An Approach to Obtain a Pairwise Potential Function from Numerical Simulations of Two-Fixed Spherical Particles at Low Particle Reynolds Number

Un enfoque para obtener una función potencial por parejas a partir de simulaciones numéricas de dos partículas esféricas fijas bajo el número de Reynolds de partículas bajas

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Abstract

In this paper a method to obtain a pairwise potential energy function from Computational Fluid Dynamic (CFD) simulation of two-fixed spherical particles is presented. A pair potential function is very helpful to evaluate the particle hydrodynamic interactions in two-phase flow systems involving a large number of particles. The hydrodynamic interactive forces play an important role in this type of flows. Using the traditional dynamic particle simulations such as direct numerical simulations (DNS), Two-Fluid Model (TFM) and discrete element (DEM), the analysis of a system of N particles, a great amount of computational work of order $O(N^2)$is required to evaluate all the pairwise particle interactions. The algorithm of the present paper only requires two-fixed spherical particles to find a pair potential that can be used in a stochastic method such as Monte Carlo (MC) or Molecular Dynamic Simulations (MDS), resulting in less computer time requirements, making it considerably more practical for large-scale problems encountered in two-phase flow systems. Thus, when someone is only interested in an equilibrium configuration of a large group of particles in two-phase flow system rather than their time-dependant particle properties, this approach could be a solution.

Key Words

Pairwise potential function, hydrodynamic interactions, two-phase flows, Computational Fluid Dynamics.

Introduction

In this paper a methodology to obtain a pairwise potential energy function $U(r)$ from numerical simulations of two-fixed spherical particles at low particle Reynolds number is presented. The study of physical phenomena by particle interactions is well established in a number of fields and is becoming increasingly important in others. The most classical example is probably magnetic fluids, which are composed of ferromagnetic particles, but much recent work has been done in particle fluid dynamics, and molecular dynamics, Greengard&Rokhlin (1997), Camp, P. J., (2006).

Greengard&Rokhlin (1997) stated that there are two major types of simulation methods. i) Dynamical simulations, which follow the trajectories of N particles over some time of interest and require an amount of work of the order $O(N^2)$. This method is based on the Newton's second law of motion.

Once given the initial positions $\{x_i\}$ and velocities, the trajectory of each particle is governed by

$$(1)\quad m_i \frac{d^2 x_i}{dt^2} = -\nabla_i \Phi \text{ for } i = 1, \ldots, N.$$

where m_i is the mass of the ith particle and the force is obtained from the gradient of a potential function Φ; ii) Stochastic technique, i. e., Monte Carlo Simulations, when one is interested in an equilibrium configuration of a group of particles rather than their time-dependant properties. In this case, a potential function becomes a paramount objective to evaluate the particle final configuration, the potential function can be evaluated for a large number of configurations as

$$(2)\quad U(r) = -\int F(r)dr$$

where $U(r)$ is the potential function, $F(r)$ is the potential force.

This paper is restricted to the case where potential or force is defined as hydrodynamic force interaction for between two-fixed particles a low Reynolds number (Re = 15). More specifically, it is based on the numerical simulations obtained by Vargas (2008), where interactive forces are considered in the form,

$$(3)\quad F_i = \left(F_{2(1)}^{2-b\,x} - F_{1(2)}^{2-b\,x}\right) sin(\grave{e}) + \left(F_{2(1)}^{2-b\,y} - F_{1(2)}^{2-b\,y}\right) Cos(\grave{e})$$

where F_i is the total interacting force, $F_{2(1)}^{2-b\,x}$ is the total drag force in the x-axis over the leading particle, $F_{1(2)}^{2-b\,x}$ stands for the total drag force in the x-axis over the trailing particle, whilst $F_{1(2)}^{2-b\,y}$ and $F_{2(1)}^{2-b\,y}$ represents the total force in the y-axis direction for the leading and trailing particle, respectively. The interaction force (F_i), can be positive if $F_i > 0$ (repulsion) or negative if $F_i < 0$ (attraction).

2. The potential energy function

As mentioned before, one of the most important parts in a stochastic method (MC) is the potential energy function. Thus, once a reliable potential function $U(r)$ is obtained, simulations using a stochastic method are straightforward. After a series of hydrodynamic interaction forces at low particle Reynolds number between two-fixed spherical particles as function of angle (θ) and separation distance (r) obtained by Vargas (2008) an analytic form of the potential energy as function of these two variables, $U(r\,\theta)$ is proposed.

A three-step procedure is used to obtain an analytic fit to the potential energy function. First, the hydrodynamic interaction forces are fitted applying a Legendre polynomial expansion; second, the fitted Legendre expansion coefficients are correlated using a superposition of two Gaussian functions, and third the force field is integrated to obtain the pairwise potential function.

