# Study of the diffusion operator by the SPH method

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**Abstract:** *The Smoothed Particle Hydrodynamics (SPH) method is a purely Lagrangian method which was developed initially to simulate the dynamic of astrophysical fluids (Lucy 1977, Gingold and Monaghan 1977, Benz 1990). The basis of the SPH method drift fundamentally of the Lagrangian description of fluids and that, considering that the movement of a control volume of a fluid can be represented by a particle carrying all physical information (mass, solicitation, energy, ... ).*
*In this work, we study the numerical behavior of the diffusion operator in the SPH method) with two different formulations. The first formulation is called the gradient formulation given by G_Liu and the second one is called Laplace.  An Application to the problem of heat conduction in a square plate is considered. The differential operators are discretized by the SPH method while for the time derivatives,we use an explicit schema based on "velocity Verlet" algorithm.*
**Keywords:** *Conduction, diffusion, particle method, SPH method*

## I.     Principal And Mathematical Formulation Of The SPH Method

**1  Principal of the SPH method**

The SPH method is based on three essential steps:

✓        The representation of a function by its integral with the definition of the interpolation kernel (« Kernel approximation »).

✓        The particle approximation with the passage of the integral form to a discrete sum of the contributions of particles in the influence domain.

✓        The application of the formalism to the conservation equations for the desired application.

**1.1 Representation of a function by its integral**

Let a function f defined and continuous on a domain $\Omega$. The concept of the representation of f by its integral used in SPH is based on the following equation:

$$f(x) = \int_\Omega  f(x') \, \delta(x - x')dx' \qquad\qquad (1)$$

Where f is a function of position vector $\overrightarrow{x}$ and $\delta(x - x')$ the Dirac function defined as follows:

$$\delta(x - x') = \begin{cases} 1 & x=x' \\ 0 & x\neq x' \end{cases} \qquad\qquad (2)$$

By replacing the Dirac function $\delta$ by the interpolation kernel $W(x - x', h)$, we obtain the integral interpolating of the function $f(x)$ over $\Omega$ noted $< f(x) >$.  It is then written in the form:

$$< f(x) >= \int f(x')W(x - x', h)dx' \qquad\qquad (3)$$

Where W must verify over $\Omega$ the condition of unity, convergence to the Dirac function when the smoothing length h tends to 0 and the substrate must be compact. These three conditions are given respectively by the following equations 4, 5 and 6:

$$\int_\Omega  W(x - x', h). dx' = 1 \qquad\qquad (4)$$

$$\lim_{h\to0} W(x - x', h) = \delta(x - x') \qquad\qquad (5)$$

$$W(x - x', h) = 0 \qquad \text{if} \qquad |x - x'| > kh \qquad\qquad (6)$$

Where $\kappa$ is a constant of the interpolation function.

If the interpolation kernel is differentiable, we can construct the differential interpolating of the function f' noted $< \nabla. f(x) >$, let :

$$< \nabla. f(x) >= \int \nabla f(x'). W(x - x', h)dx' = - \int f(x'). \nabla W(x - x', h)dx' (7)$$

We immediately notice than the gradient operator is transmitted to the interpolation function and the estimation of the derivative of a function can then be determined from the function values and derivative of the kernel.

## II.     Choice of the kernel

The chosen kernel to approximate the Dirac function can be for example a Gaussian function or a spline. The respect of conditions (4) and (5) is helping to build such functions. In practice, the support of the kernel is not the computational domain $\Omega$ but a compact support D (ie beyond a size equivalent to n times the length of the smoothing,the kernel value is zero). The most currently used kernels have a support with aray

equals to 2h or 3h. This will directly influence the number of neighbours and therefore the accuracy of the approximation. In the end we are proposing to use these kernels (where q=|r| /h):

The cubic spline proposed by Monaghan [2], on a support of size 2h:

$$W(r,h) = C_c \begin{cases} \frac{2}{3} - q^2 + \frac{1}{2}q^3 & \text{if } 0 \leq q \leq 1 \\ \frac{1}{6}(2-q)^3 & \text{if } 1 \leq q \leq 2 \\ 0 & \text{otherwise} \end{cases} \qquad (8)$$

Where the normalization constant $C_c$ allows verifying the condition 4 and is worth $\frac{1}{h}, \frac{15}{7\pi h^2}$ and $\frac{3}{2\pi h^3}$, respectively in 1, 2 and 3 dimensions.

