

Modelling Melting Ice using the Smooth Dissipative Particle Dynamics Method

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Abstract

Computational fluid dynamics (CFD) is a highly popular tool used in fluid research. It approaches fluid systems from a continuum point of view, with focus on the bulk macroscopic properties and behaviour. On the other hand, microscale modelling methods like the discrete element method (DEM) focus on the particle level — particle properties, rather than bulk constitutive relations are needed. While a DEM model is capable of reproducing bulk behaviour similar to that from a continuum model, this is only possible at great computational costs as a very large number of discrete particles would be needed. There exist many other methods which attempt to bridge the different lengthscales, for example the smoothed-particle hydrodynamics (SPH) and dissipative particle dynamics (DPD) methods. This paper describes how the smooth dissipative particle dynamics (SDPD) method, a mesoscale hybrid of both the SPH and DPD methods, could be used to numerically simulate a solid-fluid system with changing temperature like melting ice.

Introduction

As technology advances, the study of fluids via numerical experiments has become increasingly viable, yielding insights previously unattainable. One of the oldest, and most popular tools today for simulating fluid problems is computational fluid dynamics (CFD). CFD simulations involve dividing up the simulation domain into a mesh, and solving the Navier–Stokes equations using finite differences across the entire mesh in a series of spatial and temporal iterations. The method, as a whole, is a continuum approach to fluid problems as it focuses on, and is defined by, bulk macroscopic characteristics. Information can be obtained from CFD simulations only up to a scale as fine as the mesh used, and any finer details are lost. One reflection of this is in how turbulence is treated — turbulence flows involve a variety of length scales, such that very fine meshes are required to obtain higher resolution for reproducing a measure of the complexity of such flows. This is very expensive computationally, and hence numerical models are instead incorporated to approximate the small-scale effects that are not otherwise simulated.

Rather than a continuum approach, microscopic numerical methods like the discrete element method (DEM) proposed in 1979 by Cundall and Strack [3] take a discretised view of fluid problems. Admittedly such modelling methods may not be the immediate solution turned to for modelling fluid systems, as they share a lot of similarities with molecular dynamics simulation methods and are more commonly used when the fluid in question is a particulate flow. However for these methods, the focus is on the particle-level i.e. the discrete particles within a fluid flow. Interparticle relations are governed by Newton's laws of motion, and the heavily dependent on microscale properties like the particle stiffness, density or the coefficient of restitution. Naturally in contrast to CFD methods, information on the microscale behaviour is available but such a great number of particles are required to obtain enough information to reliably derive information on the macroscale, that the resulting computational costs are impractical. Another difference is that

these particle-based methods are generally not restricted to a pre-defined mesh, and thus are better able to model spatially-varying surfaces.

The smoothed-particle hydrodynamics (SPH) method is particle-based, however it is generally regarded as a macroscopic modelling method. Developed in 1977 by Gingold and Monaghan [6] and Lucy [11], SPH is similar to DEM in that the fluid is modelled with discrete 'particles'. Additionally, each 'particle' has an assigned smoothing length over which particle properties are summed according to a kernel function. In this manner, shocks and discontinuities are smoothed out from information derived from SPH simulations. This manner of averaging the information over a larger length scale is the reason for classing SPH as a macroscopic method.

In the middle ground exist the mesoscale modelling methods which involve length scales larger than microscale, that tend to be of greater physical interest. One notable mesoscale method is the relatively recent dissipative particle dynamics (DPD) method [5, 8, 12]. Introduced by Hoogerbrugge and Koelman [8] in 1992, the DPD method treats the fluid 'particles' as clusters of fluid. The Brownian motion typically seen in fluids is modelled via a random force included in the interparticle equation of motion. This random force also ensures that the DPD system maintains a constant temperature. However, the DPD formulation allows only for isothermal systems, has no direct relation to transport coefficients, and the physical parameters involved are not clearly defined. An improved version of DPD is the smoothed dissipative particle dynamics (SDPD) method [1, 4, 10] proposed by Español and Revenga [4] in 2003, which incorporates thermal fluctuations into an SPH system or, from another point of view, allows for temperature-variation in a DPD system as well as a straightforward physical interpretation.

