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Comparison and Development of Equation of State Laws in Smoothed Particle Hydrodynamics

Patrick Peacock [a], and David Holmes [b]

School of Engineering and Physical Sciences, James Cook University, QLD 4811, Australia

[a] patrick.peacock@my.jcu.edu.au, [b] david.holmes1@jcu.edu.au

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Abstract. In this paper we present a brief comparison of existing equation of state laws used in Smoothed Particle Hydrodynamics (SPH) and introduce some new expressions for the equation of state for pressure, as well as to calculate temperature. In SPH literature practical examples of heat conduction and energy are scarce when compared with fluid flow formulations that determine pressure simply from density and an artificial speed of sound. Such simplifications may be appropriate for isothermal flow problems; however, a more thermodynamically rigorous formulation is necessary for complex and thermally driven problems, particularly in geophysics. This work discusses conventional equations of state, as well as presenting some new relations. This includes having pressure depend on the energy of the system, and applying these relations to a number of proof of concept examples demonstrating natural convection and examining the parameters of the new equation of state. These developments facilitate future work towards modelling more complex physical phenomena such as heat driven convective flow.

Introduction

Heat transfer in fluids and its effect upon motion 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. 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 temperature will have upon the dynamics of a system.

SPH has been widely used since its inception in the areas of momentum dominant fluid flow to great success. However, there has been limited investigation into areas of buoyancy dominant flow. While there has been some modelling of buoyancy dominant flows, such as modelling natural convection in a closed box and of the Rayleigh-Bérnard instability [1, 2], 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 SPH should allow for these phenomena to be modelled without the utilisation of *ad hoc* relations. The logical source for motion for a thermally driven system is 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 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 [3]. 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 in SPH [1, 4], 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 little work involving coupling the energy to the equation of state. There have been examples in wider literature of using energy to influence the governing dynamic equations in SPH [5], but this has mostly been used as diffusive tuning parameters and none have taken the temperature into account. In proof of concept examples in this work, we will demonstrate our first steps towards an equation of state that has temperature influence pressure and density, and thus, its dynamics by inducing motion. 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.

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 [6] and Hu and Adams [7] 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 rate of change in internal energy due to conduction and with spatially or thermally varying conductivity is

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

where U is internal energy, κ is thermal conductivity, ρ is density and T is temperature. Applying SPH discretization methods to (1) and applying a modification to account for discontinuous thermal conductivities from Cleary and Monaghan [4], the following expression for heat conduction as a function of particle number density is obtained

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

where m is mass, n is the particle number density, $n_i = \rho_i/m_i = \sum_j W_{ij}$, W_{ij} is the smoothing function and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ are position vectors. 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.

Time Integration for Heat Conduction Dominant Problems. In this work we integrate the differential rate equations through the implementation of a *Leapfrog* numerical integration scheme. In traditional SPH formulations, the following conditions on time step length are enforced in order to achieve stable solutions [8]:

$$\Delta t \le 0.125\left(h^2/\nu\right) \qquad \Delta t \le 0.25\left(h/3c\right) \qquad \Delta t \le 0.25\min_i\left(h/3\left|\mathbf{F}_i\right|\right)^{1/2} \tag{3}$$

where ν is the particle kinematic viscosity, c is the speed of sound and $|\mathbf{F}_i|$ is the magnitude of force on a particle. These time step equations relate to the viscous dissipation condition, the CFL condition and the magnitude of acceleration on a particle condition respectively.

For a problem where heat conduction is the dominant mechanism and no motion is present, it is difficult to use any of the existing formulations to determine an appropriate time step. As such, a new condition is proposed to estimate the time step for a problem where heat conduction is dominant.

Following a finite difference approach, a generalised expression to constrain the size of the timestep for a heat conduction problem yields the following

$$\Delta t \le const\frac{\rho c_p h^2}{\kappa} \tag{4}$$

A 2D solid conduction problem was modeled in order to determine the magnitude of the constant required for Equation (4). This was done by turning off all motion within the model as it is most probable that other time constraints, such as the viscous condition, are going to more critical. The material chosen to test this equation had material properties of a density of 1000 kg/m^3, a heat capacity of 460 J/kg°C, a thermal conductivity of 52 W/m°C and problem space properties of a smoothing length of 6.03x10^{-3} m.

Using a trial and error approach, convergence was found for a constant value of 0.5. To have a reasonable factor of safety, the constant value to be used in problems is 0.25, which also brings it in line with the already present time constraint expressions for traditional SPH problems.