It is important to note that this kernel function depends only on the distance between a point i and its neighbour j. The support is then spherical and the vicinity of one ball is actually composed of all the neighbouring balls to which $r_{ij} < 2h$ .

The cubic spline viscosity given by [3], on a support of size h

$$W(r,h) = C_c \begin{cases} \frac{1}{2}q + q^2 - \frac{1}{2}q^3 - 1 & \text{if } 0 < q \leq 1 \\ \\ 0 & \text{if } 1 > q \end{cases} \qquad (9)$$

Where the normalization constant $C_c$ allows verifying the condition (4) and is worth $\frac{5}{h}, \frac{45}{7\pi h^2}$ and $\frac{15}{2\pi h^3}$, respectively in 1, 2 and 3 dimensions.

## III. The boundary conditions

The boundary conditions are a very important task for the SPH. To well succeed a simulation amounts largely to well model boundary conditions. There are different alternatives that we can adapt to the SPH method and this concerning modeling spatial boundary conditions, speed or inter-reaction. Based on the nature of the SPH, Obtaining the value of a physical quantity at a given point involves the smoothing of the neighbourhood of the point. Consequently, a problem emerges for the points in the domain boundaries as well as locations that do not have sufficient space to smooth.

In this work, we use phantom particles method; it is a question of going round the area/field by series of particles which called phantom particles. This name comes from the fact that these particles are not used for anything other than to get a neighbourhood of sufficient smoothing. The number and the spatial distribution of these sets of particles are determined so as to consider smoothing lengths of the used kernel (h, for Müller, 2h for the case of a kernel of Spline type and 4h for the case of the Gaussian).

## IV. Physical problem

Let a solid material, occupying a D domain of the three-dimensional space $x_1, x_2, x_3$ and for the mechanical point of view is on rest. Its density ρ and its specific heat C depend a priori on the three coordinates $x_1, x_2, x_3$ (for a nonhomogeneous material) but not on time t $\rho = \rho(x_1, x_2, x_3), \quad C = C(x_1, x_2, x_3)$
Suppose that this material receives, leads and absorbs some heat flow. So its temperature
u= u($x_1, x_2, x_3$: t) evolves over time and space. It is the same for the vector " heat flow density'' $\vec{q}$.
$\vec{Q} = \vec{q}(x_1, x_2, x_3 : t)$.
Recall that by definition of $\vec{q}$, $\forall \Omega \subset D$, the quantity of heat received by Ω through S= ∂Ω per unit time is equal to :

$$\iint_S -\vec{q} \cdot \vec{n} \, ds \;\equiv\; \iiint_\Omega -\vec{\nabla} \cdot \vec{q} \, dx_1 dx_2 dx_3 \qquad (10)$$

Where $\vec{n}$ is the norm to s external of Ω, the "stock'' of accumulated thermal energy through material by heating (internal energy of material) increases by : $\int_\Omega C \frac{\partial u}{\partial t} dm \equiv \iiint_\Omega \rho C \frac{\partial u}{\partial t} dx_1 dx_2 dx_3 \qquad (11)$

So the variation (10) of the stock is equal to the inflow (11) where

$$\iiint_\Omega \left( \rho C \frac{\partial u}{\partial t} + \vec{\nabla} \cdot \vec{q} \right) dx_1 dx_2 dx_3 = 0 \qquad (12)$$

From this integral, assuming that all is continuous, ie the integrant is continuous, we can, based on the fundamental lemma, conclude that the integrant is itself zero, hence the following relationship:

$$\rho C \frac{\partial u}{\partial t} = -\vec{\nabla} \cdot \vec{q} \qquad (13)$$

