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Bounding Grid Algorithm for Calculating Particle Interactions in SPH Simulations

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Abstract

A simple and easy algorithm is presented for a fast calculation of kernel evaluations which required in simulations using the Smoothed Particle Hydrodynamic (SPH) method. For a system with N particles, traditional method requires an amount of work of O(N×N) to calculate the interaction of each particle with every other particle in the system.

The algorithm described here has the amount of work to evaluate particle interactions more less the same with previous works such as sorting, linked-list, vectorized linked-list methods which can reduce the amount of work as low as O(N). The additional time required is to register all the particles inside the predefined grids and their wider bounding grids to account particles at the utmost boundary of the grids for calculation of kernel evaluations. Registration of particles to their grids and bounding grids is conducted after each time step calculation finished. Therefore, the kernel evaluations of each particle in a grid to search for its interaction particle is only necessary sought within the bounding grid. Thus, this effort results in less amount of works compared to the traditional SPH method.

Some benchmarks examples are used to show the time saved by using the present algorithm. The algorithm is easy to be implemented. Parameters study on the number of divisions for grids and amount of particles are also given to show the effectiveness of the present algorithm.

Keywords: SPH; Particle Method; Simulation; Bounding Grid.

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1. INTRODUCTION

Smoothed Particle Hydrodynamic (SPH) method which was firstly introduced (Lucy 1977; Gingold and Monaghan 1977) for modeling astrophysical phenomena is one amongst many particle methods which has been used for simulating the physical behavior of fluid and continuum solid bodies. In the SPH method, the so-called smoothing function or kernel function which is based on particle approximation plays a very important role in carrying out the integration of governing partial differential equations in the supporting domain.

One of the important issues for implementing the SPH method using the particle approximation is how to effectively perform the evaluation of functions based on a set of nodes scattered in an arbitrary manner. A lot of works have been done to improve the kernel functions as summarized in reference (Liu and Liu 2007), however less efforts have been done in the method to carry out the interaction among particles in the supporting domain. A simple and easy algorithm based on fixed and its bounding grids is presented for a fast calculation of kernel evaluations which required in simulations using the SPH method.

2. SPH FORMULATION FOR NAVIER-STOKES EQUATIONS

SPH can be considered as an interpolation method for interactions of arbitrary particles in a support domain (Monaghan 1982). In present study, SPH method is used for solving the Navier-Stokes equations problems. Figure 1 shows a typical kernel function *W*. The kernel function used in this study is taken from the cubic spline family which is known as B-spline function as given below (Monaghan and Lattanzio 1985).

$$W(R,h)=\alpha_d \times \begin{cases} \dfrac{2}{3}-R^2+\dfrac{1}{2}R^3 & 0 \le R < 1 \\ \dfrac{1}{6}(2-R)^3 & 1 \le R < 2 \\ 0 & R \ge 2 \end{cases} \tag{1}$$

here, $R=\dfrac{r}{}$, where *r* is the distance between two nodes and $\alpha_d = 1/h$, $\alpha_d = 15/7\pi h^2$, $\alpha_d = 3/2\pi h^3 h$ for one-, two- and three-dimensional space respectively. The parameter *h* is smoothing length defining the influence area of the function *W*.

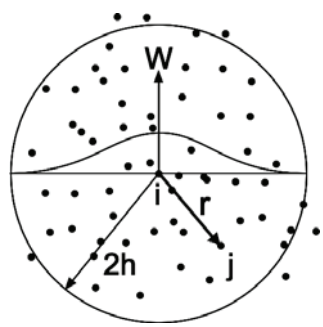

Figure 1: Support domain of the kernel function *W* of particle *i*.

For the conservation of mass governing equation, the particle approximation of density is given as

$$\frac{D\rho_i}{Dt} = \sum_{j=1}^{N} m_j \, v_{ij}^{\beta} \, \frac{\partial W_{ij}}{\partial x_i^{\beta}} \tag{2}$$

where ρ_i is the density of particle i, m_j is the mass of particle j, $v_{ij}^{\beta} = v_i^{\beta} - v_j^{\beta}$ is the relative velocity between particles i and j.

