

Dealing with density discontinuities in planetary SPH simulations

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ABSTRACT

Density discontinuities cannot be precisely modelled in standard formulations of smoothed particles hydrodynamics (SPH) because the density field is defined smoothly as a kernel-weighted sum of neighbouring particle masses. This is a problem when performing simulations of giant impacts between proto-planets, for example, because planets typically do have density discontinuities both at their surfaces and at any internal boundaries between different materials. The inappropriate densities in these regions create artificial forces that effectively suppress mixing between particles of different material and, as a consequence, this problem introduces a key unknown systematic error into studies that rely on SPH simulations. In this work, we present a novel, computationally cheap method that deals simultaneously with both of these types of density discontinuity in SPH simulations. We perform standard hydrodynamical tests and several example giant impact simulations, and compare the results with standard SPH. In a simulated Moon-forming impact using 10^7 particles, the improved treatment at boundaries affects at least 30 per cent of the particles at some point during the simulation.

Key words: hydrodynamics – methods: numerical – planets and satellites: formation.

1 INTRODUCTION

A key chapter in the Solar system’s history involves impacts between planet-sized objects. This giant impact phase of planet and satellite formation is responsible for many of the features we see today in our Solar system. To name a few: the formation of our Moon (e.g. Hartmann et al. 1975; Cameron & Ward 1976; Benz, Slattery & Cameron 1987), the tilted spin axis of Uranus (e.g. Slattery, Benz & Cameron 1992; Kegerreis et al. 2018; Reinhardt et al. 2020), the formation of the Pluto–Charon system (e.g. McKinnon 1984, 1989; Canup 2005), the Mars hemispheric dichotomy (e.g. Wilhelms & Squyres 1984), or the origin of Mercury’s high core:mantle ratio (e.g. Benz, Slattery & Cameron 1988; Chau et al. 2018).

An ideal tool for studying giant impacts is smoothed particle hydrodynamics (SPH). SPH is a particle-based method used in a wide range of astrophysical and engineering topics (Springel 2010; Monaghan 2012). It is the most commonly used option for studying giant impacts because of the complexity and anisotropy of these highly non-linear interactions. Compared with grid-based hydrodynamical codes, SPH has the advantages of naturally following the provenance of material and being readily combined with efficient gravity solvers.

Despite its many positive points, the hydrodynamical part of SPH can still have difficulties treating the mixing of particles

that represent different materials. In the standard density–energy formulation of SPH, density discontinuities cannot be accurately represented because of the smoothing inherent in the definition of the density field. However, density profiles of differentiated planets do have discontinuities, typically both between different material layers (e.g. core to mantle boundary) and the outer surface. The standard SPH formulation creates artificial forces that act like an effective surface tension at these discontinuities, repelling one material from the other and suppressing mixing between different materials. While the cause of this numerical artefact is clear, the consequences for the mixing of materials during giant impact simulations are rarely considered (e.g. Deng et al. 2019a,b, who compared SPH with another Lagrangian method). As such, this represents a significant and unquantified systematic uncertainty for standard simulations. This numerical issue could be crucial in the modelling of many giant impact problems, with examples being how much mixing would have been provoked in the core of Jupiter by a giant impact (Liu et al. 2019), and what the distribution of iron is in the debris of the hypothesized Moon-forming impact (Canup & Asphaug 2001; Ruiz-Bonilla et al. 2021).

Previous studies that have addressed the smoothing of density discontinuities in a planetary context by modifying the SPH formulation have dealt either with those arising from contact between two different materials at the same pressure (Woolfson 2007; Reinhardt et al. 2020) or with that found at the surface of a planet (Reinhardt & Stadel 2017). In this paper, we propose a novel, computationally

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cheap method to suppress the spurious numerical effects associated with density discontinuities, regardless of their context.

In Section 2, we describe the basics of SPH (Section 2.1), the details of the density discontinuity problem we aim to solve and previous attempts (Section 2.2), and finally our own method (Section 2.3). In Section 3, we perform some standard hydrodynamical tests (Sections 3.1 and 3.2), as well as testing a settling simulation of a planet (Section 3.3), and a variety of giant impacts between a proto-Earth and Theia with and without our method (Section 3.4) to search for differences. Finally, conclusions are presented in Section 4.

2 METHODS

2.1 Background theory

The fundamental idea of SPH is to reconstruct a density field from a set of discrete particles with masses m_i . The density ρ at any point in space \mathbf{r} is computed as a weighted sum of the masses of the neighbouring particles (Monaghan 1992) via

$$\rho(\mathbf{r}) = \sum_{j=1}^{N_{\text{ngb}}} m_j W(\mathbf{r} - \mathbf{r}_j, h), \quad (1)$$

where W is the kernel function, which is a function of position, and h is the smoothing length. We will be referring to the density of particle i as $\rho_i \equiv \rho(\mathbf{r}_i)$, where \mathbf{r}_i is the position of particle i .

Once the densities are computed, we can use the intrinsic specific internal energy u_i of a particle (or any other thermodynamic variable), and the equation of state assigned to it (EoS, i) to compute the pressure at the location of each particle via $P_i \equiv P_{\text{EoS},i}(\rho_i, u_i)$.

At this point, we can compute the hydrodynamical forces using

$$\mathbf{F} = \frac{\nabla P}{\rho} = \nabla \left(\frac{P}{\rho} \right) + \frac{P}{\rho^2} \nabla \rho. \quad (2)$$

Then, we can discretize the acceleration of each particle

$$\mathbf{a}_i = - \sum_{j=1}^{N_{\text{ngb}}} m_j \left(\frac{P_j}{\rho_j^2} + \frac{P_i}{\rho_i^2} \right) \nabla_i W_{ij}, \quad (3)$$

where $W_{ij} \equiv W(\mathbf{r}_i - \mathbf{r}_j, h_{ij})$. This formula was first derived using a discrete form of the action principle for an adiabatic fluid. The rate of change in internal energy for particle i can be expressed as

$$\frac{du_i}{dt} = \frac{1}{2} \sum_{j=1}^{N_{\text{ngb}}} m_j \left(\frac{P_j}{\rho_j^2} + \frac{P_i}{\rho_i^2} \right) \mathbf{v}_{ij} \cdot \nabla_i W_{ij}, \quad (4)$$

where $\mathbf{v}_{ij} \equiv \mathbf{v}_i - \mathbf{v}_j$. We will be referring to these two formulae above as the standard SPH equations of motion.

