On the treatment of entropy mixing in numerical cosmology

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ABSTRACT
For simulations of fluid dynamics in astrophysics, physical viscosity and diffusion are typically neglected. However, in this high Reynolds number regime, real fluids become highly turbulent and turbulent processes mediate substantial transport of momentum and heat that is diffusive in nature. In the absence of models for these processes, code-dependent numerical effects dominate how diffusion operates and may lead to physically incorrect simulation results. We highlight the qualitative difference in these numerical effects for smooth particle hydrodynamics (SPH) and grid-based Eulerian codes using two test problems: a buoyant gas bubble and gas in a galaxy cluster. Grid codes suffer from numerical diffusion in the absence of explicit terms, and small-scale diffusion of heat is completely absent in the Lagrangian SPH method. We find that SPH with heat diffusion added at a level similar to that expected from turbulence diffusion generates more physically appealing results. These results suggest, but do not confirm, that a flat entropy core is to be expected for gas in an idealized galaxy cluster (i.e. one without physics beyond that of a non-radiating gas). A goal of this work is thus to draw attention to the as yet unfulfilled need for models of turbulent diffusive processes in compressible gases in astrophysics.

Key words: diffusion – hydrodynamics – turbulence – methods: numerical – galaxies: clusters: general.

1 INTRODUCTION
Astrophysical studies of complex hydrodynamical systems, such as gas in clusters of galaxies and the interstellar medium (ISM), have increasingly turned to numerical simulations in recent years. A critical issue that has been largely overlooked is the high Reynolds numbers of such flows (Elmegreen & Scalo 2004), which imply highly developed turbulence and associated unresolved transport processes that can affect the evolution. Modelling such processes is challenging. In engineering fluid dynamics applications there is often a strong empirical flavour to the models used. However, unlike engineering applications, precise measurements of the astrophysical flow properties, or close laboratory analogues, are not usually possible. Thus, the engineering methodology of validating computational fluid dynamics through controlled comparisons to physical systems does not have a corresponding practice within astrophysics. Substitute practices such as statistical convergence with increasing numerical resolution and code comparisons are applied unevenly and do not provide reliable measures of whether or not the numerical models are physically correct. In this paper, test cases are presented that demonstrate shortcomings of common astrophysical numerical fluid modelling techniques due to transport process at or below the grid scale. Results are also presented that provide some qualitative understanding of the differences between Lagrangian methods, such as smoothed particle hydrodynamics (SPH), and Eulerian methods that may explain differences on standard tests such as the galaxy cluster comparison of Frenk et al. (1999). However, this work was not able to provide a suitably general and comprehensive solution to the problem. Instead, the goal of this paper is to highlight the need for more sophisticated treatments of turbulence and unresolved flow scales in real astrophysical flows.

There are several different computational fluid dynamics methods in use for research problems, particularly in astrophysics. There are also many cases in the literature where different methods disagree on specific problems. Of particular interest are systematic differences that appear to be unrelated to the effective resolution of a given scheme. Code disagreements in the astrophysical context have been explored in several code comparison papers. The Kang et al. (1994) cosmological volume comparison and the Frenk et al. (1999) galaxy cluster comparison project are two examples that involved a cross-section of workers in the field. The cluster comparison is now considered a standard test problem for cosmological hydrodynamics codes.

SPH (see Monaghan 1992 for a review) and the Piecewise Parabolic Method (PPM) of Woodward & Colella (1984) (a high-order extension of the Godunov method) are among the most popular methods used in numerical astrophysics. SPH and PPM have been compared on specific problems such as cosmological volumes (O’shea et al. 2005) and collisions of polytropes (Davies et al. 1993;
Trac, Sills & Pen 2007). In this work, we look at SPH and PPM as representing two broad classes of Lagrangian (comoving control volumes) and Eulerian (fixed mesh) methods, respectively. A notable feature of the cluster comparison (Frenk at al. 1999) was that Lagrangian methods (represented predominantly by SPH) and Eulerian methods disagreed on the inner gaseous structure of the galaxy cluster. The galaxy cluster targeted by the comparison is massive \((10^{14–15} \text{ solar masses})\) with virial temperatures of the order of \(10^8 \text{ K}\) and was simulated without radiative cooling. In the mesh code results, the temperature and thus pressure were higher in the centre and the entropy curve \([\text{approximated as } \log(P/\rho^{2/3})]\) flattened out as the radius decreased, producing a core as seen in Fig. 1. As the comparison was purely non-radiative, this implies more entropy was generated (the physical mechanism being shocks) or transported to the central region. The core radii tend to increase for the lower resolution mesh codes. However, for the ENZO PPM code (labelled ‘bryan’ in the figure) the core is significantly larger than the estimated spatial resolution. The SPH results showed no core in the radial entropy profiles. It is not known whether a large hot core is correct for the idealized non-radiative case. Real galaxy clusters are affected by radiative cooling (which are likely to result in multiple gas phases), additional sources of heating, and physical heat conduction processes strongly affected by any magnetic fields. These effects have been investigated by other authors, with particular emphasis on the evolution of hot bubbles generated by active galactic nuclei (AGN) and the impact of differing levels of conduction and viscosity due to magnetic fields with both grid codes and SPH (Reynolds et al. 2005; Sijacki & Springel 2006).