By introducing the "behaviour" law known as "Fourier" law

$$\vec{q} = -k\vec{\nabla}u \qquad (14)$$

With $k = k(x_1, x_2, x_3)$ is the thermal conductivity

So this relation expresses the fact that the heat flows are even more intense as the temperature difference is greater, and the heat goes from hot spots to cold spots. The following formula is then deduced:

$$\rho C \frac{\partial u}{\partial t} = \vec{\nabla}.\left(k\vec{\nabla}u\right) \qquad (15)$$

If the material is homogeneous, $\rho$, $C$ and $k$ are constants, hence

$$\vec{\nabla}.\left(k\vec{\nabla}u\right) = k\vec{\nabla}.\left(\vec{\nabla}u\right) = k\Delta u \qquad (16)$$

Consequently:

$$\frac{\partial u}{\partial t} = \lambda \Delta u \qquad (17)$$

With: $\qquad \lambda = \frac{k}{\rho C} = cte$

$$\frac{\partial u}{\partial t} = \lambda\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) \qquad (18)$$

This equation is called 'heat equation'' and $\lambda$ "thermal diffusivity"

## V.  Applications And Results

### 1.  Application in 1D case

Initially, we are limited to the case of one variable of space, which we will denote x : this is the case for example of a metal bar whose temperature depends only on the abscissa x and time t.
The equation (18) is reduced to:

$$\frac{\partial u}{\partial t} = \lambda \frac{\partial^2 u}{\partial x^2}$$

This equation is a model for the (parabolic) equation of the boundary layer.
We put: $Q_T = [0,1] \times ]0, +\infty[$, The overall problem is then written:

$$\begin{cases} \frac{\partial u}{\partial t} = \lambda \frac{\partial^2 u}{\partial x^2} \quad \text{sur } Q_T \\ CL: u(0,t) = u(1,t) = 0, \forall t > 0 \\ CI: u(x,0) = v(x), \forall x \epsilon [0,1] \end{cases} \qquad (19)$$

where $\lambda$ is the thermal diffusivity.

### 1.1  Discretization
- **Discretization of the differential operator by SPH**

$$\Delta u_i = \sum_j \frac{m_j}{\rho_j} u_j(t) \frac{\partial^2 W_{ij}}{\partial x^2} \qquad (20)$$

$$\frac{\partial u_i}{\partial t} = \lambda \sum_j \frac{m_j}{\rho_j} u_j(t) \frac{\partial^2 W_{ij}}{\partial x^2} \qquad (21)$$

We note that with the SPH method, following the formalism leads to derive twice the kernel, ie $\Delta = \nabla.\nabla$.

But this formula is not symmetrical; consequently it does not check Newton law. It will be replaced by :

$$\Delta u_i = \sum_j \frac{m_j}{\rho_{moyij}} (u_j(t) - u_i(t)) \frac{\partial^2 W_{ij}}{\partial x^2} \qquad (22)$$

with $\qquad \rho_{moyij} = \frac{2(\rho_i \times \rho_j)}{\rho_i + \rho_j}$

Leading to:

$$\frac{\partial u_i}{\partial t} = \lambda \sum_j \frac{m_j}{\rho_{moyij}} (u_j(t) - u_i(t)) \frac{\partial^2 W_{ij}}{\partial x^2} \qquad (23)$$

**Discretization of the temporal operator**

To treat time derivatives, we use an explicit scheme based on the 'velocityVerlet' algorithm [5] as follows: $\qquad u_i^{n+1} = u_i^{n-1} + 0.5\Delta t(D_i^n + D_i^{n+1}) \qquad (24)$

with $\qquad D_i^n = \frac{du_i(t)}{dt}$
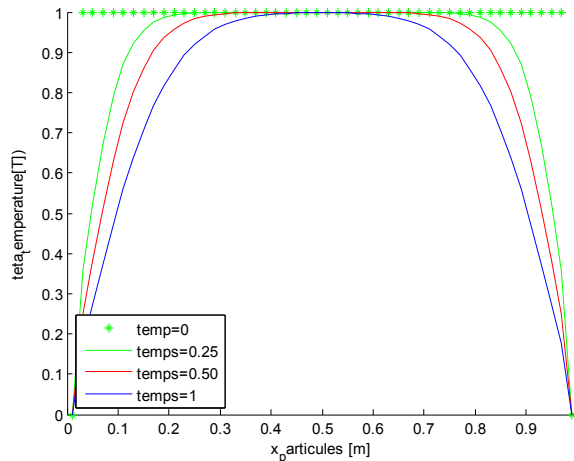
### 1.2    Results



