

Fast Calculation for Particle Interactions in SPH simulations: Outlined Sub-domain Technique

Buntara Sthenly Gan and Naohiro Kawada

Abstract—A simple and easy algorithm is presented for a fast calculation of kernel functions which required in fluid simulations using the Smoothed Particle Hydrodynamic (SPH) method. Present proposed algorithm improves the Linked-list algorithm and adopts the Pair-Wise Interaction technique, which are widely used for evaluating kernel functions in fluid simulations using the SPH method. The algorithm is easy to be implemented 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, smoothing length and total amount of particles are conducted to show the effectiveness of the present technique. A compact formulation is proposed for practical usage.

Keywords—Technique, Fluid simulation, Smoothing Particle Hydrodynamic (SPH), Particle interaction

I. INTRODUCTION

SMOOTHED Particle Hydrodynamic (SPH) method which was firstly 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 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 efforts have been done to improve the governing equations used in the simulations and variation of kernel functions as summarized in [6], however there was a few research work which has been done in enhancing the technique to carry out the interaction among particles in the supporting domain.

Classically, the particles searching algorithm is performed at a particle to find other particle inside its supporting domain within the entire simulation domain.

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The searching process is necessary at every time step, and thus the computation effort in this searching method is very time consuming, and is not feasible for problems with vast amount of particles.

The Linked-list technique was introduced in [7] before the SPH method was invented, since then; the technique is still widely being used to perform the SPH method. The Linked-list algorithm uses uniform meshes for bookkeeping with the size of $2h$. Where, $2h$ is the radius of 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 the cylindrical sub-domain is used as a bookkeeping device to simulate shocks in accretion disks. However, the circular domain will lose its capability to cover arbitrary simulation domain which is not circular, in general problems. Unlike the rectangular sub-domain, the circular sub-domain leaves the four corners of its bounding rectangle untouched, thus overlapping between circular sub-domains for bookkeeping can not be avoided, which results in less effectiveness of this technique.

The Hierarchical Tree coding has been also widely used [9-11], however due to the complexity in implementing the algorithm; this technique was not gaining any popularity in practice. In [12], the application of Hierarchical Tree coding was facilitated with parallel programming to boost its performance; nevertheless, the efforts merely increase more complexities for adopting the algorithm proposed.

In this study, a simple and easy algorithm based on creation of fixed sub-domains and its outlines is presented for a faster calculation of kernel evaluations. The present proposed technique based on the same concept with the Linked-list, but the sub-domain width need not have to the size of $2h$. In most of simulation problems, this $2h$ size is very small compared to the size of the whole simulation domain. Parametric studies conducted in this study have shown that too small sub-domain divisions' size could result in an increase of computation time considerably. For an easy use, the size of sub-domain is determined from equally dividing the size of the entire domain of simulation by a constant number. The proposed technique is then, further facilitated by the Pair-Wise Interaction method [11,13-14] to register all particles within the outlined sub-domain which contribute to the particles inside the sub-domain where the kernel functions are being evaluated.

II. 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 [15]. In present study, SPH method is used for solving the Navier-Stokes equations problems. Fig. 1 shows a typical kernel function W . The kernel function shown is used in this study was taken from the cubic spline family which is known as B-spline function (1) as given in [16].

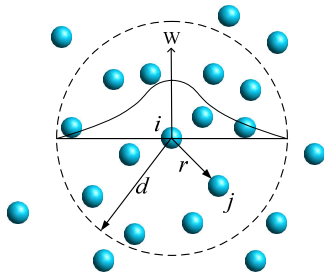


Fig. 1 Support domain of the kernel function W of particle i

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

Here, $\xi = 2r/d$, where r is the distance between two particles; $d = \kappa h$, where κ is a constant; h is the smoothing length; and $\alpha_1 = 2/d$, $\alpha_2 = 60/7\pi d^2$, $\alpha_3 = 12/\pi d^3$ are given for one-, two- and three-dimensional problem, respectively.