For the conservation of momentum and energy, the particle approximation of momentum and energy governing equations taking into account artificial viscosity are given as

$$\frac{Dv_i^{\alpha}}{Dt} = -\sum_{j=1}^{N} m_j \left(\frac{\sigma_i^{\alpha\beta}}{\rho_i^2} + \frac{\sigma_j^{\alpha\beta}}{\rho_j^2} + \prod_{ij} \right) \frac{\partial W_{ij}}{\partial x_i^{\beta}} \tag{3}$$

$$\frac{De_i}{Dt} = \frac{1}{2} \sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \prod_{ij} \right) v_{ij}^{\beta} \frac{\partial W_{ij}}{\partial x_i^{\beta}} + \frac{\mu_i}{2\rho_i} \varepsilon_i^{\alpha\beta} \varepsilon_i^{\alpha\beta} \tag{4}$$

where, σ_i , σ_j are the stresses for particles i, j, P_i , P_j are the pressures at particles i, j, ε_i is the viscous strain rate for particle i, μ_i is the dynamic viscosity for particle i, and the artificial viscosity $\prod_{ij}$ (Lattanzio et al. 1986; Monaghan 1989).

There have been many variations of the governing equations developed (Liu and Liu 2007). Regardless of the governing equations being used, finding an effective procedure for evaluating the kernel function is the main objective of the present study.

3. BOUNDING GRID ALGORITHM

The algorithm described here has the amount of work to evaluate particle interactions more less the same with previous works such as sorting, tree search algorithm, linked-list and vectorized linked-list methods (Liu and Liu 2007) which can reduce the amount of work as low as in order of O(N).

The present proposed method improved the Pairwise Interaction technique (Hockney and Eastwood 1988; Hernquist and Katz 1989; Riffert et al. 1995) which is mostly used to reduce the computational effort in the SPH simulations. The Pairwise Interaction technique is carried out with the process of nearest neighboring particle searching and stores necessary data for the SPH summation process. By dividing the whole region of simulation into smaller regions using vertical and horizontal grids, time required for storing particle data become longer but time required for searching the neighboring particle is limited inside the smaller region from which as a result total reduction in time can be achieved.

Figure 2 shows the schematic representation of bounding grid method. The whole simulation domain is first divided by horizontal and vertical grids into rectangles. Each rectangle is then used for registering all particles inside the area after each time step calculation. At the same time, a wider area bounding the inner rectangle is also used for registration. The width of the outer rectangle is determined from the size of the inner rectangle added by the radius of support domain of kernel function W at both width and height sides.

In evaluating equations from (1) to (4), the summations of governing equations are accounted for each of N_{in} particles which were registered in the inner rectangle using the index i. The searching domain for each particle i is sought within N_{out} particles with index j which are registered in the outer rectangle.

Here, for each particle inside the inner rectangle that is i indexed acts as a center for evaluating the governing equations to interact with the surrounding particles inside the outer rectangle those are j

indexed. Hence, the searching for interacting particle will only be required inside the outer rectangle which is requiring much less time rather than searching for a particle in the whole domain of simulation. The reduction of computation time of the present method depends on the number of grids, particles, and smoothing length.

The additional time required in the present method is to register all the particles inside the predefined grids and their wider bounding grids to account particles at the utmost boundary of the grids for calculation of kernel functions. Registration of particles to their grids and bounding grids is conducted after each time step calculation finished. In the next step of calculation, the kernel evaluations of each particle in a grid to search for its interaction particle is only necessary sought within the defined bounding grid.