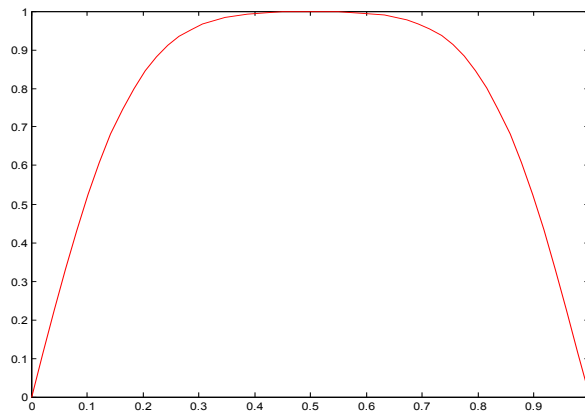Fig1Laplace_method: $DT = 0.001, NX = 50,$    $NDT = 1000$



Fig2finite difference_method: $DT = 0.001, NX = 50,$    $NDT = 1000$

### 2.    Application in 2D case

The variables of space, which we denote x and y this is the case for example of a metal cavity in which the temperature depends only on   x,y and time t.
The equation (18) is reduced to:

$$\frac{\partial u}{\partial t} = \lambda \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

This equation serves as a model for (parabolic) equation of the boundary layer.
With initial and boundary conditions :

$$u(x, y, t = 0) = 1 \qquad for \quad x, y \in \Omega$$

$u(0, y, t) = u(x, 0, t) = 0$  for    t>0    (25)
where  $\lambda$  is the thermal diffusivity.

### 2.1    Discretization of the differential operator by SPH

$$\Delta u_i = \sum_j \frac{m_j}{\rho_j} u_j \left( \frac{\partial^2 W_{ij}}{\partial x^2} + \frac{\partial^2 W_{ij}}{\partial y^2} \right) \tag{26}$$

Then  $\frac{\partial u_i}{\partial t} = \lambda \sum_j \frac{m_j}{\rho_j} u_j \left( \frac{\partial^2 W_{ij}}{\partial x^2} + \frac{\partial^2 W_{ij}}{\partial y^2} \right)$    (27)

We note that with the SPH method, following the formalism leads to derive twice the kernel, ie $\Delta = \nabla.\nabla$.

But this formula is not symmetrical; consequently it does not check Newton law. It will be replaced by:

$$\Delta u_i = \sum_j \frac{m_j}{\rho_{moyij}} (u_j - u_i) \left( \frac{\partial^2 W_{ij}}{\partial x^2} + \frac{\partial^2 W_{ij}}{\partial y^2} \right) \tag{28}$$

With $\rho_{moyij} = \frac{2(\rho_i \times \rho_j)}{\rho_i + \rho_j}$

Which leads to:

$$\frac{\partial u_i}{\partial t} = \lambda \sum_j \frac{m_j}{\rho_{moyij}} (u_j - u_i)(\frac{\partial^2 w_{ij}}{\partial x^2} + \frac{\partial^2 w_{ij}}{\partial y^2}) \tag{29}$$

This approximation which we call Laplace method, we compare it to another that we call gradient method[4] :

$$\frac{du_i}{dt} = \lambda \sum_j \frac{m_j}{\rho_j \times \rho_i} \frac{4(k_i k_j)}{k_i + k_j} (u_j - u_i)(\nabla w_{ij}) \tag{30}$$

### 2.2 Discretization of the temporal operator

To treat time derivatives, we use an explicit scheme based on the 'velocityVerlet' algorithm [5] as follows:

$u_i^{n+1} = u_i^{n-1} + 0.5\Delta t(D_i^n + D_i^{n+1})$

With $\quad D_i^n = \frac{du_i}{dt}$

## VI.    Numerical Results

The geometry of the problem is a square cavity of side L = 2. Conductivity coefficient is taken equal to1. The calculation program is tested for different values of nx and ny, npr = nx × ny with dt = $5.10^{-5}$and ndt = 1000.