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 modelled as quasi-incompressible. This also leads to most equation of states being modified on a case by case basis. The most common form for the equation of state used for incompressible flows, is the Morris [9] equation of state

$$p = c_0^2 \left(\rho - \rho_0\right) \tag{5}$$

where p is pressure, c_0 is the artificial speed of sound and ρ_0 is a reference density. The majority of state equations are similar in this regard being a function of density that is modified by a reference density and scaled by a constant (the artificial speed of sound). The other feature seen in some equation of states is an influence from a more gaseous equation of state by raising part of the equation to a power. This was first introduced by Monaghan [3] for modelling free surface flows

$$p = B\left(\left(\rho/\rho_0\right)^\gamma - 1\right) \tag{6}$$

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 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 (6) was introduced to remove nonphysical boundary effects at a free surface [8] and this has a similar effect in (5) 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 [1, 2]. To begin the development of an energy based equation of state, a simple expression was proposed to determine what effect changing different parameters would have upon a thermally dynamic system.

$$p = c_0^2 T \left(\rho/\rho_0\right)^\gamma \tag{7}$$

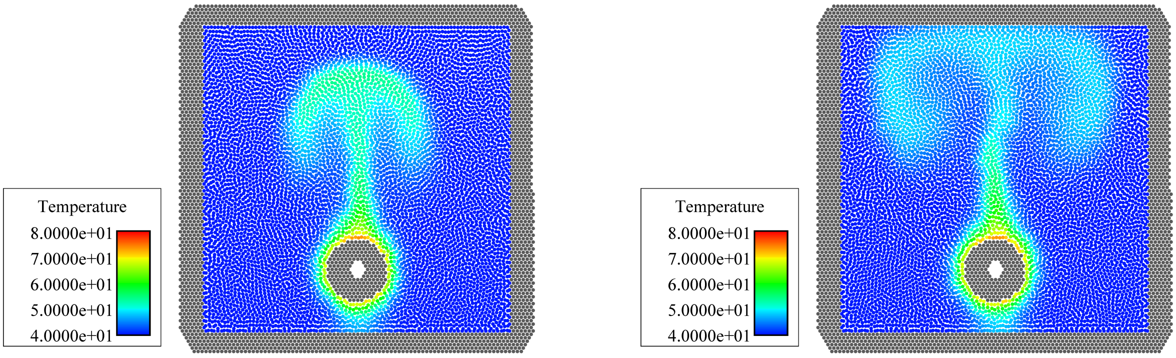
In this case, γ is free to vary and c_0^2 is simply being treated as a constant without any direct physical significance for the time being. There also isn't any term to account for free surface effects as all systems initially considered will be contained.

It is also logical to include the calculation of temperature within the scope of the equation of state instead of determining it during the *Leapfrog* time stepping and to instead iterate internal energy during that phase. As such, a straightforward expression to calculate temperature is used.

$$T = U/c_p \tag{8}$$

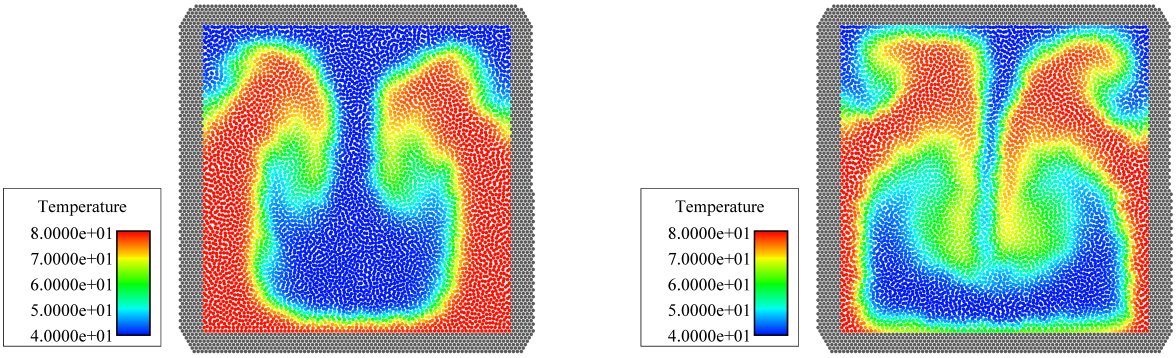
To demonstrate Equation (7), a number of proof of concept problems are presented. Figure (1) shows a cross section of a pipe with a radius of 0.1m submerged within a fluid. The pipe is held at a constant $80°$C, while the ambient fluid and adiabatic enclosure is at $40°$C with a gravitational acceleration 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.

