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Proposal for fast calculation of particle interactions in SPH simulations

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ABSTRACT

A simple and easy algorithm is presented for a fast calculation of kernel functions which are required in fluid simulations using the Smoothed Particle Hydrodynamic (SPH) method. The present proposed algorithm improves the Linked-list algorithm and adopts the Pairwise interaction technique, both of which are widely used for evaluating kernel functions in fluid simulations using the SPH method. The proposed algorithm is easy to implement without any complexities in programming. Some benchmark examples are used to show the simulation time saved by using the proposed algorithm. Parametric studies on the number of divisions for sub-domains, ratios between the sub-domain size and smoothing length and total amount of particles are conducted to determine the range of applicability and effectiveness of the proposed technique. A handy formulation which relates the ratio between the sub-domain size and smoothing length and the total amount of particles used in the simulation using the SPH method is proposed for practical usage.

1. Introduction

The Smoothed Particle Hydrodynamic (SPH) method which was first introduced [1,2] for modeling astrophysical phenomena is one amongst many particle methods that has been used for simulating the physical behavior of fluid and continuum solid bodies. Recent progress in using the SPH method has been applied in the fields of fluid and solid interaction [3,4], multi-phase fluids and free surface flows [5]. 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 within the supporting domain.

One of the important issues for implementing the SPH method using the particle approximation is how to perform effectively the evaluation of kernel functions based on a set of particles scattered in an arbitrary manner. A lot of effort has been made to improve the governing equations used in the simulations and variation of kernel functions, as summarized in [6]; however, little research work has been done in enhancing the technique to carry out the interaction among particles in the supporting domain.

Since the SPH method was introduced, three well-known particles search algorithms have been widely used in the evaluation of kernel functions. They are: the all particles searching method; the Linked-list technique; and the Hierarchical Tree technique.

The simplest of these algorithms is the all particles searching method. The search is performed at a particle to find another particle inside its supporting domain within the entire simulation domain. The searching process is necessary at every time step, and thus the computation effort required for this all particles search method is very time-consuming, and not feasible for problems with very large amounts of particles.

The Linked-list technique was introduced in [7] before the SPH method was invented, and the technique is still being widely used to perform the SPH method. The Linked-list algorithm uses uniform meshes for particle bookkeeping with the size of κh where κh is the radius of the compact support domain of the kernel function. Thus, all particles in the neighboring sub-domains can then contribute to the properties of particles in the sub-domain. An improvement was made in [8], where a cylindrical sub-domain is used as a particle bookkeeping device to simulate shocks in accretion disks. However, the cylindrical domain will lose its capability to cover an arbitrary simulation domain which is not circular, in general problems. Unlike a rectangular sub-domain, the cylindrical sub-domain leaves the four corners of its bounding rectangle untouched, and therefore overlapping between cylindrical sub-domains for particle bookkeeping is required, which makes this technique less effective.

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Hierarchical Tree coding has also been widely used [9–11]. However, due to the complexity in implementing the algorithm, this technique has not gained any popularity in practice. In [12], the application of Hierarchical Tree coding was used in parallel programming to boost its performance; nevertheless, the efforts add further complexities when adopting the algorithm proposed.

In this study, a simple and easy algorithm based on the creation of fixed sub-domains and their outlines is presented for a faster calculation of kernel evaluations, as is required in simulations using the SPH method. The proposed technique is based on the same concept as the Linked-list, but the sub-domain width does not need to be κh. In most simulation problems, the value of κh is very small compared to the whole simulation domain. Parametric studies conducted have shown that too small a sub-domain size could result in a considerable increase of the computation time. For easy use, the size of the sub-domain is determined by equally dividing the entire domain of simulation by an integer. The proposed technique is then further facilitated by the Pair-Wise Interaction method to register all the particles within the outlined sub-domain which contribute to the particles inside the sub-domain where the kernel functions are being evaluated.

Previous study [13] in internuclear distance calculations between atoms in cells inside molecular simulations also pointed out a growing computation time when the sub-divisions were increased. The so-called off-mapping algorithm was introduced to reduce unnecessary internuclear distance calculations for larger and complex systems. However, the study did not recommend the appropriate condition for applying the technique neither proposed any concrete solution for practical usage.