The particle approximation of density in the conservation of mass governing equation can be expressed as follow:

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

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 artificial viscosity into account are given as follows:

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

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

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 Π_{ij} [17,18].

There have been many variations of the governing equations which 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.

III. OUTLINED SUB-DOMAIN TECHNIQUE

The present proposed algorithm improves the Linked-list algorithm by allowing an arbitrary width for the fixed sub-domains and outlining the sub-domain with the κh width to guarantee all interacting particles are taken into account in the calculations. By dividing the entire size of simulation domain into equal size of sub-domains, time which is required for storing particle data become longer but the time which is required for searching the neighboring particle inside the sub-domain is reduced which results in considerable execution time saving.

To illustrate the present outlined sub-domain technique, a schematic two dimensional arbitrary domain as shown in Fig. 2 is used. The entire simulation domain is firstly divided into smaller squares sub-domains and their outlined squares. The width of the outer square is determined from the size of the inner square added at both width and height sides by d which is equal to the radius of kernel function W in the support domain. There are overlapping areas between the adjacent outer squares, hence the coverage of compact support of kernel function from a particle at the edge of inner squares is guaranteed. During the bookkeeping process, all the particles in the inner squares are also registered for the outer squares.

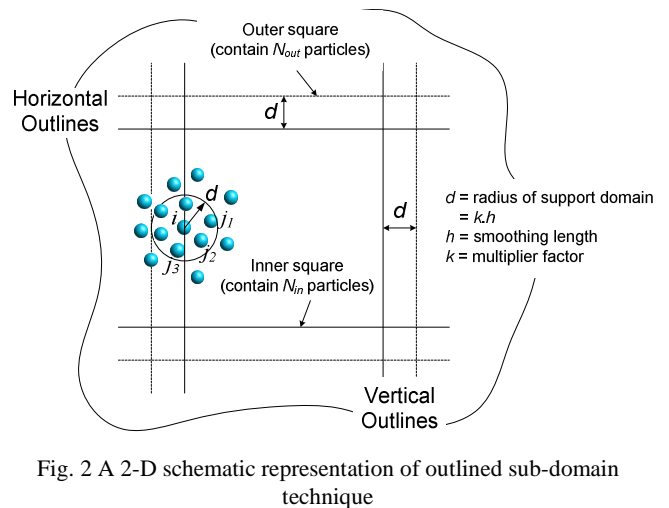


Fig. 2 A 2-D schematic representation of outlined sub-domain technique

Here, for each particle inside the inner square that is i indexed acts as a center for evaluating the governing equations of (2-4) to interact with the surrounding particles inside the outer square those are j indexed. Hence, the searching for interacting particles will only necessary sought inside the outer square which is requiring less time rather than searching for particles in

the entire domain of simulation.

The additional time required in the present technique is to register all the particles inside the predefined sub-domains and their outlined area to account particles at the utmost boundary of the sub-domains for calculation of kernel functions. Registration of particles to their sub-domains and outlined area is conducted after each time step calculation finished.

IV. PARAMETRIC STUDY USING BENCHMARKS

In the following study, 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 [6].

A. Shock tube 1-D problem

The shock tube problem is one dimensional benchmark which was comprehensively simulated by many researchers using SPH method [11,19]. The shock tube is a long straight tube filled with gas, which is separated by a membrane into two equal parts in which each part is initially in equilibrium state of constant pressure, density and temperature. When the membrane is taken away instantaneously, a shock wave, a rarefaction wave and a contact discontinuity will be produced.

The initial conditions of the simulation are similar with [11], then introduced by [14] which were taken from [20], for $x \leq 0$ ($\rho = 1$, $v = 0$, $e = 2.5$, $p = 1$, $\Delta x = 0.001875$) and for $x > 0$ ($\rho = 0.25$, $v = 0$, $e = 1.795$, $p = 0.1795$, $\Delta x = 0.0075$). Here, ρ , p , e and v are the density, pressure, internal energy and velocity of the gas, respectively. Δx is the distance between two particles. A constant time step of 0.0002 s is used for running 1000 steps calculation. A constant smoothing length $h = 0.015$ and multiplier factor $\kappa = 2$ are used in this simulation. Fig. 3 shows the scheme of outlined sub-domain technique which is applied to the shock tube 1-D problem.