3. Force fitting

Particle interactions in two-phase flows at low particle Reynolds numbers are strongly affected by the hydrodynamic interaction force between particles, Kim, et ál. (1993), Folkersma, et ál. (2000), Vargas & Easson (2005) and Prahl, et ál. (2007). A as mentioned before a series of hydrodynamic interactive forces were obtained by Equation. 3, Vargas (2008). These data were expanded on the basis set of Legendre polynomials as follows:

$$(4)\quad F_i(r,\theta) = \sum_n C_n(r) P_n(x)$$

Where P_n is the Legendre polynomial of order n, $x = cos\theta$.

By symmetry only the even values of n were used. Very good fits are obtained by including even Legendre polynomials terms up to $n = 6$. Table 1 shows the Legendre polynomials used to correlate the hydrodynamic interactive forces, Weisstein, Eric W (2011). Table 2 shows the values of the six expanded coefficients $C_n(r)$ for dimensionless particle separation, D_o, ranging from 1.1 up to 25 for particle Reynolds number of 15 and particle diameter of 1 x 10^{-4} m.

Table 1. First six even Legendre polynomials function.

N	$C_n(r)P_n(x)$, $x = cos\theta$
0	C_0
2	$C_2\left[\frac{1}{2}\left(3x^2-1\right)\right]$
4	$C_4\left[\frac{1}{8}\left(35x^4-30x^2+3\right)\right]$
6	$C_6\left[\frac{1}{16}\left(231x^6-315x^4+105x^2-5\right)\right]$

Table 2. Expanded coefficients.

D_o	C_o 1x10^{10}	C_2 1x 10^{10}	C_4 1x10^{10}	C_6 1x10^{10}
1.10	65.20	-360.44	3.61	-16.72
1.25	66.45	-357.15	-6.43	-7.11
1.50	57.97	-300.71	-29.58	-16.63
1.75	29.22	-235.79	-61.51	-15.53
2.00	12.82	-184.54	-74.69	-24.31
2.25	3.45	-152.44	-85.57	-27.96
2.50	-1.22	-128.47	-85.90	-39.91
3.00	-6.11	-95.85	-79.28	-55.07
4.00	-4.93	-55.91	-69.31	-64.29
5.00	-7.57	-43.30	-56.81	-66.34
6.00	-5.17	-26.02	-47.00	-63.47
8.00	-6.40	-20.34	-30.59	-55.46
12.00	-2.76	-8.24	-22.85	-42.24
15.00	-2.71	-5.93	-10.88	-27.22
20.00	-1.94	-3.48	-7.24	-22.30
25.00	-1.37	-2.55	-5.17	-15.38

Once $C_n(r)$ is obtained, hydrodynamic interactive forces from equation (4) are computed as function of the particle separation distance (r) and the angle position (θ), this data forces are compared with the hydrodynamic interactive forces obtained from numerical simulations. Figure 1 shows, the Legendre correlations obtained by equation (4), including terms up to n = 6. A very good correlation is observed between numerical simulation (○) and the analytic compute data (—).

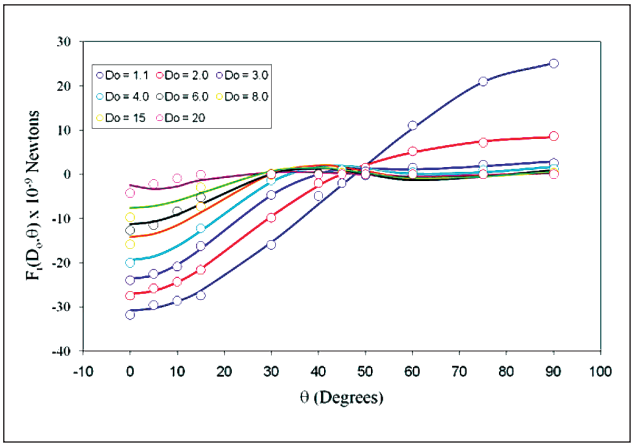

Figure 1. CFD data fit for from $1 < D_o < 20$ (○) and Legendre terms up to n = 6 (—).

The next step is to find an analytic correlation for the Legendre expansion coefficients, $C_n(r)$ from table 2. The variation of the Legendre coefficients as function of the particle separation distance between the particles is found to be very well correlated by a superposition of two Gaussian distribution in the form:

$$(5)\ r) = g_1\, exp\left| -\left(\frac{r-d_p}{h_1}\right)^2 \right| + g_2\, exp\left| -\left(\frac{r-d_p}{h_2}\right)\right.$$

Where $r\left(=D_o d_p\right)$ is the separation distance between the two particles, d_p stands for the particles diameter, g_1, g_2, h_1 and h_2 constants to be determined.

Table 3 shows the values for g_1, g_2, h_1 and h_2. These values are given in units of $1x10^{-9}$ Newtons and the values for h_1 and h_2 are given in terms of particle diameters (d_p = 1 x 10^{-4}m).

Table 3. Values of g_1, g_2, h_1 and h_2 for equation 5.