This is not the only choice of discretization that can be used. We will now briefly summarize the geometric density average force (GDF) method (Wadsley, Keller & Quinn 2017), ignoring artificial viscosity terms:

$$\mathbf{a}_i = - \sum_{j=1}^{N_{\text{ngb}}} m_j \left(\frac{P_i + P_j}{\rho_i \rho_j} \right) \nabla_i \bar{W}_{ij}, \quad (5)$$

$$\frac{du_i}{dt} = \sum_{j=1}^{N_{\text{ngb}}} m_j \left(\frac{P_i}{\rho_i \rho_j} \right) \mathbf{v}_{ij} \cdot \nabla_i \bar{W}_{ij}. \quad (6)$$

It is worth noting that these equations come from a general form of equation (2) presented already by Monaghan (1992),

$$\frac{\nabla P}{\rho} = \frac{P}{\rho^\sigma} \nabla \left(\frac{1}{\rho^{1-\sigma}} \right) + \frac{1}{\rho^{2-\sigma}} \nabla \left(\frac{P}{\rho^{\sigma-1}} \right), \quad (7)$$

with $\sigma = 1$. This choice was made in order to minimize errors in the vicinity of strong density gradients. In addition to this choice, the GDF method also requires a symmetric gradient of the kernel, in order to have symmetrized force terms, namely

$$\nabla_i \bar{W}_{ij} = \frac{1}{2} f_i \nabla_i W(\mathbf{r}_{ij}, h_j) + \frac{1}{2} f_j \nabla_j W(\mathbf{r}_{ij}, h_j), \quad (8)$$

where

$$f_i = \sum_{j=1}^{N_{\text{ngb}}} \frac{m_j}{\rho_i} r_{ij}^2 W' \left(\frac{r_{ij}}{h_i} \right) \bigg/ \sum_{j=1}^{N_{\text{ngb}}} \frac{m_j}{\rho_j} r_{ij}^2 W' \left(\frac{r_{ij}}{h_i} \right), \quad (9)$$

and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, $W(\mathbf{r}_i - \mathbf{r}_j, h_i) = \frac{1}{h_i^3} W \left(\frac{r_{ij}}{h_i} \right)$, $W'(q) = \frac{1}{q} \frac{dW}{dq}$.

This formulation of SPH minimizes surface tension effects in multiphase flows, which can be a desirable feature for planetary SPH simulations where the mixing between materials is key to some problems.

Wadsley et al. (2017) chose to use Wendland (1995) kernels over the traditional cubic spline kernel (Monaghan 1992) because they do not suffer from the pairing instability (Dehnen & Aly 2012). However, the GDF method itself does not require a specific kernel. Hence, we will use the traditional cubic spline kernel in this work when comparing different flavours of SPH, for simplicity.

An important characteristic of planetary SPH simulations is the choice of materials, or in other words, equations of state (EoS). Each particle is labelled as being a particular material and, whenever needed, its equation of state is applied to compute its pressure. One well known and widely used option is the Tillotson (1962) EoS. This analytical EoS was originally developed to model hypervelocity impacts, partly motivated by nuclear weapons research. Each material (e.g. iron, granite, etc.) is described by 10 parameters and 3 common analytical expressions describing a compressed or cold state, a hot and expanded state, and a hybrid state. As mentioned, this option is widely used for its simplicity but it has significant limitations. Materials described by the Tillotson EoS lack phase transitions, as well as not being suitable for giant impact simulations where vaporization plays an important role (Stewart et al. 2020). One example of a more modern approach is to use the ANEOS EoS (Thompson 1970; Melosh 2007; Stewart et al. 2020). This EoS model is described by the Helmholtz free energies for solid, liquid, vapour, plasma, and mixed phases. It is capable of covering a large range of pressures, densities, and temperatures, which is important for simulating giant impacts between proto-planets. ANEOS EoS have over 40 input parameters, and multiple phase transitions are present for any material. The presence or absence of phase transitions in the EoS used for the simulations, as shown in Fig. 1, will have a key role when designing a method to solve our density discontinuity problem, as described in Section 2.2.1.

In this work, we will use the open-source hydrodynamics and gravity code SWIFT (SPH with inter-dependent fine-grained tasking; www.swiftsim.com, Schaller et al. 2016; Kegerreis et al. 2019). SWIFT has been designed from scratch to run large simulations and scale well on shared/distributed-memory architectures. SWIFT runs over 30 times faster than GADGET-2 on representative cosmological problems (Borrow et al. 2018), and has enabled planetary impact simulations with 100–1000 times more particles than was previously typical. This speed is partly a result of SWIFT's task-based approach to parallelism and domain decomposition for the gravity and SPH calculations (Gonnet 2015).

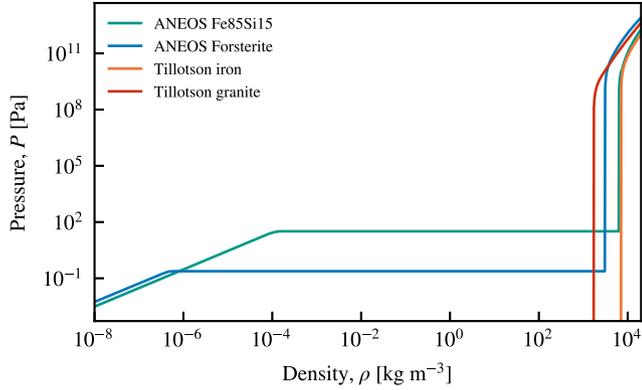


Figure 1. Pressure as a function of density at a fixed temperature, $T = 2000$ K, for different materials commonly used in planetary SPH simulations. Horizontal segments represent the phase transitions that are present only for more sophisticated equations of state like ANEOS.

2.2 Problems in planetary SPH

Given the definition of the density field in SPH (equation 1), a direct consequence is that the density varies smoothly in space, which makes density discontinuities difficult to represent. However, differentiated planets in hydrostatic equilibrium can and should contain density discontinuities both where there is a change of material (e.g. the core to mantle boundary) and at the surface of the planet.

