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DEVELOPMENT AND VERIFICATION OF A PARTICLE NUMBER DENSITY VARIANT OF SPH TO ROBUSTLY INCORPORATE ENERGY AND HEAT TRANSFER

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Abstract. In this paper we present a particle number density variation on the standard smooth particle hydrodynamics (SPH) form of the heat conduction equation and show progress towards a the development of a robust equation of state to incorporate particle energy. Including energy terms into the SPH governing equations and the equation of state will allow for more complex physical phenomena in to be modelled such as natural convection and eventually processes such as change of state. A brief derivation of a particle number density heat conduction equation is presented along with a 2D heat conduction validation problem as well as an introduction to current progress towards developing an equation of state for pressure that incorporates energy (as a function of temperature only at this stage) and a simple proof of concept example demonstrating natural convection in an enclosed square.

1 INTRODUCTION

Heat transfer in fluids and its effect upon motion within fluid dynamics is of interest in many areas within science and engineering including desalination plans, within reactor cores in power plants and in complex enhanced oil recovery techniques such as steam assisted gravity drainage used in heavy oil recovery. This is especially true when considering complex multi-fluid or multi-phase interactions that are seen in these cases. With the introduction of heat conduction into the smoothed particle hydrodynamics (SPH) framework, it is necessary to consider what effect the temperature of the fluid will have upon the dynamics of a system.

While SPH has been widely used in the areas of momentum dominant fluid flow, there has been limited investigation into areas of buoyancy dominant flow. The Rayleigh-Taylor instability [1] is one example of a well examined buoyancy dominant flow, but there has been little work into intrinsically modelling thermally driven buoyancy problems. While there has been some modelling of these flows such as modelling natural convection in

a closed box and of the Rayleigh-Bernard instability [2, 3], this has been done using an artificial modification of the body force term in typical SPH via application of the Boussinesq approximation. The use of the Boussinesq approximation is the standard approach to modelling thermally driven buoyancy flow in a number of numerical schemes [2, 3]. The use of SPH should allow for these phenomena to be modelled without the utilisation of *ad hoc* approximations such as this. The logical source for motion for a thermally driven system is to include it within the equation of state. The simplest example of an equation of state is the ideal gas law, which while used for weakly polar gases at low pressures and moderate temperatures, is indicative that temperature and energy can play an important part in the dynamics of a system. Energy is not typically considered in standard SPH formulations and thus the equation of state used is based on a the speed of sound within the fluid being modelled, as well as its density [4, 5]. With the desire to model thermally dependant problems, how we use the equation of state in SPH needs to be revised.

While there has been a number of examples of heat conduction algorithms in SPH [2, 6, 7, 8, 9], there has been little agreement in literature in regards to how to connect energy and motion in the system, or if this is even possible. There has been some examples in wider literature of using the energy of a system to influence the governing equations in SPH [10], but this has predominantly been used as diffusive tuning parameters and none have taken the temperature of a particle into account. In a proof of concept example in this work, we will demonstrate our first steps towards utilising an equation of state to have the temperature of a particle influence its pressure and density, and thus, its dynamics by inducing motion.

Natural convection is a mechanism of fluid motion and heat transport wherein density differences that arise from temperature gradients drive motion. These density differences lead into a pressure difference that, with the application of gravity, causes the fluid to move so that hotter parts rise and cooler parts fall [11]. Since the fluid is conducting heat from the heating source and throughout the rest of the fluid while also moving, it can be a difficult problem to model appropriately. Other methods, such as finite difference, have had success modelling natural convection (for further reading see [12]), but they have draw backs that motivate the use of SPH. The main motivation being how well SPH methods deal with multi-fluid and multi-phase problems [1, 13, 14, 15]. Including multiple fluids within SPH is straight forward and the tracking of interfaces is handled intrinsically in its formulation. The primary issue with natural convection in SPH is that an incompressible fluid is only being modelled as a near incompressible fluid. While this causes minimal issues for momentum dominant flows (minor fluctuations in density having only small effects on results), the generally accepted perturbations (typically of up to a few percent variation) in density can be greater than the actual density fluctuations seen in natural convection that drive fluid flow.

