Simulation and visualization of solid-liquid phase transition and interactive using particle-based method

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***Abstract*—The simulation and visualization of natural phenomena has been widely studied in computer graphics. But those studies are less involved in complex phenomena, such as solid-liquid interaction and transition. We propose a method for simulation and visualization of solid-liquid heat conduction and phase transition using Smooth Particle Hydrodynamics(SPH) based on Fourier law. To achieve a realistic phase transition, spatio-temporal discretization of solid-liquid two-phase material, we map the temperature field to solid and liquid particles and combining with the heat conduction model. Our method includes heat conduction between solid and liquid, solid and surrounding air, and latent heat caused by phase transition. The experimental results show that our method can realize stable heat conduction and smooth phase transition from solid to liquid with accurate simulation details and visualization effects.

Keywords—fluid simulation and visualization, solid-liquid transition, heat conduction

I. INTRODUCTION

Solid-liquid phase transition phenomenon widely exists in nature, such as ore melting into molten steel, chocolate melting, magma cooling and solidification, etc. The dynamics of phase transition is one of the most attractive visualization effects. Solid-liquid phase transition simulation is an interesting and challenging research direction with wide application value in film and television special effects, entertainment games and other fields.

The solid-liquid phase transition and interaction usually involve deformation and topological changes. The common method is to use an improved fluid solver, which is suitable for the simulation of viscous Newtonian fluids and viscoplastic fluids. But the motion of solid and elastic materials is more difficult to achieve using this solver. In addition, the grid-based method can better solve the problem of elastic deformation. But those methods must rely on explicit collision detection to enhance the effect, and needs to remesh according to topology changes to achieve fluid behavior. Due to the trade-off between solid and fluid simulations, many studies have explicitly coupled the two solvers, but this method is usually complicated to implement and computationally expensive.

The particle-based method is more suitable for solid-liquid phase simulation because of its simple calculation and easy handling of large deformation and transition of various materials. Therefore, the smoothed particle hydrodynamics (SPH) method was used to discretize the solid-liquid phase interactions. Combined with the first law of thermodynamics and Fourier law, the latent heat of solid and liquid caused by phase transition is considered to construct the physical quantity mapping of solid and liquid in particle state phase transition. To achieve the flow effect of liquid on solid during solid melting and liquid solidification.

II. RELEATED WORK

Particle-based method to simulate fluid has always been a research hotspot in computer graphics [1-4]. SPH method is the most typical and widely used. which was originally proposed by Lucy[5] for solving astrophysical problems. In 2003, Muller [6]et al. applied SPH method to fluid animation. In 2009, Solenthaler et al. [7] proposed the predictive correction SPH method for the simulation of incompressible fluids, which iteratively calculates and updates density fluctuations during the predictive correction. In 2014, Ihmsen et al. [8] proposed the implicit incompressible SPH method, which obtained the discrete Poisson pressure strength equation by combining the symmetric SPH pressure strength and the discrete continuity equation, and maintain the density change within 0.01%.

The common method to simulate the melting of objects is to use thermodynamic heat conduction to conduct heat and melt objects. Zhao et al. [9] based on the improved lattice Boltzmann method, simulate objects with different materials to make them melt and flow in multiple phases. Solenthaler et al. [10] proposed a unified particle model, which can simultaneously simulate multiple solid-liquid interactions and achieve melting and solidification effects. Yan et al.[11]realized solid dissolution effect based on concentration criterion.

In the simulation of phase transition between solid and liquid, the most concerned research focus is to simulate the process of ice melting into water when heated. As physical phase change models were proposed, Jone[12] designed melt models that took into account heat flow and latent heat of

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phase change. In Lagrange method, Iwasaki[13]proposed a GPU-based particle method, which can deal with the interaction between ice, water and water droplets. Lii et al. [14] endowed each particle with the attribute of virtual water by using a particle-based model. The virtual water volume of ice particles represents the water volume around the ice particles, and the virtual water is transferred between the outer ice particles to effectively simulate the thin water flow on the ice surface. In the mixed method, Stomakhin et al. [15]further realized the expansion and cracking effect caused by heat conduction effect in the MPM method based on the temperature criterion.