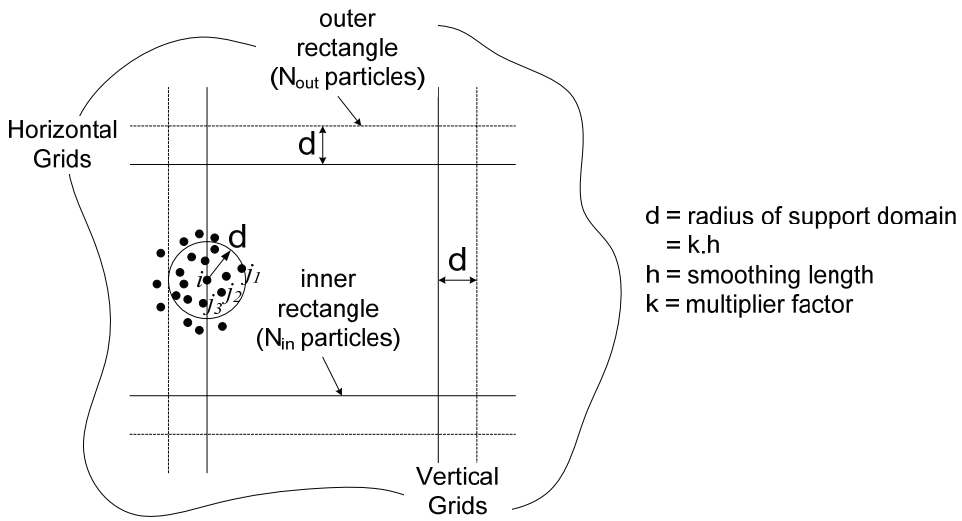

Figure 2: Schematic representation of bounding grid method.

4. EXAMPLES

In the following examples, the timing evaluations were performed on a personal computer with Core2 Duo E7500 CPU, Clock rate of 2.93 Hz, FSB speeds of 1066 MHz and 4 GB Memory of RAM. Fortran compiler was used to edit, modify, compile, debug and run the source codes available from the reference (Liu and Liu 2007).

4.1. Shock tube 1-D problem

The shock tube problem is a good one dimensional benchmark which was comprehensively simulated by many researchers using SPH method (Monaghan et al. 1983; Hernquist et al. 1989). The shock tube is a long straight tube filled with gas, which is separated by a membrane into two equal parts which each part is initially in equilibrium state of constant pressure, density and temperature. When the membrane is taken away suddenly, a shock wave, a rarefaction wave and a contact discontinuity will be produced.

The initial conditions of the simulation are similar with (Hernquist et al. 1989), then introduced by (Monaghan et al. 1983) which were taken from (Sod 1978).

$x \le 0 \quad \rho = 1 \qquad v = 0 \quad e = 2.5 \qquad p = 1 \qquad \Delta x = 0.001875$

$x > 0 \quad \rho = 0.25 \quad v = 0 \quad e = 1.795 \quad p = 0.1795 \quad \Delta x = 0.0075$

where, ρ, p, e and v are the density, pressure, internal energy and velocity of the gas, respectively. Δx is the space between two particles. A constant time step of 0.00015 *sec* is used for 1000 steps calculation. A constant smoothing length of 0.015 is used in the simulation.

Table 1 shows three different number of particles used in the SPH simulation. The parameter study is conducted similar with the reference in which the same percentage distribution of particles in two equal part of the tube was of 80% and 20% for both high density and low density regions. To keep a constant density maintained in the tube, the length of the tube is increased along with the increasing number of particles.

Table 1: Parametric study for shock tube 1-D problem

Case	*Number of Particles*		*Total Length*
	High density	*Low density*	
I	80	20	0.3
II	800	200	3.0
II	8000	2000	30.0

For each case of the three shock tubes shown in Table 1, the total length of the tube is divided by vertical grids which result in 2, 4, 6, 8, 16, 32, 64, 128 and 256 divisions.

Figure 3 shows the scheme of bounding grid method applied to the shock tube problem. Figure 4 depicts the results of timing evaluation of the present proposed method compared to the Pairwise Interaction technique for a variety number of particles and division of vertical grids.