This requires a new approach to the equation of state for a buoyancy dominant system, with the intention that this be valid for both typical momentum dominant systems and

multi-fluid systems to encompass and model more complex physical phenomena such as temperature dependent properties and change of state.

2 HEAT CONDUCTION

SPH discretization methods has been detailed widely in literature with a range of varying formulations. The direction chosen in this work is based on fundamentals formalized by authors such as Tartakovsky and Meakin [1, 16] and Hu and Adams [13] who base their SPH formulations around the concept of *particle number density* as opposed to the more standard density. This variant has been shown to perform more accurately for multi-fluid flows, which while not the focus of this particular work, will be examined in the future.

The discretization methods for particle number density SPH equations for some field quantity, A_i, and its gradient, ∇A_i, are given as

$$A_i = \sum_j \frac{A_j}{n_j} W_{ij} \qquad\qquad \nabla A_i = \sum_j \frac{A_j}{n_j} \nabla W_{ij} \tag{1}$$

where m is mass, n is the particle number density, $n_i = \rho_i / m_i = \sum_j W_{ij}$, and W_{ij} is the smoothing function.

The rate of change in internal energy due to conduction and with spatially or thermally varying conductivity is

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{1}{\rho} \nabla \left(\kappa \nabla T \right) \tag{2}$$

where U is internal energy, κ is thermal conductivity, ρ is density and T is temperature. This expression contains a number of second order spatial derivatives, which are sensitive to minor fluctuations and particle disorder for many SPH kernels [17, 6, 18]. Instead of directly calculating the second order derivative for the SPH kernel, an approximation for the second order derivative is used [18]

$$\nabla^2 A \,|_i \;\; = \;\; -2 \sum_j \frac{m_j}{\rho_j} \frac{A_j - A_i}{|r_{ij}|^2} \mathbf{r}_{ij} \nabla_i W_{ij} \tag{3}$$

where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ and are position vectors.

As this work uses a particle number density approach, a variation on (3) is used. Applying this and SPH discretization methods to (2), the following expression for heat conduction is obtained

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{1}{m_i} \sum_j \frac{1}{n_i n_j} \left(\kappa_i + \kappa_j \right) \left(T_i - T_j \right) \frac{\mathbf{r}_{ij}}{|r_{ij}|^2} \nabla W_{ij} \tag{4}$$

Since energy exchange is always balanced between a given pair of particles that are interacting, it is ensured that thermal energy conservation is maintained and that heat will flow from a higher temperature to a lower temperature inherently.

While (4) works for simple applications of heat conduction [2], it still has some minor issues. The thermal conductivity of two interacting particles are simply arithmetically averaged, which can result in the smearing of values at phase interfaces, particularly in problems where neighbouring material phases have drastically different thermal conductivities. Using a finite difference approach to look at discontinuous thermal conductivity values, Cleary and Monaghan [6] make the following substitution

$$(\kappa_i + \kappa_j) = \frac{4\kappa_i\kappa_j}{\kappa_i + \kappa_j} \tag{5}$$

An additional benefit to this is that ensuring adiabatic wall conditions becomes trivial numerically by having a thermal conductivity of 0. Previously, potentially complex setups of opposing conductivity values would need to be used, which is difficult in multi-fluid problems with a range of different thermal conductivities. With this final substitution we arrive at the final form of the heat conduction equation as a function of particle number density

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{1}{m_i}\sum_j \frac{1}{n_i n_j}\frac{4\kappa_i\kappa_j}{\kappa_i + \kappa_j}\left(T_i - T_j\right)\frac{\mathbf{r}_{ij}}{|r_{ij}|^2}\nabla W_{ij} \tag{6}$$