In this paper the simple case of a melting block of ice is chosen to assess the suitability of the SDPD method. Water has been studied and utilised in many aspects of life around us, and its solid phase is also a significant part of our environment. Naturally, the transition between ice and water is a commonly-encountered phenomenon. The melting process is particularly interesting in terms of modelling, as it is a time-varying solid-fluid system. The transition from solid ice to liquid water at 0°C is also significant as this is not spontaneous — a critical amount of energy must be gained or lost before the phase change can occur. Naturally, melting ice has been modelled before using various numerical techniques [7, 9], but there are still insights to be gained by modelling this everyday phenomenon using a mesoscale particle method like SDPD. It is expected that while the chosen 'particle' size will define the resolution of the simulation, the meshless nature of this method may simulate the formation and temporal variations of the solid-fluid interface more closely.

The following sections first describe the general SDPD formulation, followed by the specifics for implementation of an SDPD model of a melting block of ice. The paper closes with some anticipated results from this modelling method.

Smooth Dissipative Particle Dynamics

As with both the SPH and DPD methods, the SDPD system models the system as a collection of N 'particles'. Each particle i can be considered to represent a cluster of fluid, with the corresponding collective mass and velocity. The state Φ of the whole system can be characterised by the set of particle positions \mathbf{x}_i , particle velocities \mathbf{v}_i , and particle entropies S_i , for $i = 1$ to N . The equations of motion governing each particle i are then as follows:

$$d\mathbf{x}_i = \mathbf{v}_i dt, \quad (1)$$

$$m_i d\mathbf{v}_i = \mathbf{F}_C dt + \mathbf{F}_D dt + \mathbf{F}_R, \quad (2)$$

and

$$T_i dS_i = \Delta Q_V dt + \Delta Q_C dt + \Delta Q_R. \quad (3)$$

Equation (2), the momentum equation, is written as a sum of conservative, dissipative and random forces \mathbf{F}_C , \mathbf{F}_D and \mathbf{F}_R . The expressions for these are, assuming constant mass $m_i = m$, given as:

$$\mathbf{F}_C = \sum_j F_{ij} \left(\frac{P_i}{d_i^2} + \frac{P_j}{d_j^2} \right) \mathbf{x}_{ij}, \quad (4)$$

$$\mathbf{F}_D = - \sum_j \left[\gamma_{ij}^C \mathbf{v}_{ij} + \gamma_{ij}^T (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij}) \mathbf{e}_{ij} \right], \quad (5)$$

and

$$\mathbf{F}_R = \sum_j \left(A_{ij} d\overline{\mathbf{W}}_{ij} + \frac{1}{3} B_{ij} \text{tr} [d\mathbf{W}_{ij}] \right) \mathbf{e}_{ij}, \quad (6)$$

where d_i and P_i denote the diameter and pressure of particle i respectively, $\mathbf{x}_{ij} = \mathbf{x}_i - \mathbf{x}_j$ is the vector going from the centre of particle j to the centre of particle i and \mathbf{e}_{ij} is the corresponding unit vector, and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the relative velocity between the two particles in the direction of \mathbf{x}_{ij} . F_{ij} is a positive function related to the smoothing kernel function $W(\mathbf{x})$, defined as:

$$F(\mathbf{x}_{ij}) \equiv -(1/x_{ij}) dW/dx_{ij}. \quad (7)$$

Additionally,

$$\gamma_{ij}^C = \left(\frac{5\eta}{3} - \zeta \right) \frac{F_{ij}}{d_i d_j}, \quad (8)$$

$$\gamma_{ij}^T = \left(\frac{5\eta}{3} + 5\zeta \right) \frac{F_{ij}}{d_i d_j}, \quad (9)$$

$$A_{ij} = \left[8k_B \left(\frac{5\eta}{3} - \zeta \right) \frac{T_i T_j}{T_i + T_j} \frac{F_{ij}}{d_i d_j} \right]^{1/2}, \quad (10)$$

and

$$B_{ij} = \left[8k_B \left(\frac{5\eta}{3} + 8\zeta \right) \frac{T_i T_j}{T_i + T_j} \frac{F_{ij}}{d_i d_j} \right]^{1/2}, \quad (11)$$

where η is the dynamic viscosity, ζ is the bulk viscosity, k_B is the Boltzmann constant, T_i is the temperature of particle i , and $d\mathbf{W}_{ij}$ is a matrix of independent increments of the Wiener process, with $d\overline{\mathbf{W}}_{ij}$ denoting its traceless symmetric part.