The outline of the paper is as follows. First, the SPH formulation for Navier–Stokes equation is highlighted. Second, the outlined sub-domain technique is explained. Third, verifications of simulation results were conducted for some benchmark problems. Fourth, parametric studies by changing the number of particles were done to observe the varying computation times. A fifth, a handy formulation was established for practical usage. Finally, the effectiveness of the formulation was used for are presented.

2. SPH formulation for Navier–Stokes equations

SPH can be considered as a kind of interpolation method for interactions of arbitrary particles in a support domain inside the fluid simulation system [14]. In the present study, the SPH method is used for solving Navier–Stokes equations problems. Fig. 1 shows a typical kernel function W. The kernel function used in this study was taken from the cubic spline family [15], which is known as a B-spline function, as given in Eq. (1).

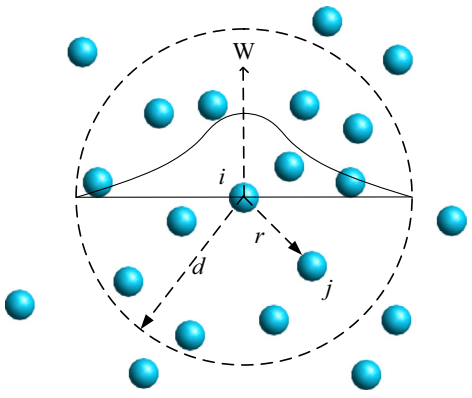

Fig. 1. Support domain of the kernel function W of particle i.

$$W(\xi,d)=\alpha_i\times\begin{cases}\frac{2}{3}-\xi^2+\frac{1}{2}\xi^3 & 0\leqslant\xi<1\\ \frac{1}{6}(2-\xi)^3 & 1\leqslant\xi<2\\ 0 & \xi\geqslant 2\end{cases}\tag{1}$$

where $\xi = 2r/d$, r is the distance between two nodes, d is the radius of the supporting domain which is given by $d = \kappa h$, κ is a multiplier factor, h is the smoothing length and $\alpha_1 = 2/d$, $\alpha_2 = 60/7\pi d^2$, $\alpha_3 = 12/\pi d^3$ for one-, two- and three-dimensional space respectively.

For the conservation of mass governing equation, the particle approximation of density can be expressed 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 $\prod_{ij}$ [16,17].

There have been many variations of the governing equations, and these are summarized in [6]. Regardless of the governing equations being used in the SPH simulations, the present technique is generally applicable and effective for evaluating the kernel functions.

3. Outlined sub-domain technique

The proposed algorithm improves the Linked-list algorithm by allowing an arbitrary spacing for the fixed sub-domains and outlining the sub-domain with the κh width to guarantee that interacting particles are taken into account in the calculations.

The proposed technique uses the Pairwise interaction technique [11,18,19] as a particle bookkeeping device that is adopted by limiting the search for interacting particles within each sub-domain. The Pairwise interaction technique is carried out with the process of searching for the nearest neighboring particle and stores the necessary data for the SPH summation process. By dividing the whole of the simulation domain into equal size sub-domains, the time needed for storing particle data becomes longer, but the time required for searching for the nearest neighboring particle is reduced, which results in a considerable total time saving.

To illustrate the present outlined sub-domain technique, a schematic two-dimensional arbitrary domain as shown in Fig. 2 is adopted. The whole simulation domain is first divided into smaller rectangles and outlines the sub-domain of the rectangles. Each rectangle is then used for registering all the particles inside the area after each time step calculation. At the same time, an outer rectangle outlining the inner rectangle is also used for particle registration. The width of the outer rectangle is determined from the size of the inner rectangle increased by the radius d of the support domain of kernel function W in both its width and height. There are overlapping areas in the adjacent sub-domains due to this outline sub-domain technique, hence coverage of the compact support of the kernel function from a particle at the edge of the inner sub-domain is guaranteed.