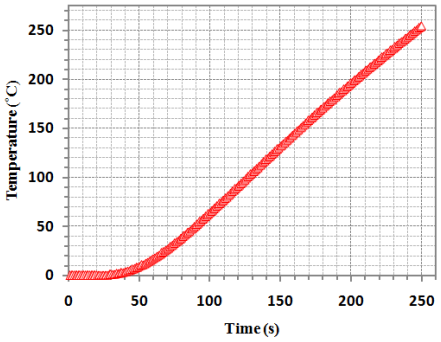
2.1 Verification of Heat Conduction Equation

The derived equation for heat conduction present earlier needs to be verified to ensure that it produces an accurate representation of heat conduction. The current commonly seen form for heat conduction is

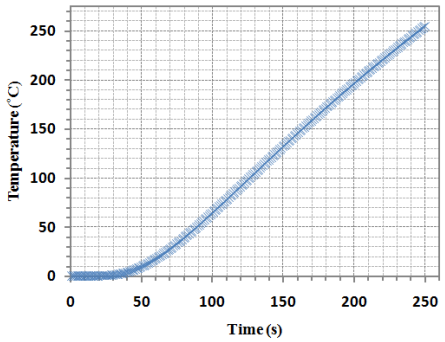
$$\frac{\mathrm{d}U}{\mathrm{d}t} = \sum_j \frac{m_j}{\rho_i\rho_j}\frac{4\kappa_i\kappa_j}{\kappa_i + \kappa_j}\left(T_i - T_j\right)\frac{\mathbf{r}_{ij}}{|r_{ij}|^2}\nabla W_{ij} \tag{7}$$

While the substitution appears trivial, it was necessary to robustly derive this equation from the first law of thermodynamics as it was dependant on density, and thus, also on particle number density when that approach is taken, and it has been shown in the past a straightforward substation would not necessarily yield the correct formulation [1]. The primary motivations for utilising this *NForm* of the heat conduction equation is twofold. In work done within our group, all forms of the SPH equations used are based on their particle number density forms as there is a focus upon multi-phase and multi-fluid problems and the utilisation of this approach has proved necessary for a more accurate representation of problems [15, 19].

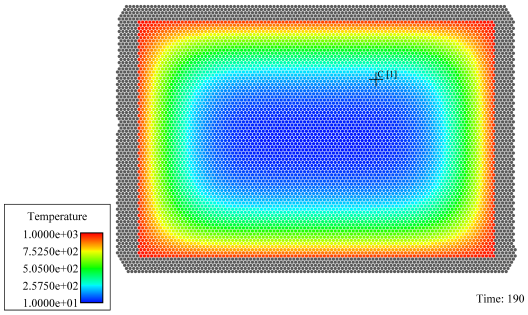
A simple 2D problem with a known solution was examined to determine if there was any differences between the standard and *Nform* variations. A domain of 0.6 x 0.4 meters with an internal domain initially at 0°C, with boundaries held at a constant temperature of 1000°C and material properties being a density of 7850 kg/m^3, a heat capacity of 460 J/kg°C and a thermal conductivity of 52 W/m°C. A provided solution is given for a point



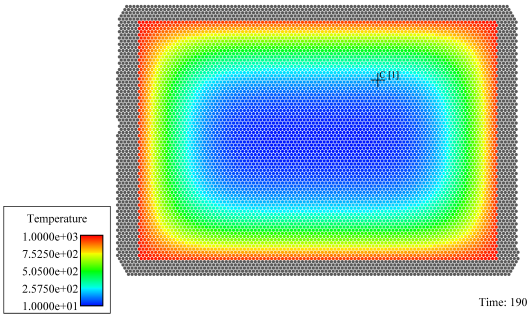
(a) Temperature over time for standard heat conduction



(b) Temperature over time for *NForm* heat conduction



(c) Particle temperatures for standard heat conduction



(d) Particle temperatures for *NForm* heat conduction

Figure 1: Figures comparing standard and *NForm* heat conduction at 190s with point of interest indicated.

of interest inside the domain. The benchmark result for a the point incident at $x = 0.4$ m and $y = 0.3$ m after 190s is a temperature of 186.5°C.