Figure (2) shows a simple Rayleigh-Bénard instability problem in a 1m x 1m domain. The fluid is split via a sinusoid of $y = 0.6 + 0.2\sin\left(-\pi x\right)$ with the upper portion initially being at $40°$C and



(a) $t = 375s$ (b) $t = 500s$

Fig. 1: Temperature visualisation of a submerged pipe with equation of state parameters $c_0^2 = 0.05$ and $\gamma = 4$.



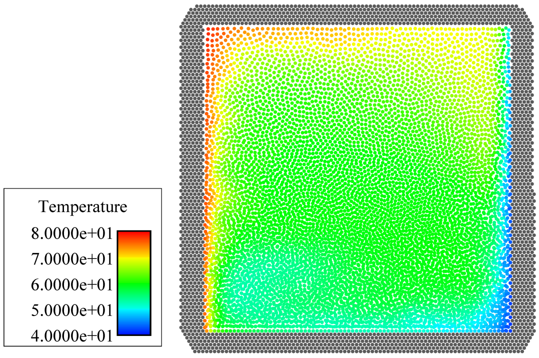
(a) $t = 200s$ (b) $t = 250s$

Fig. 2: Temperature visualisation of a Rayleigh-Bénard problem with equation of state parameters $c_0^2 = 0.05$ and $\gamma = 4$.

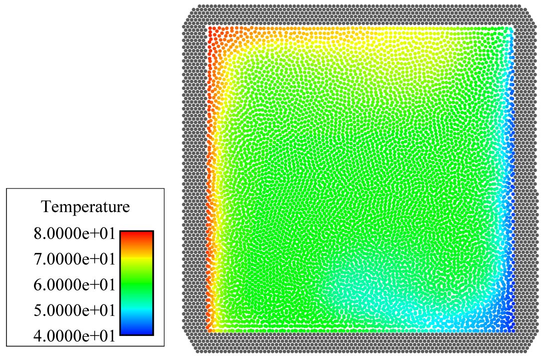
the lower portion initially at $80°$C with a gravitational acceleration of 0.001 m/s^2 in the negative y direction. The fluid used in this problem has the same properties as that seen in Figure (1).

Having demonstrated that Equation (7) is capable of reproducing natural convection phenomena without the use of the Boussinesq approximation, the next stage is refining its parameters and establishing what effect they have upon a given system. The problem chosen to test the parameters of Equation (7) is a 1 m by 1 m 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.

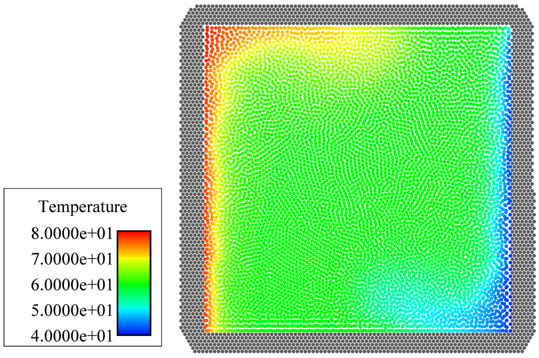
Figure (3) shows the effect increasing the value of γ has upon the system. In these cases, the influence of the ratio of a particles current density to its initial density is increased. The greater this influence, the less of a tendency there is for particles to clump together due to external forces. This has the result of decreasing the amount of compressibility that is possible within the system. However, if this value is too large, it may restrict motion in the system by not allowing any displacement due to the small amount of compression (however temporary) this may cause. Allowing for motion in this way can be related back to the requirement that there be some degree of quasi compressibility in SPH. Figure (4) shows the effect increasing 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 present and so will be dependant on the type of problem and the values of parameters within the 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



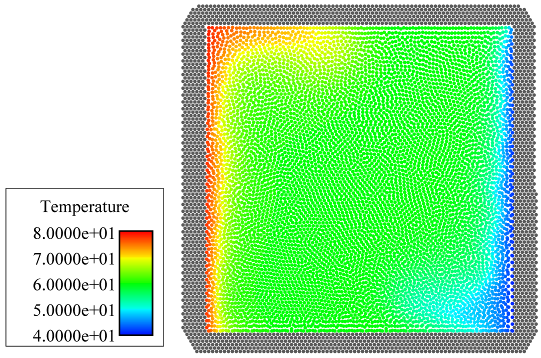
(a) $\gamma = 2$



(b) $\gamma = 4$



(c) $\gamma = 6$



(d) $\gamma = 8$

Fig. 3: Temperature visualisation of enclosed box with $c_0 = 0.01$, varying γ and after 500s.