Equation (3), the entropy equation, is likewise written as a sum of viscous, conductive and random components ΔQ_V , ΔQ_C and ΔQ_R respectively. Their corresponding expressions are:

$$\Delta Q_V = \frac{1}{2} \sum_j \left[\gamma_{ij}^C (\mathbf{v}_{ij} \cdot \mathbf{v}_{ij}) + \gamma_{ij}^T (\mathbf{e}_{ij} \cdot \mathbf{v}_{ij})^2 \right], \quad (12)$$

$$\Delta Q_C = -2 \sum_j \kappa \frac{F_{ij}}{d_i d_j} T_{ij}, \quad (13)$$

and

$$\begin{aligned} \Delta Q_R &= -\frac{1}{2} \sum_j \left(A_{ij} d\overline{\mathbf{W}}_{ij} + \frac{1}{3} B_{ij} \text{tr} [d\mathbf{W}_{ij}] \right) : \mathbf{e}_{ij} \mathbf{v}_{ij} \\ &+ \sum_j \left(4\kappa k_B T_i T_j \frac{F_{ij}}{d_i d_j} \right)^{1/2} dV_{ij}, \end{aligned} \quad (14)$$

where κ is the thermal conductivity and dV_{ij} is an antisymmetric, independent increment of the Wiener process.

Additionally, an equation of state is required to relate the internal energy and entropy of the system. The pressure and temperature can then be determined from this equation of state. For general cases, a Taylor expansion can be used, assuming that the system state is close to the chosen reference state (pressure P_0 , volume V_0 , temperature T_0 and entropy S_0):

$$\begin{aligned} U &= U_0 - P_0 (V - V_0) + T_0 (S - S_0) + \frac{1}{2} \beta_0 (V - V_0)^2 \\ &+ \frac{1}{\alpha_0 V_0} (V - V_0) (S - S_0) + \frac{1}{2} \frac{T_0}{C_{V,0}} (S - S_0)^2. \end{aligned} \quad (15)$$

The subscript 0 refers to a reference state, while the adiabatic bulk modulus β_0 , coefficient of thermal expansion α_0 and heat capacity at constant volume $C_{V,0}$ determined from the internal energy U as follows:

$$\beta_0 = V_0 \frac{\partial^2 U}{\partial V^2}, \quad (16)$$

$$\alpha_0 = \frac{1}{V_0} \left(\frac{\partial^2 U}{\partial V \partial S} \right)^{-1}, \quad (17)$$

and

$$C_{V,0} = T_0 \left(\frac{\partial^2 U}{\partial S^2} \right)^{-1}. \quad (18)$$

The temperature T and pressure P of the system are then given as:

$$T = T_0 + \frac{1}{\alpha_0 V_0} (V - V_0) + \frac{T_0}{C_{V,0}} (S - S_0), \quad (19)$$

and

$$P = P_0 - \frac{\beta_0}{V_0} (V - V_0) - \frac{1}{\alpha_0 V_0} (S - S_0) \quad (20)$$

respectively.

Implementation for Melting Ice Model

First the physical system to be modelled has to be chosen — in this case, an ice cube allowed to melt on a flat, horizontal surface at room temperature. Initial conditions are that the ice cube is at 0°C, and the room temperature remains at 20°C.

The ice cube will be modelled by particles held fixed in a crystalline structure. Each of these particles, with equal mass m and radius r , represent a small cluster of ice. As long as they remain in the solid phase, their spatial position will remain unchanged. The solid flat surface beneath the ice can be modelled either by a horizontal wall (assigned infinite mass) or a series of smaller particles (radius $r_w < r$) held permanently fixed in position. The melted ice-water will be represented by the previously-ice particles, but no longer constrained spatially. The surrounding air will not be modelled.

Parameters that need to be pre-determined include:

- the particle radius r , as this determines the resolution of the numerical simulation results,

- the smoothing kernel function $W(\mathbf{x})$ from which the function $F(\mathbf{x}_{ij})$ can then be determined using equation (7),
- the two independent increments of the Wiener process, $d\mathbf{W}_{ij}$ and dV_{ij} , and
- the latent heat of fusion, U^* , required for the phase change of a single ice particle at 0°C .

U^* is the product of mass m and the specific heat of fusion, given in [2] as 334 J/g .