Figure (1) shows a comparison between the results obtained from using the standard SPH algorithm for heat conduction and the *Nform* algorithm, both of which were simulated using 9470 particles. It can be seen that as expected the results are identical between the two results with a value obtained of 183.52°C.

3 DEVELOPMENT OF AN ENERGY BASED EQUATION OF STATE

The equation of state is used in SPH to determine the pressure a given particle exerts on its surroundings. For standard incompressible flow problems, using a truly physical equation of state will result in prohibitively small time steps. As such, fluids are effectively modelled as quasi-incompressible. This also leads to most equation of states being modified on a case by case basis to suit the problem at hand. The most common form for the equation of state used for incompressible flows, and used in previous work, is the

Morris [20] equation of state

$$p = c_0^2 (\rho - \rho_0) \tag{8}$$

where p is pressure, c_0 is the artificial speed of sound and ρ_0 is a reference density. The vast majority of state equations are similar in this regard. They are almost all a function of density that is modified by a reference density and scaled by a constant (the artificial speed of sound) and it is this constant that is varied to obtain a convergent solution for a problem. The other feature seen in some equation of states is a minor influence from a more gaseous equation of state by raising part of the equation to a power. This was first introduced by Monaghan [4] for modelling free surface flows

$$p = B \left(\left(\frac{\rho}{\rho_0} \right)^{\gamma} - 1 \right) \tag{9}$$

where γ is a constant that is usually taken to be 7, similar to what is used in a gaseous equation of state and B is again a problem dependant parameter. It is simple to see how both equations of state are in actuality quite similar. The subtraction of 1 seen in (9) was introduced to remove nonphysical boundary effects at a free surface [21] and this has a similar effect in (8) but rearranged and is a common feature of state equations that are also valid for free surface flows.

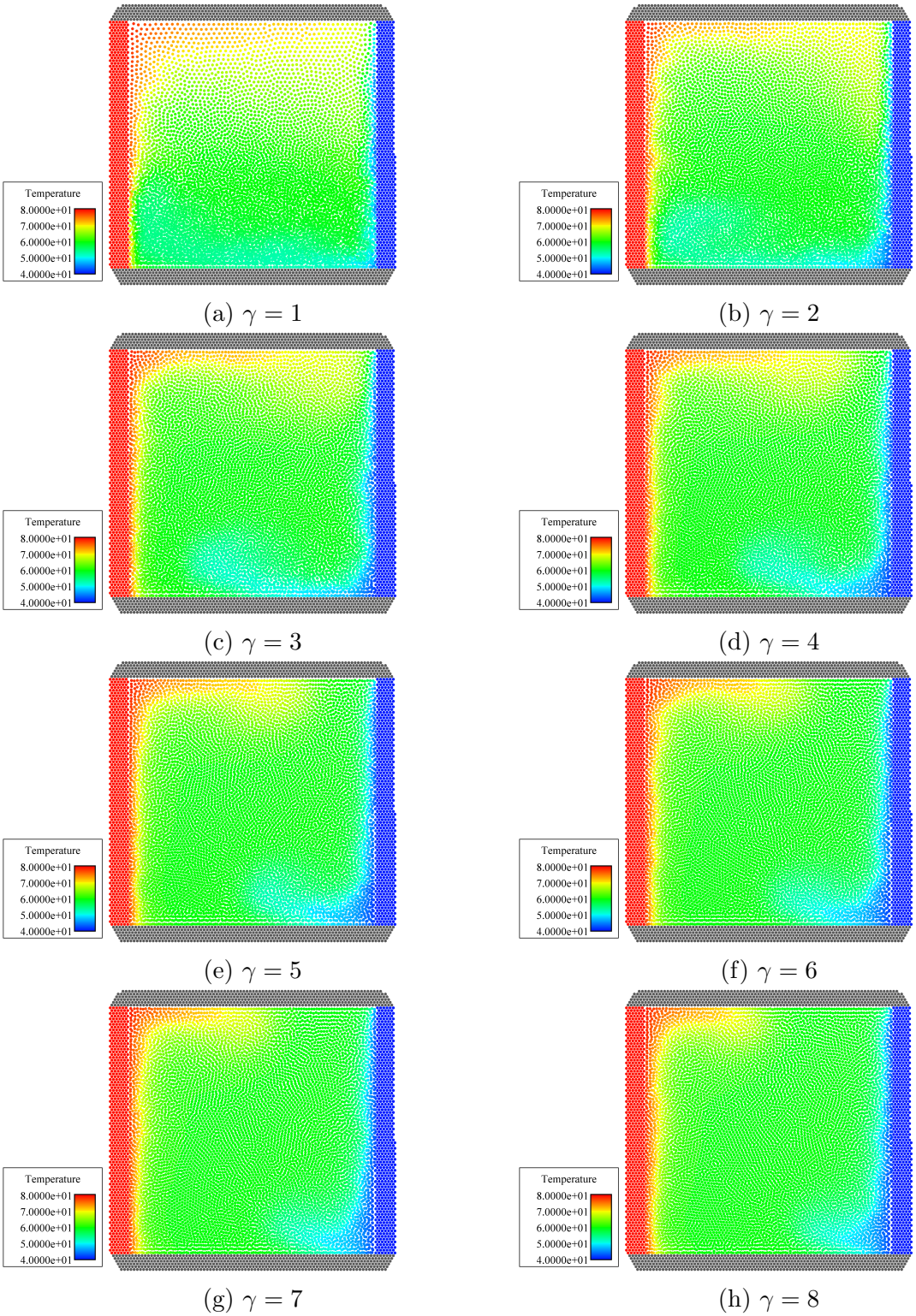
An equation of state incorporating temperature was developed to model a simple natural convection test case. The aim was to determine if it is possible to observe natural convection flow without the use of the Boussinesq approximation [2, 3].