When trying to represent a planet in SPH simulations, the smoothing of SPH particle densities across these discontinuities gives rise to well-known problems (Woolfson 2007), with poorly quantified consequences. The incorrect pressures induced by the smoothed densities in these regions effectively create an artificial force that repels different material layers from each other. In the case of the free surface, particles in the outermost regions of the planet will have their densities underestimated. This will subsequently lead to underestimated pressures that will accelerate the system away from the desired equilibrium configuration. We illustrate the initial problems using a Theia-like body, with mass $M = 0.133 M_{\oplus}$, in Fig. 2. The analytical profile and particle placement for this, and all examples in this paper, have been produced by the open-source code WoMa (Ruiz-Bonilla et al. 2021), which uses the SEAGen method (Kegerreis et al. 2019) to make particle realizations of planets. Note that the artificial effective surface tension is equally present for both the standard and GDF flavours of SPH, because it arises from the definition of the density field, which is common to both methods.

2.2.1 Density discontinuities between different material layers

Previous studies have attempted to address the issue of density discontinuities between different materials by changing the formulation of SPH (Price 2008; Hosono, Saitoh & Makino 2016). Woolfson (2007) and later Reinhardt et al. (2020) proposed solutions based on computing correction factors, f_{ij} , for the SPH density, which was corrected via

$$\rho_i = \sum_{j=1}^{N_{\text{ngb}}} f_{ij} m_j W_{ij},$$

$$f_{ij} = \frac{\rho_{\text{EoS},i}(P, T)}{\rho_{\text{EoS},j}(P, T)}. \quad (10)$$

The density of particle i is calculated with the inclusion of the correction factor, which varies for each neighbouring particle j . The correc-

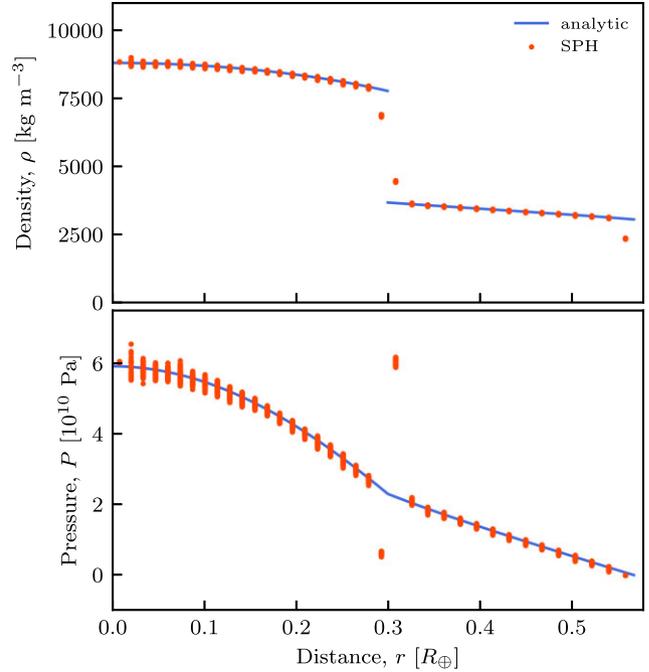


Figure 2. Initial density (upper panel) and pressure (lower panel) profiles of a spherical Theia-like planet, $M = 0.133 M_{\oplus}$, using standard SPH density calculations. The core:mantle mass ratio is 30:70, and the temperature at the surface of the planet is 2000 K with an adiabatic entropy profile. 10^5 particles are used to represent the planetary body. The smoothing in the density field introduces spurious pressures at the material boundary and, to a lesser extent, the edge of the planet.

tion factors represent the ratio of densities that particle i would have at pressure P and temperature T if it were made from material i versus material j . Thus, if neighbour j is the same material as particle i , then $f_{ij} = f_{ji} = 1$. Woolfson (2007) applied this modification to equilibrium models of planets, where the temperature and pressure vary smoothly with radius. Reinhardt et al. (2020) suggested using the kernel-averaged temperature and pressure as better estimates to account for dynamical evolution of the system during a giant impact simulation.

This approach can reduce the problem, especially for stationary planets, but has a couple of inconvenient drawbacks. The first is that, computationally, it requires three loops over all particles to compute the density, compared with the single loop used in the standard density definition: the first loop is used to compute the standard SPH density, the second one to compute the kernel averages of temperature and pressure, and the third one to recompute the density using equation (10). In addition to these, there is a final fourth loop to compute the hydrodynamical forces using equations (3) and (4) for standard SPH or equations (5) and (6) for GDF. The second and more serious downside appears when using more sophisticated equations of state like ANEOS. As shown in Fig. 1, for the same temperature and pressure, two materials could have different densities by many orders of magnitude. For example, at 10 Pa and 2000 K, the density ratio between Tillotson iron and granite is 0.2, but between ANEOS $\text{Fe}_{85}\text{Si}_{15}$ and forsterite is 9.5×10^7 . This occurs because one material (in this case $\text{Fe}_{85}\text{Si}_{15}$) has undergone vaporization whereas the other (forsterite) has not. When computing the final density using equation (10), the f_{ij} factors could produce hugely unrealistic densities if particle i has a significant number of neighbours j of a different material. This issue would not only affect the density estimation of a few particles and hence the evolution of

the system, but the high densities will also yield high pressures and hence forces that will dramatically decrease the value of the time-step needed to continue evolving the simulation. Reinhardt et al. (2020) do not perform any correction if a particle has a density below an empirically determined threshold, in order to avoid this problem (private communication).

2.2.2 The free surface problem

Reinhardt & Stadel (2017) also proposed a solution, distinct from those described above, to the problem of the density discontinuity present at the surface of any planet. Their approach consisted of defining a statistic

$$f_i = \frac{\left| \sum_{j=1}^{N_{\text{ngb}}} (\mathbf{r}_j - \mathbf{r}_i) m_j W_{ij} \right|}{2h_i \sum_{j=1}^{N_{\text{ngb}}} m_j W_{ij}} \quad (11)$$

that is computed for every particle. The density of each particle is corrected by a factor that depends upon the value of this statistic, f_i , with the correction factor derived by assuming that the particle configuration involves a plane boundary between mass and vacuum in the kernel. This assumption may be appropriate to explain non-zero f_i values during a simulation of a planet in hydrostatic equilibrium. However, there could be different scenarios where this is not the case during a planetary impact SPH simulation, for instance a satellite being tidally disrupted into some distorted geometry. Thus, a more general approach to correcting densities near the boundary with a vacuum is desirable.