In the simulation of phase transition between solid and liquid, the most concerned research is to simulate the process of ice melting into water when heated. Due to the complex coupling problem of solid-liquid phase transition, non-physical models were used in the early methods. In Euler method, Fujishiro et al. [16] used the voxel method to simulate solid ice and modeled the phase transition process of ice through the grid automaton to approach the real physical effect, but this method could not deal with the fluid formed by melting. Subsequently, physical phase change models were proposed. Jones[17] designed a melting model that took into account heat flow and latent heat of phase change, and Matsumura et al. [18] simulated the melting process of ice when natural convection occurs in the surrounding air based on this heat flow model. In Lagrange method, Iwasaki[19] proposed a GPU-based particle method, which can deal with the interaction between ice, water and water droplets. Lii et al. [20] endowed each particle with the attribute of virtual water by using a particle-based model. The virtual water volume of ice particles represents the water volume around the ice particles, and the virtual water is transferred between the outer ice particles to effectively simulate the thin water flow on the ice surface. In the mixed method, Stomakhin et al. [21] further realized the expansion and cracking effect caused by heat conduction effect in the MPM method based on the temperature criterion.

III. METHOD

A. *Fluid simulation methods for smooth particle hydrodynamics—SPH*

In fluid simulation based on SPH method, the value of any physical field at coordinates in the simulated region can be approximated as (1) according to the properties of Dirac function:

$$A(\mathbf{x}) \approx (A * W)(\mathbf{x}) = \int A(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)dv' \quad (1)$$

where W is the normalized Gaussian kernel function, h is the smoothing length of the kernel function, this paper selects the cubic spline function as the smooth kernel function, dv' is the volume integral variable corresponding to x' The formula indicates that the physical quantity of physical quantity A at $\mathbf{x}$ can be approximated as the volume integration process of the product of the physical quantity and the smooth kernel function on the smooth length.

In the computer SPH numerical calculation process, the continuous space needs to be discretized into the form of uniform volume particles. According to formula (1), for the particle i at position x_i, the value A_i of any physical quantity A can be taken according to its own value. And the value A_j of all neighbor particles j within the smooth length h is approximately:

$$A_i = \sum_j A_j \frac{m_j}{\rho_j} W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (2)$$

and the gradient of A_i can be obtained directly by approximating the gradient of the smooth kernel function:

$$\nabla A_i = \sum_j A_j \frac{m_j}{\rho_j} \nabla W(\mathbf{x}_i - \mathbf{x}_j, h) \quad (3)$$

Due to the SPH method has poor stability in calculating the second derivative, the Laplacian form of A_i can be expressed in artificial form as:

$$\nabla^2 A_i = 2(d+2)\sum_j \frac{m_j}{\rho_j} \frac{A_{ij} \cdot \mathbf{x}_{ij}}{\left|\mathbf{x}_{ij}\right|^2 + 0.01h^2} \nabla W_{ij} \quad (4)$$

where $A_{ij} = A_i - A_j$, $\mathbf{x}_{ij} = \mathbf{x}_i - \mathbf{x}_j$, and d are the dimensions of the simulation space. The simulation process in this paper is all three-dimensional, so $d=3$. The advantage of this approximation is that it has Galileo invariance and has no effect on the uniform velocity field. The $0.01h^2$ term is used to ensure that the denominator is not 0.

B. *Lagrangian particle heat conduction solution*

The physics-based solid-liquid transition is mainly based on the realization of heat conduction. In this paper, the heat conduction phenomenon caused by the temperature difference between the solid and the liquid, the solid and the surrounding air and the latent heat caused by the phase change are numerically simulated, and a realistic phase transition animation is generated. The specific process is shown in the Figure 1.