N	g_1 1 x 10^{-9}	h_1 1 x 10^{-4}	g_2 1 x 10^{-9}	h_2 1 x 10^{-4}
0	7.78144	0.890645	-0.6684	15.3592
2	-24.5916	0.909302	-12.1709	3.92072
4	-8.50118	7.26746	9.18018	0.651117
6	-6.85526	16.6977	5.86892	1.78035

A comparison of the computed values of g_1, g_2, h_1 and h_2 using equation (5) with values from Table 3 is shown in Figure 2, excellent correlation is found. The solid lines represent the values obtained by equation (5) and symbols represent the values from Table 3. The abscissa is on a log-linear scale in order to highlight de points at small distances.

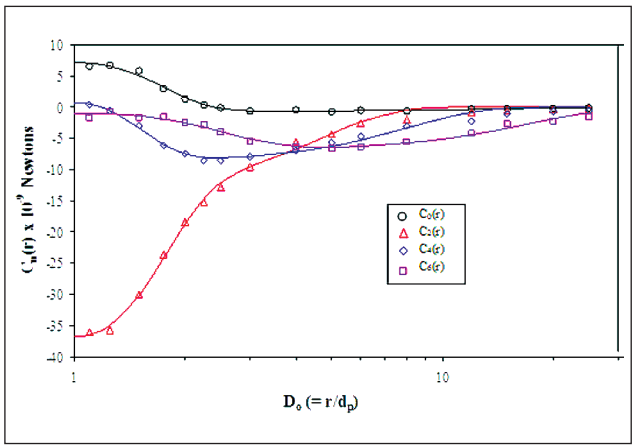

Figure 2. Fit correlations for Legendre expansion coefficients $C_n(r)$.

4. The Pair potential

The final step is to find the pairwise potential energy function. Pairwise potential functions *U(***r***)* as mentioned before are commonly used to study many particle systems applying Monte Carlo method or Molecular Dynamics Simulations. If the interactive force is considered conservative, the pair potential energy *U(***r***)* is straightforwardly obtained from equations (4) and (5) as an expansion of Legendre polynomials as following:

$$(6)\quad U(r,\grave{e}) = \sum_n U_n(r) P_n\left(Cos\grave{e}\right)$$

where

$$(7)\quad U_n(r) = \int_r^{\infty} C_n(\tau)\, d\tau = \frac{\pi}{2} \cdot \left[g_1 h_1 erfc\left(\frac{r-d_p}{h_1}\right) + g_2 h_2 erfc\left(\frac{r-d_p}{h_2}\right)\right]$$

Where τ is only a variable change equal to *r*.

Given the forces from equations (4) and (5), the coefficients $U_n(r)$ are obtained. Figure 6 shows the four Legendre polynomial expansion coefficients as functions of the non-dimensional particle separation.

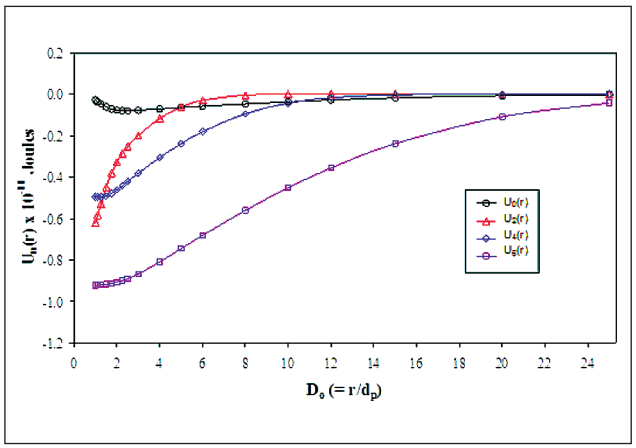

Figure 6. Legendre polynomial expansion coefficients $U_n(r)$

By using equations (6) and (7) the pair potential energy can be calculated as a function of the particles' separation at different angle positions. Figure 7 shows the pair potential energy for several angles as function of the particle separation distance. From Figure 7 is observed that the minimum potential energy ($U_{min} = -2.0\ x10^{-1}$ *Joules*) is found for θ = 0° at the minimum separation distance, $D_o = 1$.

Figure 7. Pair potential energy as function of the separation distance.

Conclusions

A three-step approach was applied to obtained a pairwise potential energy function from hydrodynamic interactive forces of CFD simulations from two-fixed spherical particles at low particle Reynolds number (Re_p = 15). The angular part of the hydrodynamic interactive forces was described by a series of Legendre polynomials, very good fits are obtained by including Legendre polynomials even terms up to

n = 6. The radial dependence of the potentials was fitted, $C_n(r)$, by a superposition of two Gaussian distributions. And the pairwise potential energy function, $U(r)$ was obtained by integration of the forces as an expansion of Legendre polynomials as $U(r,\theta) = \sum_n U_n(r) P_n(\cos\grave{e})$.

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