To begin with, a simple equation of state was proposed to to determine what effect changing different parameters would have upon a thermally dynamic system.

$$p = c_0^2 T \left(\frac{\rho}{\rho_0} \right)^{\gamma} \tag{10}$$

In this case, γ is free to vary and c_0^2 is simply being treated as a constant without any direct physical significance for the time being. There also isn't any term to account for free surface effects as all systems initially considered will be contained.

The problem chosen to test Equation (10) is that of a 2D box enclosing a fluid at 60°C with one side held constant at 80°C, the other at 40°C, an adiabatic top and bottom, and a gravitational acceleration of 0.001 m/s^2 in the negative Y-direction. The fluid has a density of 1000 kg/m^3, a dynamic viscosity of 0.001 kg/ms, a heat capacity of 4181 J/kg°C and a thermal conductivity of 50 W/m°C. All thermal and viscous properties are assumed to be constant and independent of temperature. Tests were performed to establish to what degree natural convection behaviour would be observed for varying values of γ and c_0.



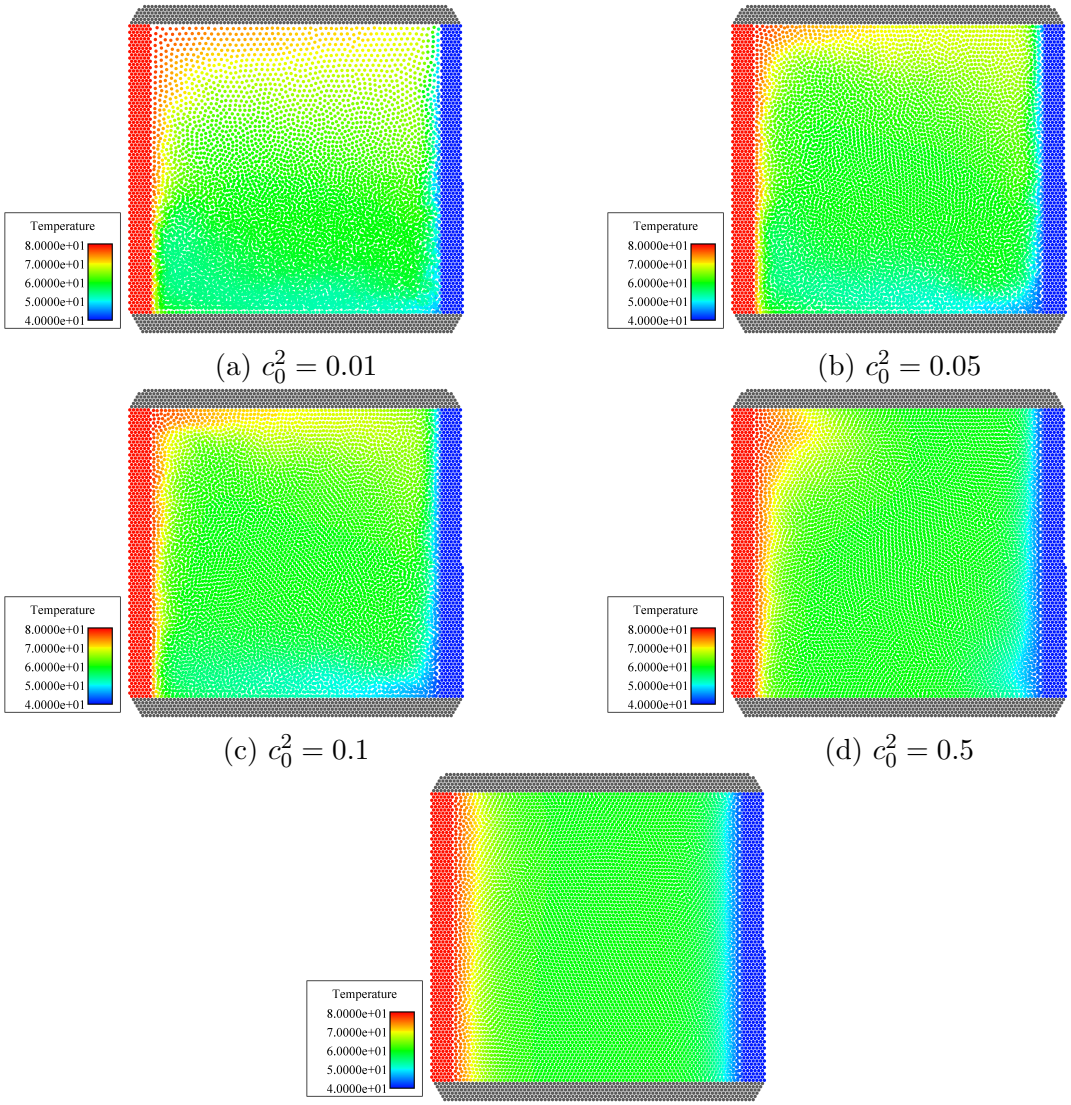
(a) $\gamma = 1$ (b) $\gamma = 2$

(c) $\gamma = 3$ (d) $\gamma = 4$

(e) $\gamma = 5$ (f) $\gamma = 6$

(g) $\gamma = 7$ (h) $\gamma = 8$

Figure 2: Temperature visualisation of enclosed box with $c_0 = 0.01$, varying γ and after 500s.



(a) $c_0^2 = 0.01$ (b) $c_0^2 = 0.05$

(c) $c_0^2 = 0.1$ (d) $c_0^2 = 0.5$

(e) $c_0^2 = 1$

Figure 3: Temperature visualisation of enclosed box with varying c_0^2, $\gamma = 1$ and after 500s.