Table I shows three different total numbers of particles used in the SPH simulation. The parametric study is conducted 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.

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

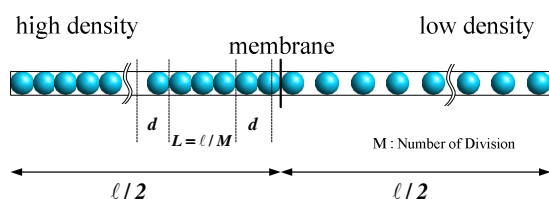


Fig. 3 Outlined sub-domain scheme in the shock tube problem

TABLE I
 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

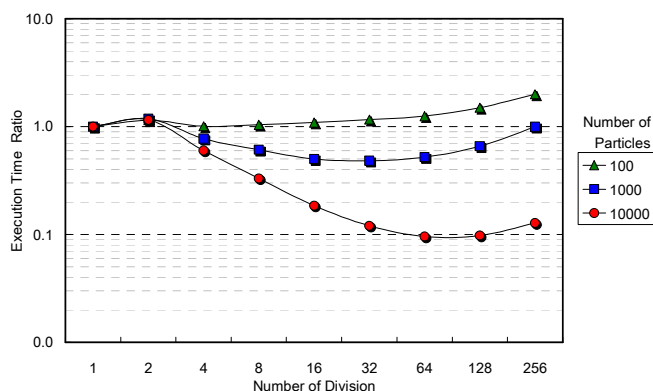


Fig. 4 Results of execution time for shock tube 1-D problem

Fig. 4 depicts the ratios of timing evaluation of the present proposed technique compared with the results from the original technique without improvement, for a variety number of particles and division of vertical sub-domains.

From Fig. 4, the present proposed outlined sub-domain technique shows less computing times for larger number of particles used in the simulation. For 100 total number of particles used in the simulation, time for registering the particles became longer than for evaluating the kernel functions, thus less effectiveness were resulted. However, the present technique shows its effectiveness for larger number of particles used in the simulation. In case, the number of particle is 10,000; the reduction in execution time of less than 10% can be achieved when the divisions of sub-domains in between 64 and 128 are used.

B. Shear driven cavity 2-D problem

The classic shear driven cavity 2-D 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 $\nu = 10^{-6}$ m²/s and $\rho = 10^3$ kg/m³ 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 II shows four different total numbers of particles used in the simulation to conduct a parametric study on the present proposed technique. For each case of the four shear driven cavity 2-D problems shown in Table II, the simulation domain is divided equally by vertical and horizontal sub-domains of 2, 4, 8, 16, 32, 64 and 128 divisions. Fig. 5 shows the scheme how the outlined sub-domain technique is applied to the shear driven cavity 2-D problem.

TABLE II
 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	1000
II	100×100	0.00250	1000
II	200×200	0.00500	1000
IV	1000×1000	0.02500	10