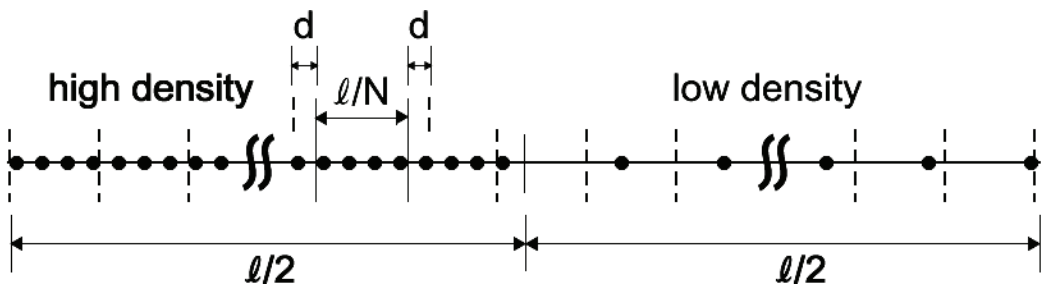

Figure 3: Bounding grids in the shock tube problem.

From the Figure 4, the effectiveness of the present proposed grid bounding method is giving better results for larger number of particles used in the simulation. As shown in the Figure 4, for the number of particle of 100 used, the time for registering the particles became higher than evaluating the kernel functions, thus less effectiveness will be resulted if the number of particle used in the simulation is less. However, the present method shows the good results for larger number of particle used, as shown for the number of particle of 10000 the computation time reduced to less than 10% can be achieved when the divisions of grid from 64 to 128 are used.

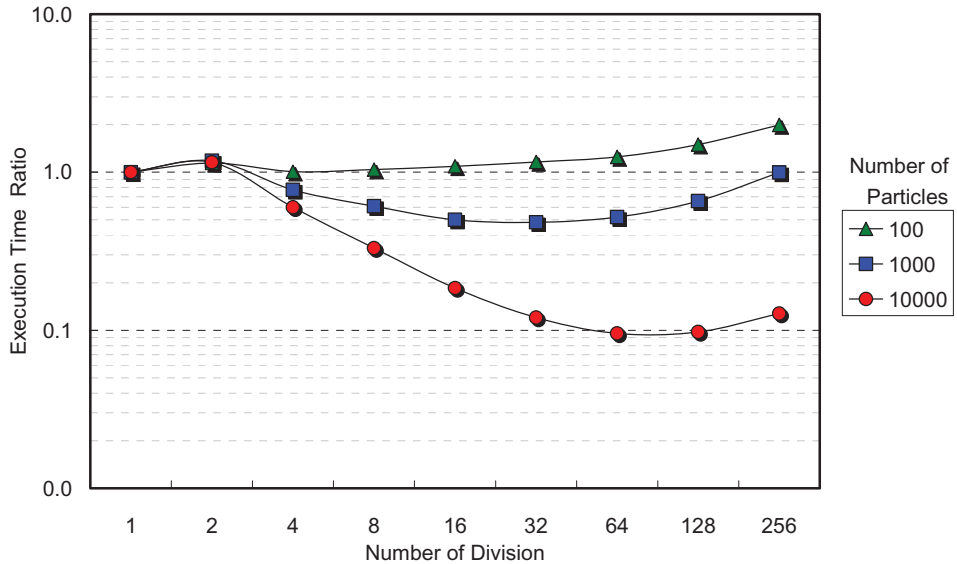

Figure 4: Results of execution time for shock tube problem for different divisions.

4.2. Shear driven cavity 2-D problem

The classic shear driven cavity problem is the fluid flow within a closed square generated by moving the top side of the square at a constant velocity while the other sides remain fixed. The flow will reach a steady state and form a recirculation pattern. In the simulation, the dimension the kinetic viscosity and density are $\nu = 10^{-6}$ m^2/s and $\rho = 10^3$ kg/m^3 respectively. The top side of the square moves at a velocity of $V = 10^{-3}$ m/s, thus the Reynolds number for this case is one. A constant time step of 5×10^{-5} s is used. A constant smoothing length of 2.5×10^{-5} is used.

Table 2 shows four different numbers of particles used in the simulation to show the efficiency of the present proposed method.