2.3 Density corrections

Here, we present our method to address both the material boundary and free surface problems at once. In addition, this method is relatively computationally cheap since it only uses one extra loop over all particles compared with the standard SPH density computation. We define a statistic that measures how afflicted a particle is by being close to a density discontinuity. The densities of these particles are then corrected in a smooth way using that same statistic.

The method can be summarized as two steps: first, we identify problematic particles, then we fix their densities. Our first goal is to identify particles close to a material boundary or free surface. Our proposal, which is similar to that of Reinhardt & Stadel (2017), is

$$I_i = \alpha \frac{\left| \sum_{j=1}^{N_{\text{ngb}}} \kappa_{ij} (\mathbf{r}_j - \mathbf{r}_i) m_j W_{ij} \right|}{h_i \sum_{j=1}^{N_{\text{ngb}}} m_j W_{ij}}, \quad (12)$$

$$\kappa_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are the same material,} \\ -1 & \text{if } i \text{ and } j \text{ are different material.} \end{cases}$$

where α is a dimensionless parameter whose value we discuss later. We will refer to I_i as the ‘imbalance statistic’ for particle i .

Particles sitting in the middle of a perfectly regular grid of the same material particles will have an imbalance statistic equal to zero, and this will be approximately the case for most of the particles in our initial planet in hydrostatic equilibrium. Particles sitting at the surface of a planet will have about half of their kernel filled with particles of the same material and the other half empty. Their imbalance statistics should be somewhat greater than zero and, for the choice of α we

describe in due course, they will be of order unity. Similarly, for particles placed at the boundaries between two materials, one half of their kernel is full of particles of the same material whereas the other hemisphere is full of particles of a different material; hence, the inclusion of the minus sign in κ_{ij} to account for the contributions from particles of the other material and produce a comparable unity-order value for I_i .

Now that we have defined the imbalance statistic that locates the problematic particles, we need to correct their densities. First, we compute the standard SPH density using equation (1), and the pressure, P_i , and temperature, T_i , for every particle using their corresponding equation of state with their density, ρ_i , and specific internal energy, u_i , which is used in the hydrodynamical simulation rather than the temperature. Then, assuming that pressure and temperature vary smoothly on the scale of the smoothing length everywhere within the simulation, we compute, for every particle, estimated values for their temperature and pressure via

$$\tilde{T}_i = \frac{\sum_{j=1}^{N_{\text{ngb}}} T_j e^{-I_j^2} W_{ij}}{\sum_{j=1}^{N_{\text{ngb}}} e^{-I_j^2} W_{ij}}, \quad \tilde{P}_i = \frac{\sum_{j=1}^{N_{\text{ngb}}} P_j e^{-I_j^2} W_{ij}}{\sum_{j=1}^{N_{\text{ngb}}} e^{-I_j^2} W_{ij}}. \quad (13)$$

These estimates represent pressures and temperatures averaged over neighbouring particles, weighted to favour nearby neighbours with low imbalance statistics. Recall that low imbalance statistic particles typically have neighbours sitting in regular grids, so those particles should be away from sharp density discontinuities and thus in regions where pressures and temperatures are computed accurately. In addition, we would like to have a smooth transition between the standard SPH computation and our modified one, such that the modification is only used when needed and without any sudden transitions. Hence we can define a pressure, \tilde{P}_i , and temperature, \tilde{T}_i , for every particle as

$$\begin{aligned} \tilde{P}_i &= e^{-I_i^2} P_i + (1 - e^{-I_i^2}) \tilde{P}_i, \\ \tilde{T}_i &= e^{-I_i^2} T_i + (1 - e^{-I_i^2}) \tilde{T}_i, \end{aligned} \quad (14)$$

such that the more problematic a particle is (the higher the imbalance statistic) the greater the contribution from the modified estimate. Now that we have estimated a corrected pressure and temperature for every particle, we use the corresponding equation of state to infer a corrected density for every particle via

$$\tilde{\rho}_i = \rho_{\text{EoS},i}(\tilde{T}_i, \tilde{P}_i). \quad (15)$$

Finally, we compute a particle pressure based upon this corrected density and the unaffected specific internal energy, using $P_i = P_{\text{EoS},i}(\tilde{\rho}_i, u_i)$. $\tilde{\rho}_i$ and P_i are the values that are used in the equations of motion.

We determine the value of α with the following condition: a particle with a kernel that is half full of particles of the same material organized in a regular grid, and with the other half empty must have imbalance statistic equal to 1.5. We have chosen this value empirically, since an imbalance statistic of 1 has very little effect on the densities of particles one shell away from a different material, and a value of 2 significantly affects particles two shells away from a different material. This ensures particles at the surface of the planet and the material boundaries will have big enough imbalance statistics for the method to have a significant impact, without overcorrecting. This parameter may need to be adjusted if the kernel and/or the resolution parameter η (i.e. the number of neighbours within the kernel) is changed. Fig. 3 shows the reduced imbalance statistic, I/α , for different kernels and numbers of neighbours. The minimum

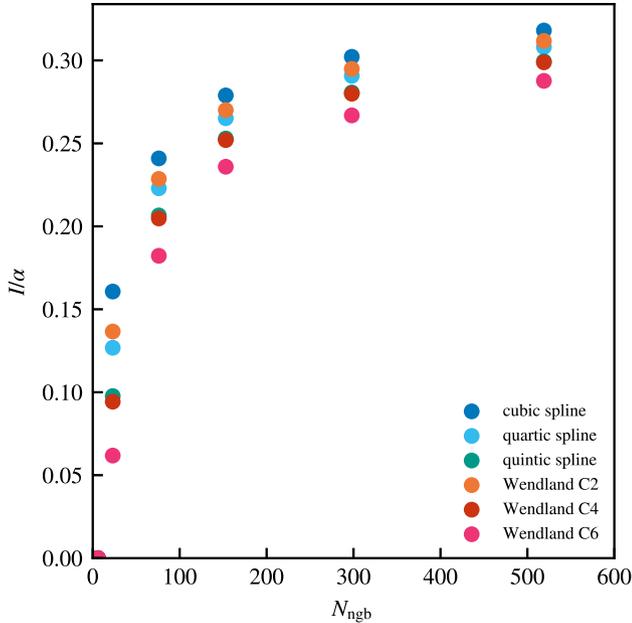


Figure 3. The scaled imbalance statistic, I/α (equation 12), calculated at the centre of a sphere, only half of which is filled by particles in a regular cubic grid, as a function of the numbers of neighbours. This value is computed to normalize the value of the imbalance statistic so that it affects the first shell of particles at a density discontinuity, but not the rest. Different colours represent a variety of kernels, as detailed in the legend.

number of particles used to compute I/α is 6 [(0, 0, 0), ($\pm 1, 0, 0$), (0, $\pm 1, 0$), and (0, 0, -1)]. By making that grid finer, we can compute it with 23, 76, 153, 298, and 519 particles. Finally, we interpolate linearly to obtain the value of α that yields $I = 3/2$, depending on the desired number of neighbours.