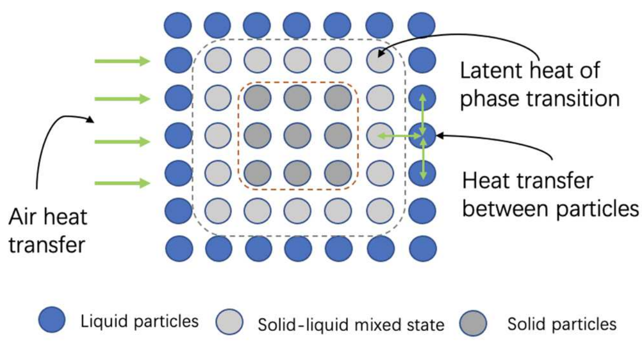

Figure 1 Simulation of particle heat conduction process

In the Lagrangian simulation system, solids and liquids can be discretized into particle forms, and the solid-solid and solid-liquid heat conduction process can be expressed as heat exchange between particles. This paper simulates the heat conduction process based on Fourier's law , the law states that

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the amount of heat conduction through a given section in a unit time is proportional to the temperature change rate in the direction perpendicular to the section and the area of the section, expressed as:

$$\frac{dQ}{dt} = -ks\frac{dT}{dx} \tag{5}$$

where s is the heat conduction area, dQ/dt is the heat conduction rate, Q is the heat, x is the coordinate on the heat conduction surface, and the constant k is the thermal conductivity, the unit is $W \cdot m^{-1} \cdot K^{-1}$, which is regarded as a constant in this paper.

C. Air heat conduction calculation

Due to the large proportion of air in the simulation space, if the rest of the space is discretized by particles, the simulation efficiency will be greatly affected and the simulation dynamics process will not be significantly affected. In order to calculate the air heat conduction efficiently, the global air temperature is set as constant, and the implicit heat conduction simulation is carried out based on Newton's cooling law.

Newton's law of cooling states that when there is a temperature difference between the surface of an object and its surroundings, the heat loss per unit area per unit time is proportional to the temperature difference, which can be expressed as:

$$Q_i = h(T_{air} - T_i)\delta S \tag{6}$$

where Q_i is the heat received by the particle i, h is the heat conduction coefficient, and δs is the surface area of the particle in contact with the air.

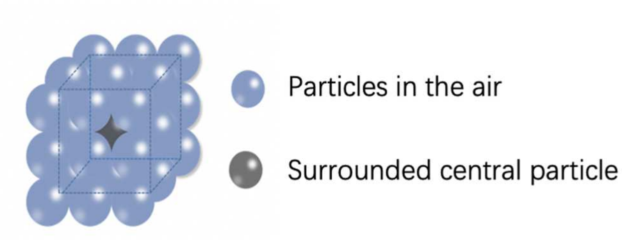


Figure 2 Particles and their neighbors in three-dimensional space

As shown in Figure 2, in the microscopic state, the particles can be approximately regarded as cubes. Considering the incompressibility of liquids and the uniform sampling of solids, when a particle is completely surrounded, the number of surrounding particles is at most about 26. , Therefore, the contact area of the particle with the air can be obtained indirectly by calculating the number of neighbors of the particle. Suppose the total surface area of the particle is s, then the surface area exposed to the air is approximately:

$$\delta S = \frac{26 - n_i}{26} * S \tag{7}$$

where n_i means that the particle i has n neighbor particles. If the number of neighbor particles is less than 26, it can be judged that the particle has a certain surface area exposed to the air; if the neighbor particle is equal to or greater than 26, it can be considered that the particle is completely surrounded and not exposed to the air, there is no heat exchange with the air.

D. Solid-Liquid phase transition simulation

Based on the above method, the state and motion process of each particle can be calculated, so as to simulate the phase change. Figure 3 shows the simulation process within a time step.