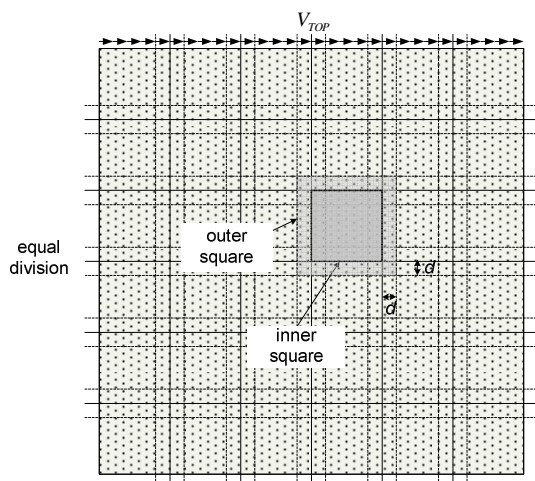


Fig. 5 Outlined sub-domain scheme in the shear driven cavity 2-D problem

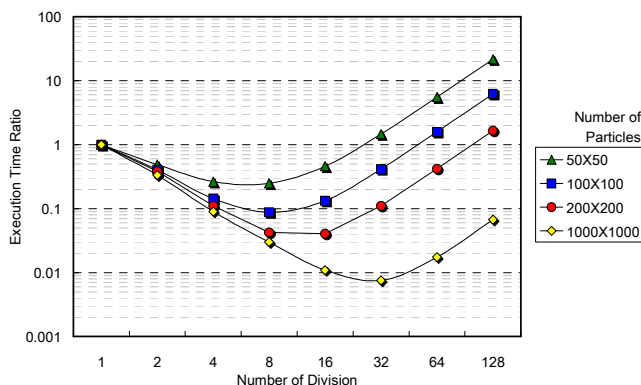


Fig. 6 Results of execution time for shear driven cavity 2-D problem

Similar tendency with the results obtained from the shock tube 1-D problem is also observed. The present proposed outlined sub-domain technique shows significant time reductions for larger number of particles used in the simulation. As shown in Fig. 6, for small number of particle, the time for registering the particles became longer than evaluating the kernel functions, thus less effectiveness will be resulted. The present technique shows much time reduction for larger number of particle used, as shown in the number of particle of 1000×1000 used in the simulation. The computation time can be reduced to less than 1% when the divisions of sub-domains about 32 are used. On the contrary, further increasing of number divisions will result in longer execution time.

C. Shear driven cavity 3-D problem

The shear driven cavity 2-D problem is extended to a 3-D closed cube problem by moving the top side of the cube at a constant diagonally 45 degree x-z direction of velocity generated while the other sides remain fixed. By using the same parameters in the 2-D problem, the flow will reach a steady state and form a recirculation pattern. In the simulation, the dimension the kinetic viscosity and density are $\nu=10^{-6} \text{ m}^2/\text{s}$ and $\rho=10^3 \text{ kg/m}^3$ respectively. The top side of the cube moves at a velocity of $V=10^{-3} \text{ m/s}$ in the diagonal x-z directions. A constant time step of $5 \times 10^{-5} \text{ s}$ is used. A constant smoothing length of 2.5×10^{-5} is used. Fig. 7 shows the scheme how the outlined sub-domain technique is applied to the shear driven cavity 3-D problem.

Table III shows four different total numbers of particles used in the simulation to show the effectiveness of the present proposed technique. For each case of the four 3-D shear driven cavity problems shown in Table III, the simulation domain is divided by sub-domains of 2, 4, 8 and 16 equal divisions in all Cartesian axes directions.

TABLE III
 PARAMETRIC STUDY FOR SHEAR DRIVEN CAVITY 3-D PROBLEM

Case	Number of Particles inside the cube	Side Length	Computation Steps
I	30×30×30	0.00100	1000
II	40×40×40	0.00100	1000
II	50×50×50	0.00100	1000
IV	60×60×60	0.00100	1000

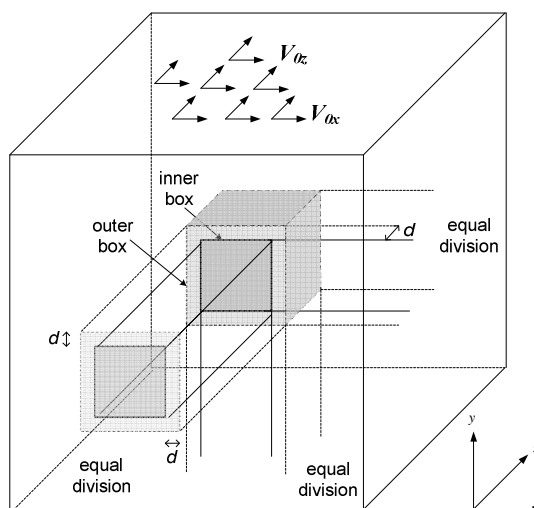


Fig. 7 Outlined sub-domain scheme in the shear driven cavity 2-D problem

In similar tendencies with the results obtained from the previous studies, the present proposed outlined sub-domain technique is showing less execution time for larger total number of particles used in the simulation. As shown in Fig. 8, for less number of particles, the time required for registering interacting particles became longer than evaluating the kernel functions, thus less effectiveness will be resulted.