This method only uses two loops over the neighbours of all particles. The first loop is used to compute the standard SPH density, pressure, and temperature, as well as the imbalance statistic for every particle; the second loop is used to evaluate equation (13), which leads to the corrected density, $\tilde{\rho}_i$, and final pressure. To illustrate how our method works, Fig. 4 shows the imbalance statistic, the intermediate estimate of the pressure, and the final corrected density, for the same Theia-like planet that was shown in Fig. 2. The imbalance statistic targets the right particles and the weighted and smoothed pressure estimate erases the pressure jump that is present for standard SPH. Finally, using the equation of state, we compute corrected densities that have values close to the analytical solution.

Fig. 5 demonstrates the different calculations of density produced for one (identical) snapshot of a simulation by the three methods: standard SPH (equation 1), the Reinhardt & Stadel (2017) method described in Section 2.2.1, and our method described above. The exact same particle configuration is used in all cases, a mid-collision snapshot of a giant impact between a proto-Earth and Theia, using ANEOS materials. The different densities produced by the three methods would lead to different subsequent evolution of these cases, if they were evolved forward from this common starting point using the different methods. The distinction between core and mantle material in the proto-Earth is quite diffuse in the standard SPH computation compared with the other two methods. The Reinhardt & Stadel (2017) method yields particles with densities over 10^5 kg m^{-3} , highlighted in red in the figure. This is due to the problem described in Section 2.2 when using equations of state with phase boundaries like ANEOS. Finally, the iron particles scattered within the mantle of

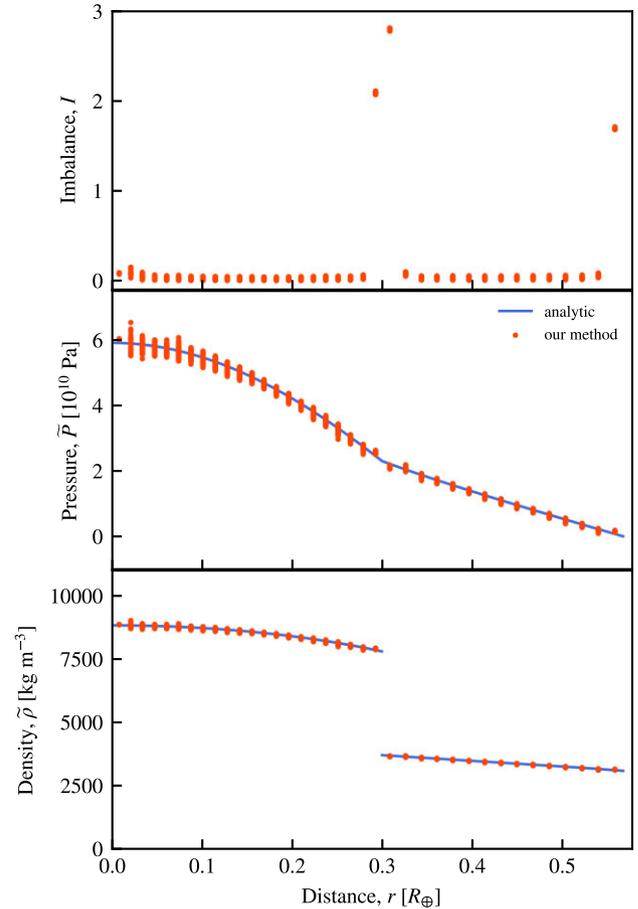


Figure 4. Imbalance statistic, I , estimated pressure from equation (14), \tilde{P} , and corrected density, $\tilde{\rho}$, for the same spherical Theia-like planet, $M = 0.133 M_{\oplus}$, used in Fig. 2.

the proto-Earth are assigned significantly higher densities using the Reinhardt & Stadel (2017) method or our method than for standard SPH, and thus are more clearly visible in the figure. This is because their method acts whenever a particle has a neighbour of a different material, whereas in our method having a regular grid of particles of random materials will yield a density identical to the standard SPH one, up to the noise in the particle distribution for each material. Hence, our method produces high densities for iron particles in the mantle when they have other iron particles as neighbours, but not when they are just surrounded by granite particles.

3 TESTS AND EXAMPLES

Up to this point, we have been using static distributions of particles to compare different ways to compute the density field in SPH simulations. Now, we will perform some dynamic tests and example simulations combining these density estimators with the two different equations of motion that were presented in Section 2.1, standard SPH and GDF SPH (Wadsley et al. 2017).

3.1 2D square test

One of the most common tests of contact discontinuities is the square test (Saitoh & Makino 2013; Deng et al. 2019a; Reinhardt et al. 2020). A 2D box of a certain material and density is surrounded by a medium of the same or different material at a different density