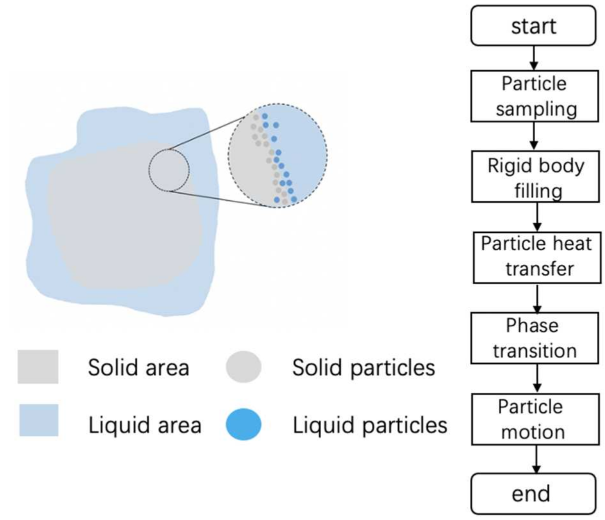
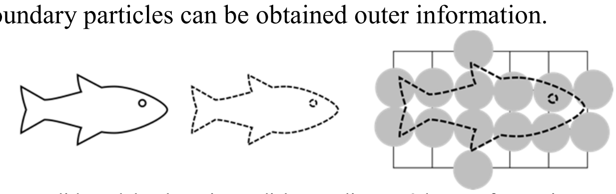


Figure 3 Solid melting process and phase transition treatment

The solid and liquid in this paper are represented by particles. Each particle stores information such as initial position, initial velocity, static density, temperature, etc. In order to prevent only the solid surface information after sampling, and the interior is hollow, resulting in a splash effect after liquefaction. First of all, the solid is sampled with a Poisson disk, as shown in Figure 4. The position information of each particle after sampling can be calculated to obtain the distribution of the solid model in the three-dimensional space. The space is formatted with the particle radius as the side length, and divided three-dimensional space into cubes, and the formatted particles are located at the intersection of the cube grid. By calculating the distance between the sampled point and the intersection, and taking the intersection with the sampling point of the Poisson disk less than the particle radius to place the solid particles, the boundary particles can be obtained outer information.



a. Solid model b. Poisson disk sampling c. 3d space formatting

Figure 4 Schematic diagram of uniform grid sampling method

After obtaining the boundary information of the solid, it is necessary to determine the position properties of particles at the intersection point, that is, internal particles or external particles. It is possible to explore whether there are sampled boundary particles in each direction along the three dimensions and six directions of the space where the

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intersection point is located. If there are boundary particles in all six directions from an intersection point, it indicates that the intersection point is inside the solid. If the boundary of the grid has been explored in a certain direction and no boundary solid particles are found, the intersection is outside the solid. A solid particle model with ideal uniform sampling can be obtained by this method. The smaller the particle radius, the smoother the surface, and the more realistic the details of the original model appear.

After completing solid sampling and filling, we need to find the neighbor particle of each particle, calculate the heat conduction between the neighbor particle and the particle, and determine whether the particle will undergo phase transition. In reality, when the solid reaches the melting point, will not immediately melt, but also need to absorb a certain amount of heat, this heat is called latent heat, usually the solid melting heat absorption is called latent heat of melting. Different substances have different latent heat, and different latent heat coefficients can be set according to the different substances to be simulated. When the temperature of a solid particle is higher than the melting point and the latent heat is consumed, the solid particle becomes a liquid particle.

The liquid particles formed by melting will move along the solid surface. When the liquid particles on the solid surface converge into water droplets, and the gravity of the droplets exceeds the force between the two particles, the water droplets will fall. SPH method can be used to simulate the liquid particles to achieve a realistic effect.