Table 2: Parametric study for shear driven cavity 2-D problem

Case	*Number of Particles inside the square*	*Side Length*	*Computation Steps*
I	50×50	0.00125	1,000
II	100×100	0.00250	1,000
II	200×200	0.00500	1,000
IV	1000×1000	0.02500	10

For each case of the four shear driven cavity problems shown in Table 2, each side of the simulation domain is divided by vertical and horizontal grids of 2, 4, 8, 16, 32, 64 and 128 equal divisions.

Figure 5 shows the scheme how the bounding grid method applied to the shear driven cavity problem. Figure 6 depicts the results of timing evaluation of the present proposed method compared to the Pairwise

Interaction technique for a variety number of particles and equal division of both horizontal and vertical grids.

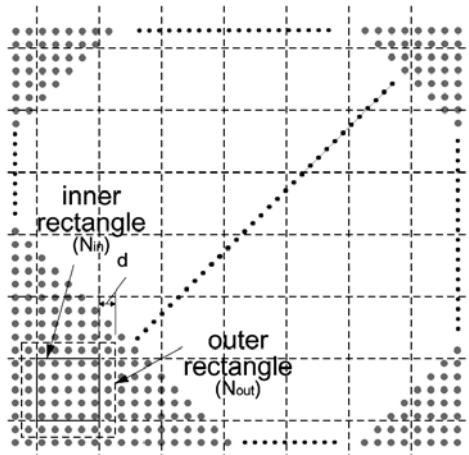

Figure 5: Bounding grids in the shear driven cavity problem.

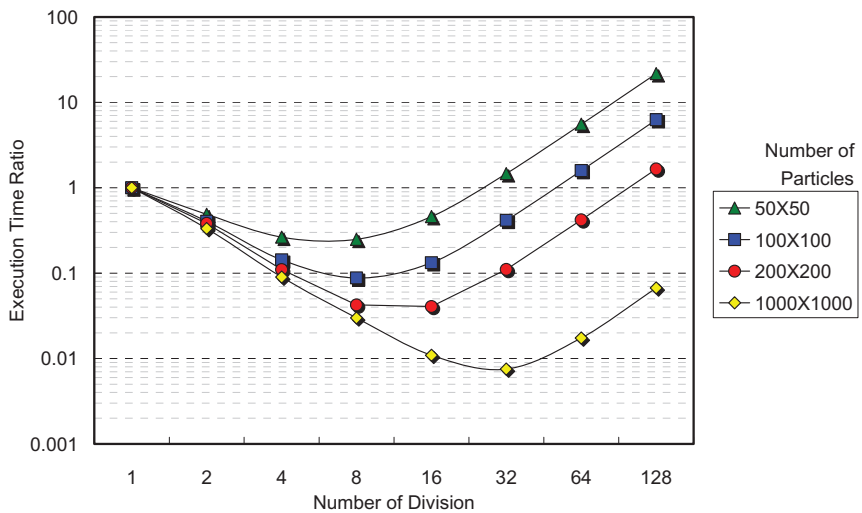

Figure 6: Results of execution time for shear driven cavity problem for different divisions.

Similar tendency with the results from the shock tube problem, the effectiveness of the present proposed grid bounding method is giving better results for larger number of particles used in the simulation. As shown in the Figure 6, for lesser number of particle, the time for registering the particles became higher than evaluating the kernel functions, thus less effectiveness will be resulted. The present method shows even better results for larger number of particle used, as shown for the number of particle of 1000×1000 the computation time reduced to less than 1% can be achieved when the divisions of grid around 32 is used. However, further increasing of number divisions will result in longer computation time.

5. CONCLUSIONS

From both examples, it can be concluded that the present proposed method shows good results for larger number of particles, in which larger number of particle is mostly required for general usage in order to obtain a reasonable simulation results. Less number of particles used in the simulation is not recommended, since the time for registering particle positions is more time consuming than directly evaluating the governing equations. However, further parameter study need to be conducted in order to grasp the most appropriate conditions where the current method has the most effectiveness. For future works, depend on the nature of simulation problem, a study on parameters such as smoothing length and number of division relationship that influencing the computation time will be investigated.

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