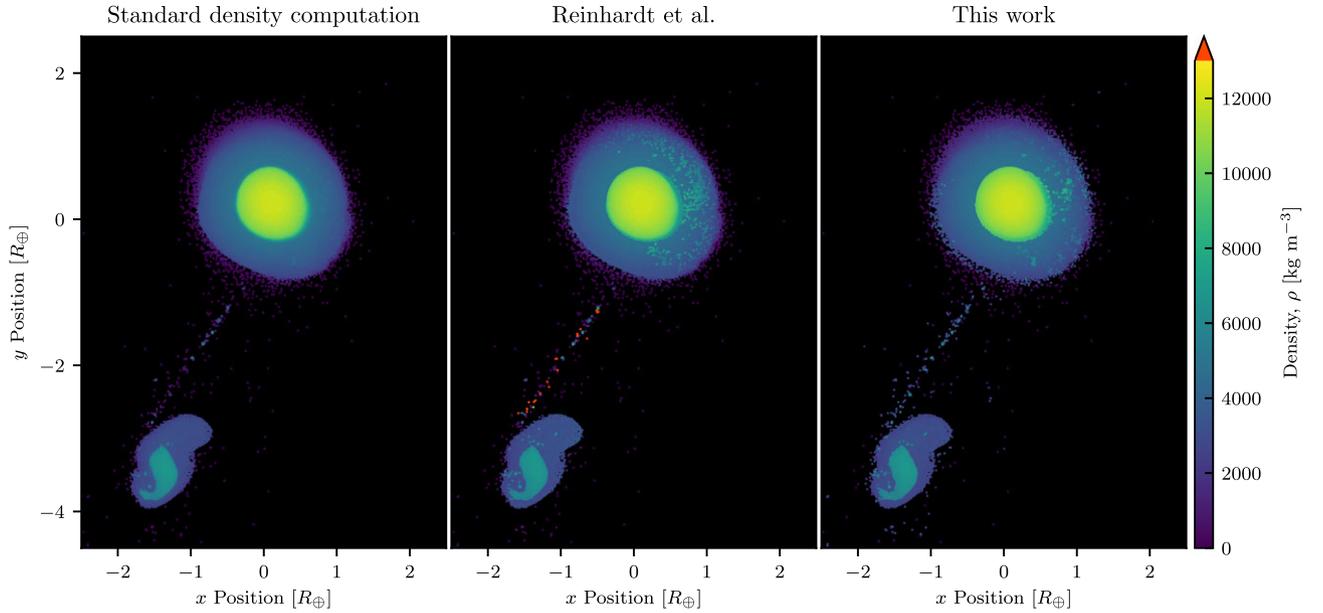


Figure 5. Different methods for computing the density for the exact same particle configuration, a mid-collision snapshot of a canonical impact using ANEOS materials. Higher density particles are plotted on top of lower density ones. Red particles are at least one order of magnitude higher in density than the maximum shown by the colour bar.

in pressure equilibrium. If the code does not capture the density discontinuity correctly, then the pressure at the material interphase becomes discontinuous. This creates an artificial tension, similar to that shown in Fig. 2, which effectively acts to round the corners of the box.

For this test, we use Tillotson (1962) materials, which are often used in planetary SPH simulations. The central square contains iron whereas the surroundings are composed of granite. The side length of the simulation box is $l_x = l_y = 0.5 R_\oplus$, and the depth of the box is $l_z = 0.001 R_\oplus$. This small thickness, together with periodic boundary conditions, allows densities to be computed in 3D despite particles being confined to 2D. The set-up is designed such that the pressure everywhere is 10^{10} Pa and the temperature is 1000 K. These constraints dictate the mass (i.e. density) and internal energy of each particle, and result in a density jump from $\rho_{\text{granite}} = 3251 \text{ kg m}^{-3}$ to $\rho_{\text{iron}} = 7980 \text{ kg m}^{-3}$. Iron particles, located in the inner square of side length $l_x/2$, are given a larger mass than granite ones such that the 2^{14} total particles in our simulations can be placed on to a regular square grid. Each simulation is evolved until 100 ks, which corresponds to roughly 300 sound crossing times of the central iron square.

We tested four different flavours of SPH: standard SPH; standard SPH with our method for improving densities; GDF SPH (Wadsley et al. 2017); and GDF SPH with our method. Adding our method on top of the standard SPH equations of motion has little effect on the overall evolution, so we will not discuss this combination for any of the tests in this paper. Fig. 6 shows the initial conditions and the result for the remaining three flavours of SPH following 100 ks of evolution. Relative to standard SPH, GDF SPH better maintains the shape of the central square, and our method further improves the sharpness of the corners.

3.2 2D Kelvin–Helmholtz test

The Kelvin–Helmholtz test is a common way to determine how well methods capture the instability that arises between adjacent

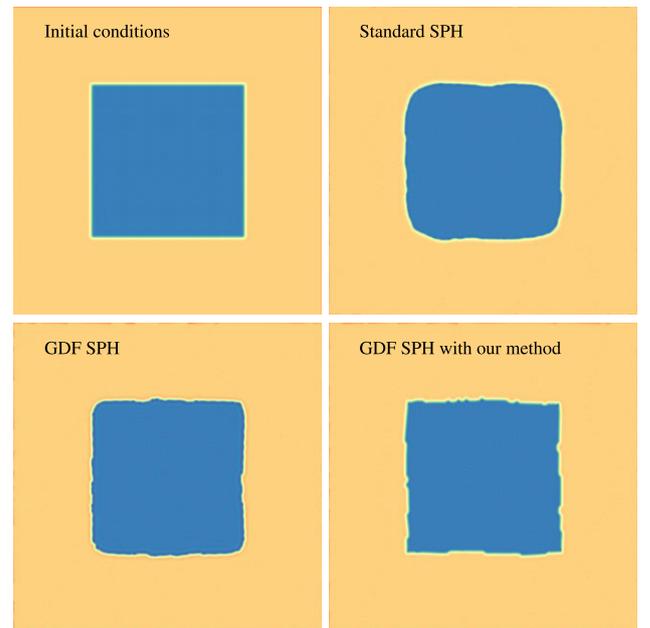


Figure 6. 2D square test for three different flavours of SPH: standard SPH, GDF SPH, and GDF SPH with our method. Blue and orange represent higher and lower density values, respectively. All panels, except for the initial conditions, show the result of the test after 100 ks, which corresponds to ~ 300 sound crossing times of the central iron square.

fluids moving with different velocities. This is particularly relevant for giant impact simulations where velocity shear between different materials is common. This test does not have a known analytical solution, so we compare with different hydrodynamic codes, how our method handles the Kelvin–Helmholtz instability.