IV. Results and Discussion

In order to verify our method can efficiently simulate the solid-liquid phase transition phenomenon based on heat conduction, this paper experimented the heat conduction changes of the solid rabbit in high-temperature liquid and in the air, and the melting process of the cocktail block in the wine glass. The experimental platform is Intel (R) Xeon(R) E7-8870, 385G RAM, Quadro P1000 GPU.

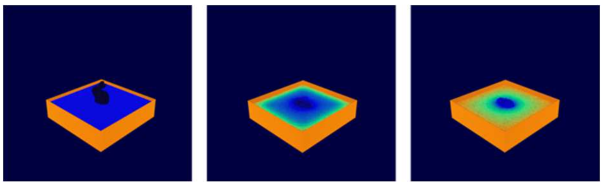
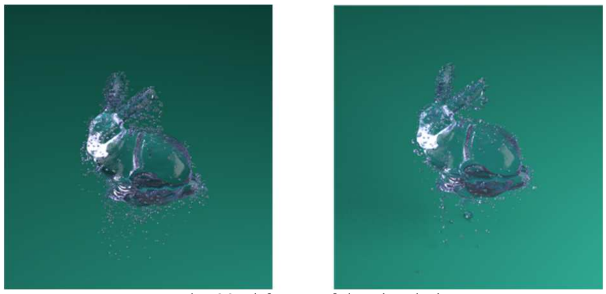
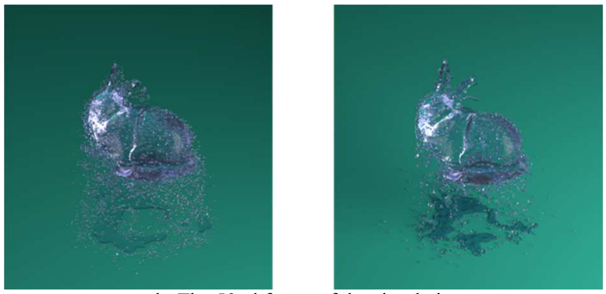


Figure 5 Heat conduction of a cryogenic solid rabbit falling into a high-temperature liquid

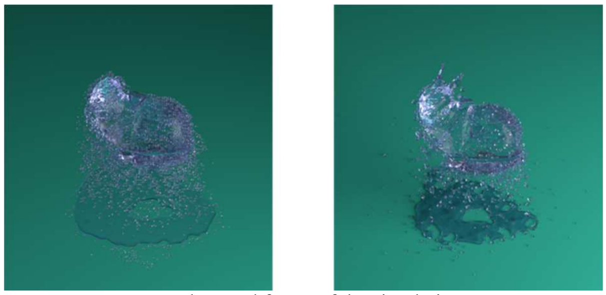
Figure 5 shows the experimental effect of a cold solid rabbit falling into a hot liquid. In order to display the temperature information in real time, RGB values of particles are used to represent the corresponding temperature information in the temperature field graph. The darker the color, the lower the temperature, and the lighter the color, the higher the temperature. As shown in Figure 5, the outer layer is a constant temperature wall, and heat conduction begins after the low-temperature solid rabbit falls into the center of the high-temperature liquid. As time goes by, heat is gradually transferred to the inner circumference, and the overall color tends to be uniform. This scene mainly shows the heat conduction process between solid and liquid.