Taking the reference state to be at 0° , the change in internal energy can be set to the latent heat of fusion in equation (15). The volume remains unchanged prior to melting, leading to:

$$U^* = T_0(S - S_0) + \frac{1}{2} \frac{T_0}{C_{V,0}} (S - S_0)^2$$

$$S - S_0 = -C_{V,0} \left(1 \pm \sqrt{1 + \frac{2U^*}{C_{V,0}T_0}} \right). \quad (21)$$

The change in entropy should be positive, so the critical change in entropy S^* required for the phase change is:

$$S^* = C_{V,0} \left(\sqrt{1 + \frac{2U^*}{C_{V,0}T_0}} - 1 \right). \quad (22)$$

The general numerical algorithm carried out at each timestep is outlined as follows:

1. The force components \mathbf{F}_C , \mathbf{F}_D and \mathbf{F}_R , as well as the components ΔQ_V , ΔQ_C and ΔQ_R are calculated based on the values of \mathbf{x}_i , \mathbf{v}_i , P_i and T_i at the previous time-step, using equations (4–6) and (12–14).
2. Equations (1–3) are used to update the values of \mathbf{x}_i , \mathbf{v}_i and S_i .
3. If the particle is still in the solid phase and the change in entropy $\Delta S_i = S_i - S_0 < S^*$, then the temperature and pressure are kept constant at T_0 and P_0 respectively. Otherwise, if $\Delta S_i \geq S^*$, the particle is then considered to have changed from solid to liquid phase.
4. When the particle has entered the liquid phase, the pressure P_i and temperature T_i are updated using equations (19) and (20).

It must be noted that certain parameters may have different values before and after melting, for instance the dynamic viscosity η , bulk viscosity ζ and thermal conductivity κ , so the appropriate values should be used for particles in the liquid phase.

An important issue in melting is that the density of ice is less than that of water, which results in melted liquid taking up a larger volume than the equivalent mass in ice. This can be accounted for by decreasing the density and increasing the particle radius for the liquid phase, such that the mass remains constant. This leads to an explicit increase in volume as the ice melts.

Anticipated Results

The discrete nature of SDPD will result in the simulated melting process appearing less ‘continuous’ than in reality. Both the volume of ice melted (figure 1), as well as the temperature profile (figure 2), will show jumps over time. Figure 1 shows a sketch of the decreasing width of an ice block over time. Each

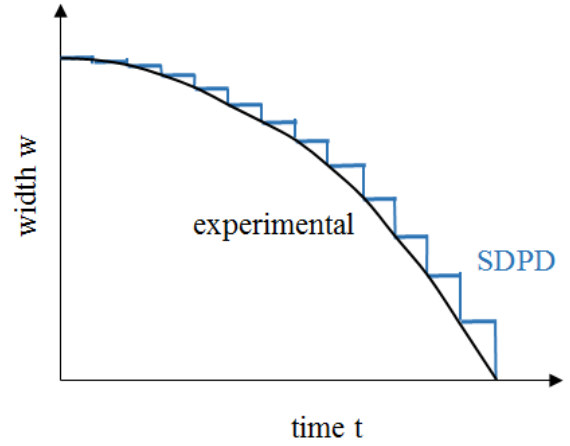


Figure 1: Sketch of the variation of the width of a melting ice block over time. The thin black line represents physical reality while the thick blue line shows anticipated SDPD results.

frozen SDPD particle has a definite volume which in turn requires a definite amount of time to melt, and hence the transformation from solid phase to liquid phase appears to be discrete.

Similarly, the temperature profiles shown in figure 2 are discrete as each SDPD particle has a single temperature i.e. there is no temperature variation across a single SDPD particle. Continuity (in terms of temperature) is not enforced between particles, unlike with finite volume methods, resulting in a non-continuous temperature profile. These jumps can be reduced as the model resolution (particle size) becomes finer.