For this experiment, we used the same box dimensions and materials as in the square test (Section 3.1). The pressure and

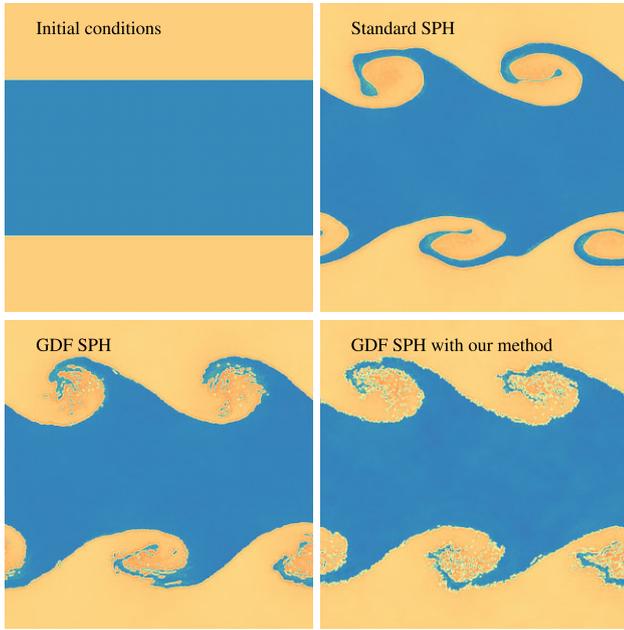


Figure 7. 2D Kelvin–Helmholtz test for three different flavours of SPH: standard SPH, GDF SPH, and GDF SPH with our method. Blue and orange represent Tillotson iron and granite respectively. All panels except that for the initial conditions show the result of the test after 2500 s.

temperature throughout the box were set to 10^{10} Pa and 1000 K, and the number of particles on the x -axis for the low-density material was $N = 256$. We chose all particles to have the same mass, so the denser layer contained ~ 2.5 times more particles. The central strip of iron particles were given an initial x velocity of $v_x = 1000 \text{ m s}^{-1}$, whereas the granite particles had $v_x = -1000 \text{ m s}^{-1}$. An initial perturbation in the y velocity, $v_y = 20 \sin(4\pi x/R_\oplus) \text{ m s}^{-1}$, was introduced in order to seed the instability.

We observe that all three flavours of SPH create roll-like structures after 2500 s, as shown in Fig. 7. At that time, a particle travelling at the original x velocity will have traversed just over three quarters of the box length. We can see clear qualitative differences between all three flavours of simulation and, relative to the other two cases, GDF SPH with our method shows enhanced mixing between different material particles at the end of the swirls.

We tested the numerical convergence for a range of resolutions up to $N = 2048$ and calculated the time evolution of the maximum y -direction kinetic energy density and the amplitude of the y -velocity mode of the instability. All three flavours of simulation produced very similar shapes to the SPH code results shown by McNally, Lyra & Passy (2012). Using the smoothed y velocity field values, rather than the individual SPH particle values, made the maximum y -direction kinetic energy density grow slightly slower, but in neither case was the evolution in this statistic comparable with that found for grid codes (McNally et al. 2012). We conclude that our method does not converge significantly faster or slower than previous formulations of SPH for this particular test.

3.3 Planetary profiles after settling simulations

Prior to running a planetary giant impact simulation, a settling simulation is typically undertaken for every proto-planet. This is done in order to reduce any noise from the initial positions of the particles, as well as to obtain an object that is in hydrostatic equilibrium.

Ideally the SPH densities, which are computed using the positions and masses of the particles, should match those obtained from solving the hydrostatic equilibrium equation. However, particle placement algorithms always introduce some perturbations and, as is the focus of this study, density discontinuities are not well captured with the traditional SPH density computation.

We consider a proto-Earth like planet, $M = 0.887 M_\oplus$, made of an ANEOS $\text{Fe}_{85}\text{Si}_{15}$ core and forsterite mantle (Stewart et al. 2020) with a surface temperature of $T = 2000$ K and adiabatic temperature profile. The core:mantle mass ratio is 30:70. We use approximately 10^6 particles and let the simulation run for 20 ks, which is many times the sound crossing time of the planet.

Fig. 8 shows the results for standard SPH, GDF SPH, and GDF SPH with our method. For standard SPH, we see the evolved versions of the same issues that were highlighted for the initial particle arrangement in Fig. 2. The density discontinuity in the material boundary is smoothed over, leading to a spurious jump in pressure across the boundary. Also, the underestimated density, and hence pressure, in the outermost shell of particles of the planet has decreased the radially outwards hydrodynamical force (see equation 3). Consequently, the planet has contracted to find its numerical equilibrium, leaving it slightly smaller than desired.

For GDF SPH with the standard density computation, the situation is even worse because it does not even reach an equilibrium state. The density discontinuity is somewhat smoothed, although not quite as badly as in the standard SPH case. However, there is an additional problem whereby particles at the edge of the planet continually leak away; note the expanded horizontal scale for these panels. The reason for this is the factor f_i described in equation (9). Consider the particles sitting at the edge of the main planet. Their neighbours are predominantly interior with higher densities. These outermost particles will have underestimated densities because of the exterior vacuum increasing their smoothing lengths. However, this problem will not affect the interior particles, which will have densities that more accurately reflect the input profile. As a consequence, f_i will be inappropriately large for the outermost particles, producing an outward hydrodynamical acceleration (equation 5) that exceeds the inward pull of gravity. Within two hours of simulation time, particles are already flying outwards. f_i can reach values of the order of 100, where the typical value should be around 1, and this effect gradually peels off more layers from the outer edge of the planet.

GDF SPH with our method solves the problems mentioned above, as illustrated in Fig. 8. Not only is the density discontinuity well represented, which means that there is no jump in the pressure profile between the core and mantle, but the outer boundary also closely matches the analytical profile, meaning that the planet has the intended radius.

3.4 Giant impacts

In this section, we compare features that occur during giant impacts between planets for different flavours of SPH. In Section 3.3, we saw that GDF SPH needs to be accompanied by our method in order to have stable planets; therefore, we will just consider standard SPH and GDF SPH with our method.

We use the proto-Earth and Theia described in Sections 3.3 and 2.2, respectively, increase the number of particles by a factor of 10, and collide them with a range of impact angles and velocities. The total number of particles in our simulations is approximately 10^7 , with all particles having the same mass.