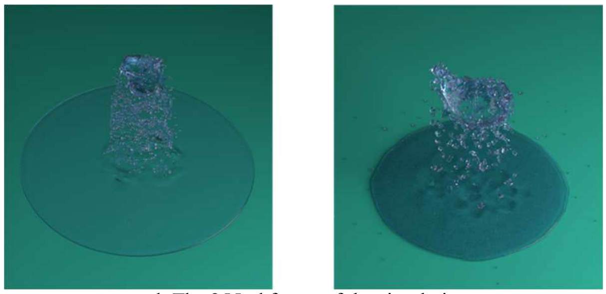
a. The 22nd frame of the simulation



b. The 50nd frame of the simulation



c. The 75nd frame of the simulation



d. The 255nd frame of the simulation

Figure 6 The melting process of a solid rabbit in the air

Figure 6 shows the process of heating and melting of a rabbit exposed to the air. When the rabbit is subjected to heat conduction from the surrounding air, it first begins to melt from a place with a larger surface area and volume, and gradually changes from an irregular shape to a spherical shape. The left row shows the pure melting process of the solid rabbit in the air. The liquid particles formed by the melting are very scattered and cannot be close to the solid surface. After falling to the ground, they form a disc; the surface tension model and adhesion force model are added to the right row, and the liquid formed by melting is added. The particles gather to form larger droplets, and then slide down along the surface. The water that falls on the ground produces irregular arrangements and hollow effects due to surface tension. This is the same as the details of the solid melting into liquid to form droplets in real situations. This scene mainly shows the process of heat conduction between solids and air.

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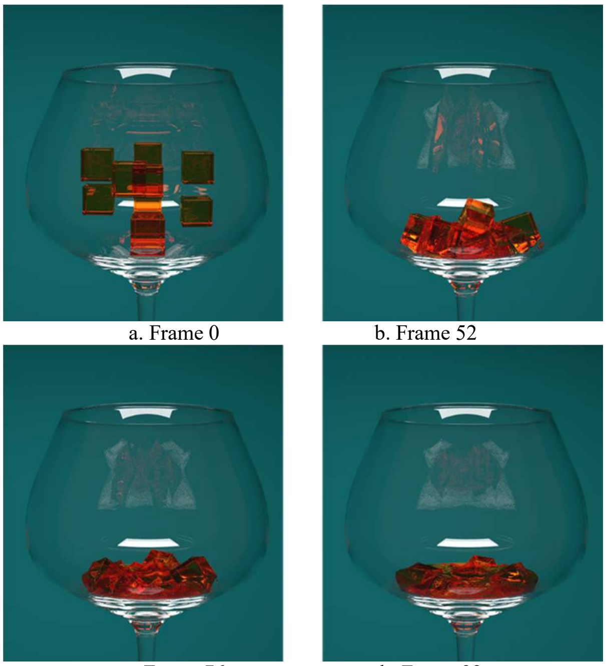

a. Frame 0 b. Frame 52

a. Frame 76 b. Frame 93

Figure 7 Cocktail block melting in the glass simulation

Figure 7 comprehensively considers the heat conduction between solids, liquids and air, and verifies the application of this method in comprehensive complex scenarios.

After falling into the glass, the cocktail block is not only subjected to heat conduction from air, but also from solid to solid and solid to liquid. During the phase transition, when the temperature of the liquid in the glass reaches the melting point and the heat absorbed by the cocktail block exceeds the latent heat of the phase transition, the cocktail block completely melts into a liquid state. It can be seen from the scene that latent heat of phase transition is considered in the process of phase transition, which makes the phase transition process more natural and achieves realistic effect.

V. CONCLUSION

We propose a solid-liquid heat conduction phase transition animation simulation model based on SPH method. By simulating the heat conduction between discrete material points and between implicit air and Lagrangian particles, the gas-solid-liquid three-phase heat conduction is established. The model realizes realistic fluid simulation and phase transition visualization.

This method also has some limitations. Due to some numerical errors in the calculation of solid absorption latent heat of melting, the voxelized fluid particles may melt inside the surface first, which makes the pressure calculation of fluid simulation unstable. It is planned to introduce Euler grid data model to realize smooth particle phase transition based on more uniform and stable heat conduction. Meanwhile, based on the mixed discretization model, the stability of the force analysis at the solid-liquid interface was improved.

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REFERENCES

[1] Koschier D, Bender J, Solenthaler B, et al. Smoothed particle hydrodynamics techniques for the physics based simulation of fluids and solids[C]. Eurographics 2019-Tutorials, 2019.