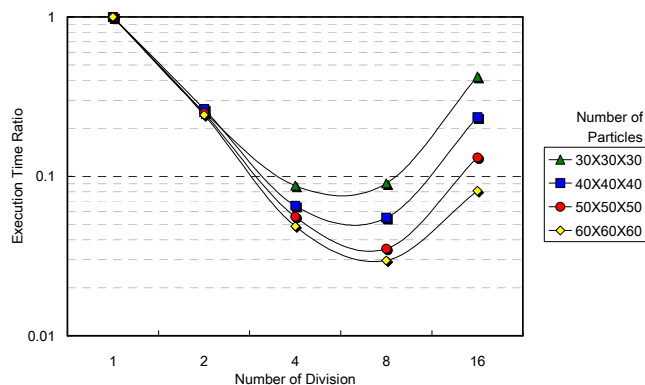


Fig. 8 Results of execution time for shear driven cavity 3-D problem

The present technique shows less execution time for larger number of particle used, as shown for the number of particle of $60 \times 60 \times 60$ the computation time can be reduced to less than 3%. This value is achieved when the divisions of sub-domains about 8 is used. However, further increasing the number divisions will result in longer execution time.

V. PROPOSAL FOR PRACTICE

From the results of parametric studies, the effectiveness of the present technique in reducing the execution time depends on the dimensional type problem, total number of particles in the simulations and number of divisions adopted in the simulations as shown in Figs. 4, 6 and 8. The most reduced execution time ratios resulted from parametric studies are collected and summarized in Table IV. Here, an additional non-dimensional ratio of L/h is introduced to represent physical characteristic of the simulation. In Table IV, L is the size of sub-domain; h is the smoothing length; N is the total number of particles used in the simulation.

For practical purpose, a simple formulation that relates all the parameters in the simulation is to be sought. A unique relationship between the total number of particles, radius of smoothing length and number of division is formulated.

Fig. 9 shows a logarithmic relationship between the L/h ratio and ND which is defined as $ND = N^{1/D}$, where D is the dimension of the simulation type. By using the linear regression analysis to the data plotted in Fig. 7, a straight line relationship can be formulated as follow.

$$ND = 0.5 (L/h)^{2.4} \quad (5)$$

In term of total number of particles used in the simulation, N , the expression (5) can be rewritten as follows.

$$N = ND^D = 0.5^D (L/h)^{2.4D} \quad (6)$$

Depends on the problem type and number of particles used in the simulations, the reduction of execution time varies from one-hundredth to one-tenth ratio can be achieved.

TABLE IV
THE MOST REDUCED EXECUTION TIME FROM PARAMETRIC STUDIES

Case	Total Number of Particles	L/h ratio	ND
Shock Tube 1-D	II 1,000	9.563	1000
	III 10,000	31.313	10,000
Shear Driven Cavity 2-D	I 50x50	9.375	50
	II 100x100	12.500	100
	III 200x200	18.750	200
	IV 1000x1000	31.250	1000
Shear Driven Cavity 3-D	I 30x30x30	5.682	30
	II 40x40x40	6.250	40
	III 50x50x50	7.031	50
	IV 60x60x60	7.485	60

