0 = 30 \text{ m} \cdot \text{s}^{-1} \), external force acceleration \( g = 9.81 \text{ m} \cdot \text{s}^{-2} \) and constant which prevents zero value of denominator \( \epsilon = 0.0001 \). Next, we start with initial position of fluid particle \( x = (0; 5h) \text{ m} \) and initial velocity \( v = (0.7; 0) \text{ m} \cdot \text{s}^{-1} \). We use Wendland C2 kernel as a smoothing function and for the numerical integration we use Semi-Implicit Euler method.

For DBC formulation, we are using equations 8-13. Numerical solution of this single particle problem can be seen in the figures 3 and 4.

![Graph of dependency of normalized height on time (for DBC)]

Figure 3: Dependency of normalized height of the fluid particle on time for DBC
Variant with Boundary integral is described by equations 14-20. We can notice that in equation 16 for \( x \)-axis, the right hand side is equal to zero, so there is not any interaction between fluid particle and boundary in tangential direction and thus velocity remains unchanged. Numerical solution of BI formulation for the above-mentioned problem is shown in the figure 5. Figure with dependency of tangential velocity on time is therefore unnecessary, since velocity is constant.

The main difference between both formulations is in the interaction in tangential direction as we described above. Another difference occurs in normal direction. We can notice that fluid particle for DBC reaches equilibrium position way faster than for BI formulation. The reason is that DBC is more dissipative (viscous) than BI. This is caused by two things. First, for DBC more boundary particles interact with fluid particle than in BI variant. Second reason is in the formulation itself. For DBC in momentum equation (11), the viscous term is multiplied by weight and corresponding element of gradient of weight function. In BI case, in the momentum equation (16), the viscous term is multiplied by density of boundary particle, length between boundary particle and value of weight function. This sum is then normalized by Shephard renormalization factor. We can analyze value of viscous term of each formulation. First, for DBC we assume density of particle \( \rho = 0.16 \text{ kg/m}^{-3} \), which is the maximum value of density during this computation (so this estimate provides lower bound of resulting viscous behaviour). We can estimate the contribution of one boundary
particle as

\[ m\frac{-2\alpha c_0 \mu_{ij}}{2\rho} \nabla_y W_{ij} \approx 0.1 \frac{-2\alpha c_0 \mu_{ij}}{0.32} \nabla_y W_{ij} \approx 0.3125(-2\alpha c_0 \mu_{ij}) \nabla_y W_{ij}. \]

For BI variant, the density is reduced but we have to take into account Shephard renormalization factor. Fluid particle moves around height of one smoothing length above boundary so we set \( \gamma = 0.75 \). We can estimate the contribution of one boundary particle as

\[ \frac{1}{\gamma_i} \rho \frac{-2\alpha c_0 \mu_{ik}}{2\rho} s_k W_{ik} \approx \frac{1}{0.75} (-2\alpha c_0 \mu_{ik}) \frac{0.5}{2.0} W_{ik} \approx 0.266(-2\alpha c_0 \mu_{ik}) W_{ik}. \]

It is clear that viscous term in DBC variant has stronger effect. We should add that in interval where fluid particle moves (in area of boundary particle effect - (0.75h; 2h)), following inequality holds \( |W_{ij}| < |\nabla W_{ij}| \).

### 4.1 Additional term in BI formulation

The BI formulation is simple to implement, event for complex geometries. However if we want use this formulation for solving viscous problems we have to improve the current BI formulation so it contains tangential interaction with fluid particle. In the following part new additional term will be presented.

We propose additional term based on second Newton’s law of motion and Newton’s law of viscosity. This term approximates the force contribution of the tangential stress in the fluid. Force is determine by tangential stress operating on length of secant line between kernel radius and the wall. We define the acceleration term as

\[ \frac{Dv_i}{Dt} = - \sum_{k \in B} \xi_{ik} t_k, \tag{21} \]

where

\[ \xi_{ik} = \begin{cases} \frac{2\mu \sqrt{\kappa h} - (n \cdot x_{ik})^2}{m_i} v_{ik} \cdot t_k, & W(x_i - x_k, h) > 0 \\ \frac{1}{(-n_{ik}) \cdot x_{ik}} \cdot x_{ik}, & W(x_i - x_k, h) = 0, \end{cases} \]

and \( t_k \) is tangential vector of the wall, \( \mu \) is dynamic viscosity and \( \kappa \) is the constant determining the size of the kernel support. If we add this term into equation 16 we get numerical solution of the case described in the figure 2, as it is shown in the figure 6. It is clear that fluid particle slows down when it is in the boundary particle area of effect and eventually stops completely.

**Figure 6: Dependency of tangential velocity of the fluid particle on time for BI with additional term**
Dependency of normalized height above the wall on time for modified BI is almost identical to standard BI in the figure 5 and thus is not shown. In figure 7, we compare evolution of tangential velocity in time for DBC and BI with proposed additional term.

Figure 7: Dependency of difference in tangential velocity of the fluid particles (DBC-BI) on time (red), dependency of tangential velocity of the fluid particle for DBC (blue) and BI (orange) formulation

From the results, it is clear that DBC formulation is still more viscous than modified BI formulation. However, we should note that although the DBC allows us to capture the viscous interaction with the wall, we are not guaranteed that it corresponds to the exact physical behavior. In contrast, our additional term, which is driven by physical background can be appropriately tuned and ensuring proper scaling will be the subject of future work.

5 Conclusion

We compared DBC and BI formulations of boundary condition on simple model case of horizontal motion of single fluid particle above the wall. We observed that DBC are more viscous (more dissipative) than BI variant. It is due to the fact that contribution of single boundary particle to viscous term is greater in DBC variant than in BI. It was explained why BI formulation cannot cover tangential interaction between fluid and wall. We presented possible solution of this problem based on second Newton’s law of motion and Newton’s law of viscosity. Based on these principles, we designed additional term to momentum equation and this term was demonstrated on the same case. Comparison between the DBC and improved BI was made. At first, we compared viscous behaviour of both standard formulations. Then we compared tangential interaction between fluid and boundary particle for standard DBC and modified BI formulations. We observed that BI with additional term is qualitatively similar to DBC but quantitatively different. The next step (prior to further work) should be to compare both variants with the physical behaviour and possibly tune the additional member of the BI formulation to match the physical reality.

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