We run three different impact scenarios, varying the angle of impact β and the impact velocity at contact v_c : a ‘canonical’ impact

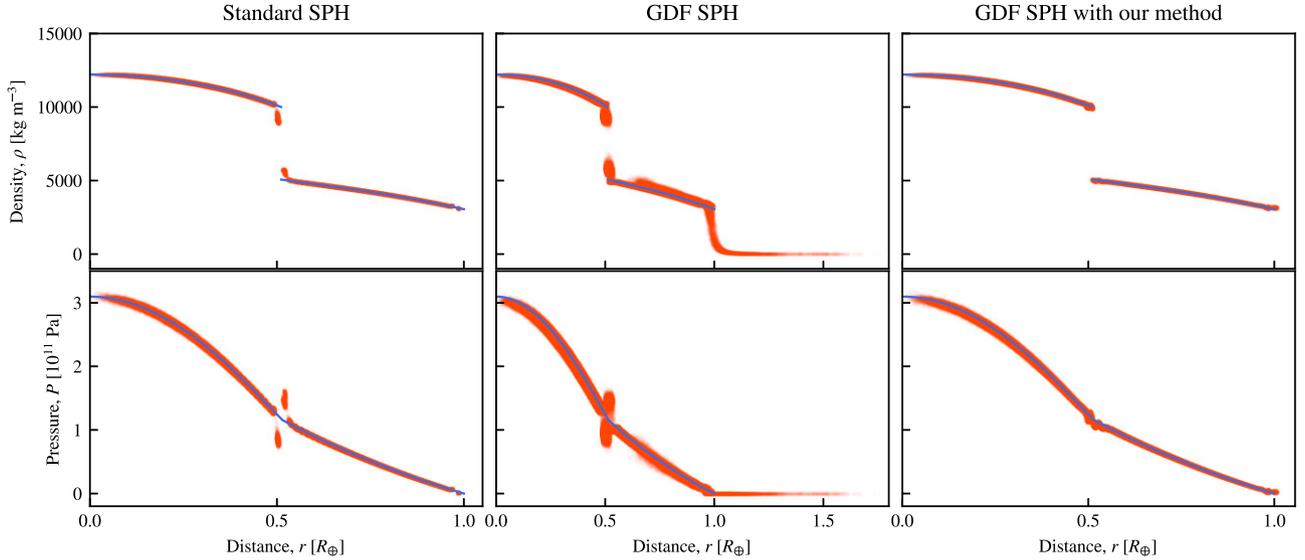


Figure 8. Density (top row) and pressure (bottom row) profiles after 20 ks of a settling simulation of a proto-Earth in hydrostatic equilibrium, for different flavours of SPH (different columns). The blue line represents the analytical profile, and red dots represent particles in the simulation. The central column, showing the GDF SPH results, has an expanded radial scale to show the extent to which particles are leaking away.

($\beta = 45^\circ$, $v_c = 1v_{\text{esc}}$), a faster low-angle impact ($\beta = 15^\circ$, $v_c = 2v_{\text{esc}}$), and a hit-and-run grazing impact ($\beta = 65^\circ$, $v_c = 1.5v_{\text{esc}}$). The mutual escape velocity of the system is $v_{\text{esc}} = 9026 \text{ m s}^{-1}$. Each impact is run four times using different random reorientations of the particle realizations of the planets. This provides an estimate of the stochastic noise and allows us more confidently to ascribe any observed differences to the different flavour of SPH being used. Depending upon just how chaotic the impact and its aftermath are, this can be an important consideration (Kegerreis et al., in preparation).

We have now resolved the density discontinuity issues we previously had, and can thus be confident that these are not causing big unknown errors. Beyond the broad similarities, we observe some key differences between both flavours of SPH. These are common to all of the randomly reoriented resimulations and so appear to be robust differences between the standard SPH case and that with GDF SPH plus our method.

Changing between the two SPH flavours leads to significant differences in the distribution of post-impact iron in our low-angle collisions. The mass fraction of iron in the debris beyond $3 R_\oplus$ is ~ 8 per cent using our flavour of SPH. This is about three times higher than the corresponding value for standard SPH. Within the final planet, the transition region between core and mantle, defined as the region where the relative iron content as a function of distance drops from 99 per cent to 10 per cent, is $0.12 R_\oplus$ for standard SPH and $0.41 R_\oplus$ for GDF SPH with our method. This demonstrates how mixing of materials can increase if the spurious boundary pressure gradients associated with standard SPH are suppressed using GDF SPH and our method. For both the canonical-like and hit-and-run impacts, the core of the target is barely disrupted by the impactor and the distribution of post-impact iron is insensitive to the flavour of SPH used.

In the initial conditions for our iron and rock bodies, the fraction of particles that have their densities badly mis-estimated by standard SPH as a result of their proximity either to a material boundary or the edge of the planet is ~ 14 per cent for a 10^5 -particle realization. This drops to a still large ~ 7 per cent with 10^6 particles, and ~ 3 per cent for 10^7 particles. The fraction of particles that at some point during an impact simulation have $I > 1.5$, the value at the surface of a

planet, is much larger. For 10^7 -particle simulations, this fraction is 10 per cent, 30 per cent, and 70 per cent for hit-and-run, ‘canonical’, and low-angle impacts, respectively. The spurious density is often sufficiently wrong that the particle will be translated across a phase boundary in its EoS. In addition to producing spurious pressure, this will complicate efforts to track the thermal evolution of the material, both during the impact simulation and when providing inputs for subsequent long-time-scale thermal evolution codes. This is relevant for material in the target and the resulting debris, be it a diffuse disc or in coherent clumps (Ruiz-Bonilla et al. 2021). The combination of GDF SPH with the method we have described here practically eliminates these problems that are present in standard SPH approaches, opening up the opportunity to use SPH planetary giant impact simulations for such studies reliably.

4 CONCLUSIONS

We have presented a novel method to compute the density field in SPH simulations with particular reference to scenarios of planetary giant impacts. It solves problems that arise in SPH for systems with sharp density discontinuities between different materials and between any material and a vacuum, with low computational cost. We combine this method with the GDF SPH (Wadsley et al. 2017) equations of motion because of their treatment that minimizes spurious numerical surface tension effects in multiphase flows. An implementation of our method is publicly available as an option in the open-source code SWIFT (Schaller et al. 2016).

This new method produces improved performance in the 2D square test with a better maintained square shape, and enhanced mixing between different material particles in the 2D Kelvin–Helmholtz test. Simulations of impacts between a proto-Earth and Theia, where the core of the Earth has been highly disrupted by the impactor, reveal a partially diffused iron core and a higher mass of iron in the debris disc. This method also prevents smoothed densities from placing particles into inappropriate places in their material phase diagram. As a consequence, the thermodynamic evolution of material can be tracked more realistically throughout an impact and its aftermath.

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The research in this paper made use of the SWIFT open-source simulation code (www.swiftsim.com, Schaller et al. 2016) version 0.9.0.

DATA AVAILABILITY

The data underlying this article will be shared on reasonable request to the corresponding author.

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