Figure (2) shows the effect increasing the value of γ has upon the system. In these cases, the influence of the ratio of a particles current density to its initial density is increased. The greater this influence is, the less of a tendency there is for particles to clump too close together due to external forces. This in turn has the result of effectively decreasing the amount of compressibility that is possible within the system. However, if this value is allowed to be too large, it may have the effect of restricting motion in the system by not allowing any physical displacement due to the small amount of compression (however

temporary) this may cause. Allowing for motion in this way can be thought of relating back to the requirement that there be some minor degree of quasi compressibility in SPH systems.

Figure (3) shows the effect of increasing the value of c_0 has upon the system. The effect here is more straight forward as it is essentially a scaling factor on the magnitude of pressure that will be present in the system and so will be very dependant on the type of problem and the values of various parameters within a given system. In the example shown, it can be seen that the larger this scaling value, the more *resistant* the particles are to motion due to the relatively weaker effect gravity has by comparison. When the scaling value is too low, the inter-particle pressures are insufficient compared to gravity and thus are overpowered and end up compacted together at the bottom of the problemspace as time goes on with smaller values than presented here having the effect of a complete collapse of particles.

Table 1: Comparison of equation of state parameters.

γ	c_0^2	Max ρ (kg/m^3) $\pm$% from ρ_0	500s ρ (kg/m^3) $\pm$% from ρ_0	500s $\lvert v_{max} \rvert$ (m/s)	Convection	Fig Ref
1	0.01	241.86	151.96	0.01613	Particles clump.	2(a) & 3(a)
2	0.01	90.91	74.15	0.00696	Yes, minor clumping.	2(b)
3	0.01	71.47	46.59	0.00819	Yes.	2(c)
4	0.01	69.04	31.93	0.00676	Yes.	2(d)
5	0.01	57.58	30.20	0.00582	Yes.	2(e)
6	0.01	55.71	23.93	0.00493	Yes, minor.	2(f)
7	0.01	45.53	19.52	0.00426	Yes, minor.	2(g)
8	0.01	45.67	19.38	0.00393	Yes, restricted.	2(h)
1	0.05	75.53	67.46	0.01028	Yes, minor clumping.	3(b)
1	0.10	58.02	53.61	0.01094	Yes.	3(c)
1	0.50	40.49	40.49	0.00611	Very minor.	3(d)
1	1.00	38.17	38.17	0.00236	No.	3(e)

Table (1) provides a summary of the tests performed in this analysis showing the variation in density, velocity magnitude and to what degree convection is present for each. For this unrefined equation of state, the densities are varying considerably at this stage, but do show a measure of correlation with the velocities produced and the degree of convection identified. There are clear trends demonstrating how the increasing value of γ is reducing the amount of compression experienced with the amount of reduction being less pronounced between γ's of 6, 7 and 8, especially so between the latter two

values. Increasing the c_0 term also has the effect of reducing the amount of compression experienced, but this would be due to the increasing magnitude of pressure as indicated by still having a relatively high degree of compression whilst also having restricted or no apparent convection for higher c_0 values.

In a more true representation of the equation of state, various parameters would be included in this c_0 term and will also serve as a guide to determine an appropriate value. One such parameter would be the heat capacity of the fluid since it would be more physically true for an equation of state to have the energy of the particle influence the pressure as a function of its energy instead of simply as its temperature. This will be considered in future work for a full and rigorous development of an energy based equation of state for a SPH formulation to more robustly include heat transfer and the flow on phenomena associated with this in fluid dynamics.

The concept has been proven through clear convection phenomena being modelled. Now true and accurate forms of the equation of state need to be developed based on subsequent verification work. This robust equation of state will be useful in a wider range of problems than are currently possible to be modelled.

4 CONCLUSIONS

In this paper we have presented and validated a particle number density form of the standard heat conduction equation seen in SPH. It has been shown to produce accurate results compared to existing forms of heat conduction in literature and will be further tested in the future for potential benefits in multi-fluid flow problems. Initial progress towards a more encompassing equation of state in relation to including the energy of a system was also presented. Current ongoing work is involved in refining and further investigating the parameters of the equation of state to determine the most effective variables for a system that is both thermally active and physically driven.

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