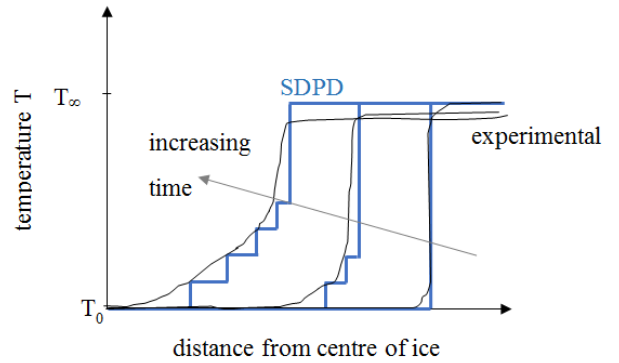


Figure 2: Sketch of the temperature profile of a melting ice block and the surrounding air over time. The thin black line represents physical reality while the thick blue line shows anticipated SDPD results.

Another difference between the SDPD results and reality portrayed in figure 2, is the variation in the room temperature. Naturally, the far-field temperature remains constant (this is not shown explicitly in the small length-scale of figure 2); but it is expected that the temperature of the air nearest the melting ice cube should be lower than the far-field, before the whole system reaches a steady state. The SDPD system, however, does not explicitly include air and hence its temperature variation is not modelled. This could be resolved by including particles representing the air, governed by similar equations as the ice/water but with properties corresponding to air. This solution, however, requires more computational power, and the air transport properties may vary greatly with temperature.

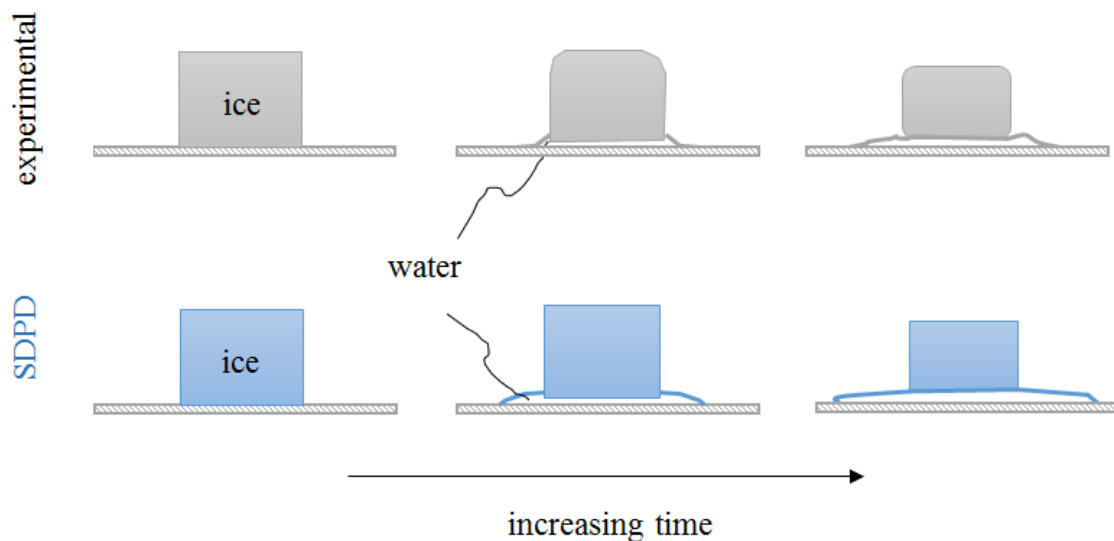


Figure 3: Sketches of the cross-sectional view of a block of melting ice over time (left), with corresponding anticipated cross-sectional views of the SDPD model (right).

The closeness of the simulated shape to reality depends largely on the resolution of the SDPD model. However it is expected that the SDPD model will likely be more blocky (angular) than in reality, as sketched in figure 3. As a whole however, this SDPD model will be able to model the motion of the ice and water more closely compared to other numerical methods — specifically the spreading of the ice-water as well as the vertical motion of the ice as it floats on the melted water. This is shown in figure 3: due to ice being less dense than water, it is expected that the ice will float in the melted water. After a sufficient amount of ice has melted, a thin layer of water will be present under the remaining ice.

Conclusions

This paper outlines a general formulation and implementation of an SDPD model for a block of ice melting at room temperature. Due to the phase change from solid ice to liquid water, an additional criteria for the change in entropy has to be included in the typical numerical algorithm. This model can potentially simulate the melting process more closely than grid-based methods, in that the liquid water and solid ice are free to move and unconstrained by position. Unfortunately as the air is not included explicitly, the temperature variation of the air will not be modelled. The resolution of the model is also very important in how closely the simulation comes to the continuous process of melting.

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