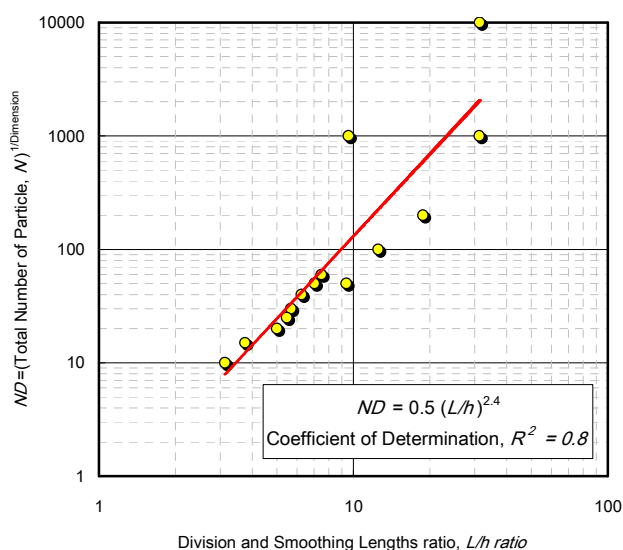


Fig. 9 Results of parametric study with the most reduction time ratio

Unlike the other techniques proposed in the past, expression in (6) is very simple and provides a handy formulation for implementation, thus recommended for practical simulation purpose.

VI. APPLICATION

In order to verify the effectiveness of the present proposed technique, a 1-D type fluid simulation problem is presented. The proposed formula in (6) was used to determine the division number of the sub-domains.

The original shock tube problem which was used as the benchmark problem is modified by dividing the long straight tube filled with gas into four equal parts. The tube is separated by membranes at three locations. All parts of the tube are initially in equilibrium state of assumed constant pressure, density and temperature. When all the membranes are taken away instantaneously, shock waves, rarefaction waves and contact discontinuities will be produced. Fig. 10 shows the scheme of outlined sub-domain technique applied to the

modified shock tube 1-D problem. Considering the flow of gas inside the tube is adiabatic in smooth regions, the functional entropy can be set as a constant, thus the relationships between density and pressure follows the isentropic law.

The initial conditions of the simulation are given as: for $x \leq 0.15$ ($\rho = 1.0$, $v = 0$, $e = 2.5$, $p = 1.0$, $\Delta x = 0.0000375$); for $0.15 < x \leq 0.30$ ($\rho = 0.5$, $v = 0$, $e = 1.895$, $p = 0.379$, $\Delta x = 0.000075$); for $0.30 < x \leq 0.45$ ($\rho = 0.8$, $v = 0$, $e = 2.287$, $p = 0.732$, $\Delta x = 0.000046875$); and for $x > 0.45$ ($\rho = 0.3$, $v = 0$, $e = 1.544$, $p = 0.185$, $\Delta x = 0.000125$).

Here, ρ , p , e , and v are the density, pressure, internal energy and velocity of the gas, respectively. Δx is the distance between two particles. A constant time step of 0.00005 s is used for 3000 steps calculation. There were 10400 particles used in the simulation. The radius smoothing length used in the simulation was determined from the largest radius of smoothing length, $d = 2h = 0.00025$ which is two times of distance between particles in the least density region, $\Delta x = h = 0.000125$. By using (5), the division length L can be calculated; hence number of division of the tube length calculated is 80.

Figs. 11-14 show the mixture processes of different pressure regions at varying simulation times along the x-axis after all the membranes that separated density varied regions are taken instantaneously at the same time.

The CPU time required for conducting the 1000 steps simulation was recorded to be 86 s which is only about 7.1% of the time required when no sub-domains along the length that was 1211 s. From the comparison of both execution CPU times, the present proposed technique shows its effectiveness in reducing the time required for conducting the modified Shock Tube 1-D simulation.

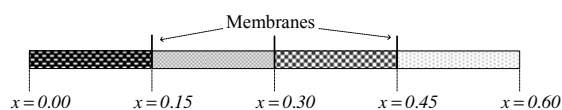


Fig. 10 Modified Shock Tube 1-D problem

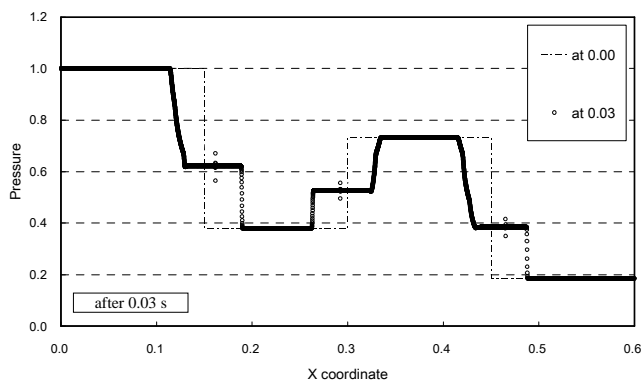


Fig. 11 Pressure distributions along the tube from the modified shock tube 1-D simulation results at 0.03 s