We have found that the Laplace method and the gradient method give the same result when the number of particles is small (100 real particles and 40 virtual particles (phantoms)). But when the number of particles increases, Laplace method gives results comparable to those found by other authors while with the gradient method, we obtain practically the same result regardless of the number of particles engaged. In Figures 3 and 4, the results are presented with the two methods fornx = ny = 40. In figure 3, we give the results obtained by Liu for the same number of particles.
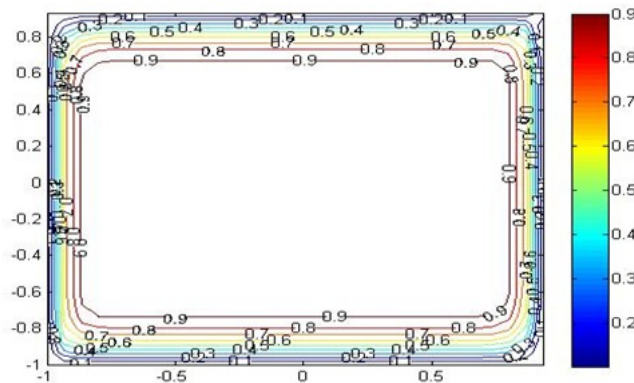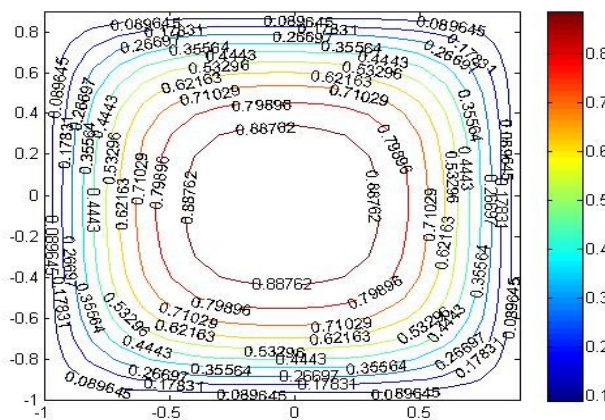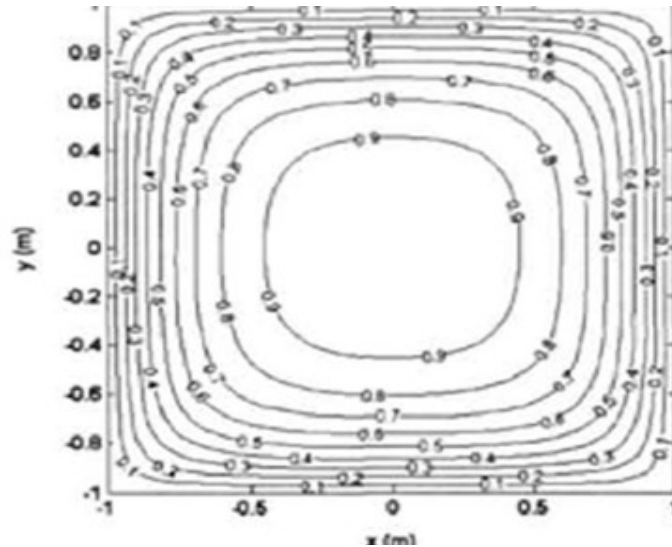


Fig3gradient_method



Fig4Laplace_method

Fig5Liu_method: [1]

## VII.    Conclusion

In this paper, we have proposed a model based on SPH method to simulate conduction problem. The main advantage of this technique involves the approximation of functions on the edge around the tool which is difficult to achieve with other numerical methods such as finite element method.

We are working now on extending the proposed model to simulation process of natural convection with consideration of a bill of more realistic behavior depending on both temperature model, the fluid velocity as well as in the case 2D and 3D.

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