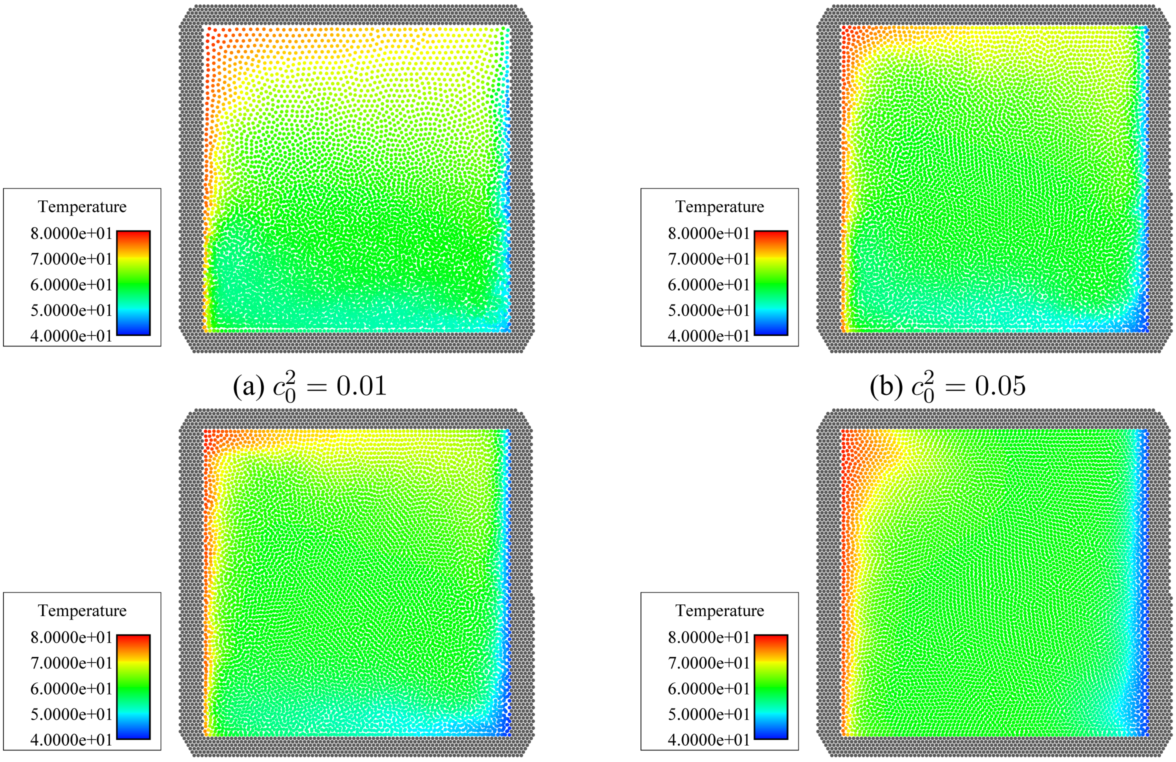
weaker effect gravity has by comparison. When the scaling value is low, the inter-particle pressures are insufficient compared to gravity and end up compacted together at the bottom of the problemspace.

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, that are not possible using traditional forms for the equation of state. Now true and accurate forms of this 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.

Conclusions

In this paper we have presented a comparison of existing equation of state laws, as well as introducing some new expressions for calculating pressure and temperature based on an energy approach. A candidate for determining the critical time step value for a heat conduction problem was also presented, however, it will almost always be the case that in dynamic problems, other constraints upon the timestep size will be more critical. A number of proof of concept problems demonstrating the potential of an energy based equation of state to model thermally dynamic systems was presented and this will work towards a more physical equation of state used in the future. 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.



(a) $c_0^2 = 0.01$

(b) $c_0^2 = 0.05$

(c) $c_0^2 = 0.1$

(d) $c_0^2 = 0.5$

Fig. 4: Temperature visualisation of enclosed box with varying c_0^2, $\gamma = 1$ and after 500s.

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