[2] Ren B, Yang X Y, Lin M C, et al. Visual Simulation of Multiple Fluids in Computer Graphics: A State-of-the-Art Report[J]. Journal of Computer Science and Technology, 2018, 33(3): 431-451.

[3] Z. Yalan, X. Ban, Y. Xu, and X. Liu, "Boundary handling for non-newtonian fluid simulation,"JournalofComputer-AidedDesign&ComputerGraphics, vol. 31, p. 1341, 01 2019. Wang X, Liu S, Ban X, et al. Recovering turbulence details using velocity correction for sph fluids[M]//SIGGRAPH Asia 2019 Technical Briefs. 2019: 95-98.

[4] Wang X, Liu S, Ban X, et al. Recovering turbulence details using velocity correction for sph fluids[M]//SIGGRAPH Asia 2019 Technical Briefs. 2019: 95-98.

[5] Lucy L B. A numerical approach to the testing of the fission hypothesis[J]. The astronomical journal, 1977, 82: 1013-1024.

[6] Müller M, Charypar D, Gross M. Particle-based fluid simulation for interactive applications[C]//Proceedings of the 2003 ACM SIGGRAPH/Eurographics symposium on Computer animation. Eurographics Association, 2003: 154-159.

[7] Solenthaler B, Pajarola R. Predictive-corrective incompressible SPH[C]//ACM transactions on graphics (TOG). ACM, 2009, 28(3): 40.

[8] Ihmsen M, Cornelis J, Solenthaler B, et al. Implicit incompressible SPH[J]. IEEE transactions on visualization and computer graphics, 2013, 20(3): 426-435.

[9] Ye Zhao,Lujin Wang,Feng Qiu,Arie Kaufman,Klaus Mueller. Melting and flowing in multiphase environment[J]. Computers & Graphics,2006,30(4).

[10] Solenthaler B, Jürg Schläfli, Pajarola R. A unified particle model for fluid-solid interactions[J]. Computer Animation and Virtual Worlds, 2007, 18(1):69-82.

[11] Yan X, Jiang Y T, Li C F, et al. Multiphase SPH simulation for interactive fluids and solids[J]. ACM Transactions on Graphics (TOG), 2016, 35(4): 1-11.

[12] Jones M W. Melting Objects.[J]. Smalltalk Report, 2003, 11:155--158.

[13] Iwasaki K , Uchida H , Dobashi Y , et al. Fast Particle-based Visual Simulation of Ice Melting[J]. Computer Graphics Forum, 2010, 29(7):2215-2223.

[14] Lii S Y , Wong S K . Ice melting simulation with water flow handling[J]. The Visual Computer, 2014, 30(5):531-538.

[15] Stomakhin A, Schroeder C, Jiang C, et al. Augmented MPM for phase-change and varied materials[J]. ACM Transactions on Graphics, 2014, 33(4):1-11.

[16] Fujishiro I, Aoki E. Volume Graphics Modeling of Ice Thawing.[J]. Volume Graphics, 2001:69-80.

[17] Jones M W. Melting Objects.[J]. Smalltalk Report, 2003, 11:155--158.

[18] Matsumura M, Tsuruno R. Visual simulation of melting ice considering the natural convection[M]//ACM SIGGRAPH 2005 Sketches. 2005: 61-es.

[19] Iwasaki K , Uchida H , Dobashi Y , et al. Fast Particle-based Visual Simulation of Ice Melting[J]. Computer Graphics Forum, 2010, 29(7):2215-2223.

[20] Lii S Y , Wong S K . Ice melting simulation with water flow handling[J]. The Visual Computer, 2014, 30(5):531-538.

[21] Stomakhin A, Schroeder C, Jiang C, et al. Augmented MPM for phase-change and varied materials[J]. ACM Transactions on Graphics, 2014, 33(4):1-11.

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