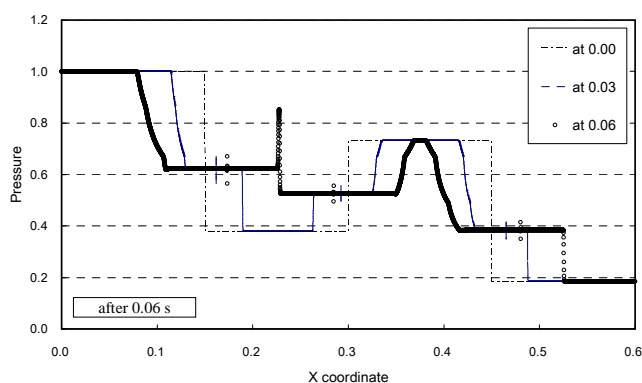


Fig. 12 Pressure distributions along the tube from the modified shock tube 1-D simulation results at 0.06 s

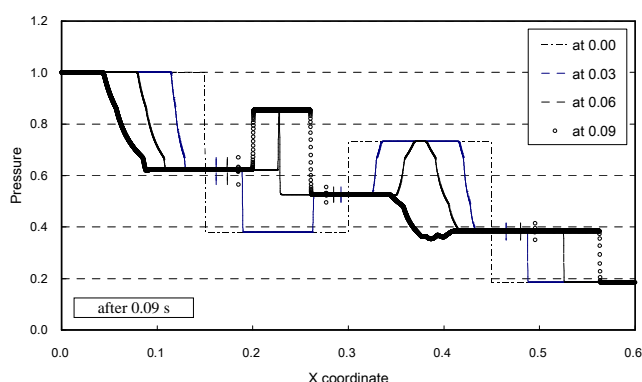


Fig. 13 Pressure distributions along the tube from the modified shock tube 1-D simulation results at 0.09 s

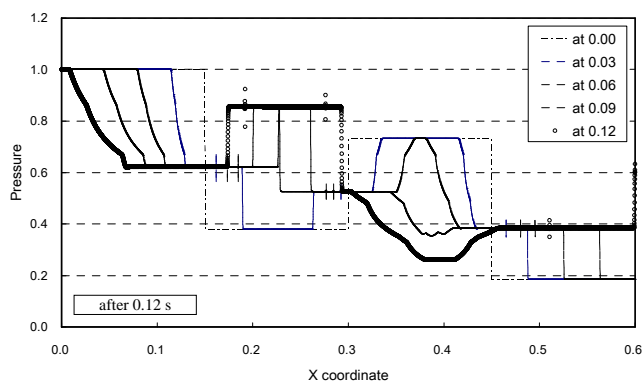


Fig. 14 Pressure distributions along the tube from the modified shock tube 1-D simulation results at 0.12 s

VII. CONCLUSION

From parametric studies, it can be concluded that the present proposed technique shows its effectiveness in the optimum ranges of number division which gives the most reduction in execution time, especially when larger number of particles is used in the SPH simulation.

An easy and handy formulation for practical purpose for conducting a simulation using SPH method is proposed. Equal division of sub-domains; and the longest smoothing length

selection for the outlines; are the two simple algorithms which are seamlessly implement able to the existing SPH simulation codes.

For future works, application of parallel programming to the bookkeeping and evaluation of kernel functions in sub-domains could further boost the performance of the present proposed technique in reducing the execution time for simulation using SPH method.

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