Even a non-radiative, unmagnetized galaxy cluster is complex, incorporating substructure and a long, chaotic evolutionary process spanning the age of the universe. Timing differences in the passage of substructure can substantially alter the measured or observed properties over short-time periods (Wadsley, Stadel & Quinn 2004). The dominant hydrodynamic process is the creation of entropy in shocks associated with interactions between infalling overdense material in the cluster core and the subsequent rise of the higher entropy gas to the outskirts of the cluster. The process is driven by buoyancy and inhibited when and if entropy is redistributed. Over the long term, this results in a relatively stable trend of increasing mass, central temperature and central pressure as seen in Frenk et al. (1999). To investigate the key differences between the classes of methods, we elected to start with a simpler analogue. We constructed a toy problem to probe the adiabatic gas physics, examining the behaviour of buoyant compressible fluid in an externally applied gravitational field. In the tests, an initially warmer gas bubble rises and the fluid mixes due to Kelvin–Helmholtz (KH) instabilities at the interface between the rising warm gas and the colder but otherwise identical background fluid. The mixing redistributes the entropy that is driving the flow. This toy problem is quite similar to the Rayleigh–Taylor problem, and is related to problems in classical convection cells. It has the capacity to shed light on a range of astrophysical situations, including hot supernova bubbles rising in the gravitational field of the galaxy, collisions between stars with the resulting entropy-driven settling into a single larger star and jets from active galaxies or young stars creating bubbles in the surrounding medium. Not least, it is a model of how pockets of hotter gas should behave in the gravitational field of a galaxy cluster. The convective processes studied are important in meteorology and fluid dynamics generally, including the modelling of atmospheric explosions.

In the following sections, we start with a discussion of the treatment of physical diffusion and turbulence. In the absence of physical diffusion terms, Lagrangian and Eulerian methods differ substantially in how thermal energy is redistributed on the smallest resolved scales. The hot bubble problem is used to illustrate this difference with SPH representing Lagrangian methods and PPM representing Eulerian methods. We examine convergence at multiple resolutions and the effect of variations of code parameters, particularly the artificial viscosity coefficients in SPH. The tests show that PPM includes a numerical diffusion that is intrinsic for Eulerian methods and that is absent for purely Lagrangian methods. We briefly explore adding physically motivated diffusive transport to SPH which we compare to the results from numerical diffusion in Eulerian PPM. We show how added diffusion can improve the agreement between SPH and grid codes for both the hot bubble problem and the cluster comparison. We conclude by discussing prospects for validating astrophysical simulation codes and for modelling the turbulence present in astrophysical flows.

\section{Simulating Turbulence and Diffusive Processes}

Astrophysical simulations operate in a particularly challenging regime. The Reynolds number is defined as \(\text{Re} = vL/\nu\), where \(v\) is a characteristic velocity on the larger length-scales \(L\) and \(\nu\) is the viscosity. It characterizes the importance of advective terms versus dissipation in the momentum equation that governs fluid flow. The Reynolds number of astrophysical flows is typically very large, implying that the gas is extremely turbulent. For example, in a galaxy cluster Reynolds number estimates range as high as \(10^{26}\) (Fujita, Takizawa & Sarazin 2003). Tangled magnetic fields in galaxy clusters are expected to severely inhibit other diffusive mechanisms with the result that hydrodynamic turbulent diffusion may be the dominant mechanism for heat transport (Cho & Lazarian 2004). By way of comparison, Reynolds numbers in engineering applications vary from small values of order unity up to values of the order of
$10^6$ in extreme situations such as aerodynamics and aeronautics. The following paragraphs are intended to provide background for the astrophysical reader who may not be overly familiar with the numerical approaches to turbulence used in other fields.

The high values of the Reynolds number, Re, in astrophysical flows make it impractical to model the real situation via the direct inclusion of viscous terms as it is not possible to resolve the viscous scale. Simulations of the Navier–Stokes equations, resolving the viscous scale, are referred to as direct numerical simulation (DNS) by the turbulence community. The key requirement is that the physical dissipation dominates the numerical dissipation. This allows the modeller to determine the actual Reynolds number of the simulated flow and avoid spurious numerical effects. Directly simulating a flow with a Reynolds number, Re, for a single dynamical time requires computational effort proportional to $Re^4$ (Yakhot & Sreenivasan 2005). Some groups modelling astrophysical magneto-moments of the SGS flow. The Reynolds stress tensor is the term arising in the momentum equation and the turbulent (eddy) heat flux $(v_i \theta - (v_i) \langle \theta \rangle)$ is the term in the temperature equation, where $v_i$ is velocity and $\theta$ is the temperature. Due to the nonlinearity of the Navier–Stokes equations, the evolution of low-order moments depends on high-order moments and a division based on a particular filter scale does not result in a closed system of equations. Closure approximations based on statistical arguments or intuition are employed. In the popular Smagorinsky (1963) SGS model, the terms are assumed to be diffusive in nature with coefficients proportional to the magnitude of the strain rate in the resolved flow field. This model has been qualitatively very successful, is simple to implement and is very widely used outside astrophysics. In this approach, turbulent diffusion of heat is modelled using the Laplacian operator applied to the temperature or internal energy with a coefficient proportional to the magnitude of the local velocity shear field multiplied by the square of a length comparable to the grid or resolution scale.

The picture of turbulence as a diffusive energy cascade from large to small scales is, however, only correct in a statistically averaged sense. There is two-way energy flow to and from the small scales. Energetic small-scale structures, particularly vortices, intermittently strongly influence the large-scale flow. As a result, SGS models can only reliably extend the Reynold’s number by a factor of 10–100 above the viscous scale if high-order statistical features of the flow need to be captured or the simulation needs to model complex boundaries (Kevlahan, private communication). For flow far from boundaries, the operational criteria are that the resolved flow contains the bulk of the kinetic energy and that the smallest numerically resolved scale is in the inertial range of the turbulence. In this case, the turbulent part of the flow can be considered locally homogeneous and isotropic, and LES models are thought to provide a good approximation to the correct dissipation rate for extracting energy from the larger scales (Pope 2000). It is important to note that these assumptions have been primarily tested for incompressible flows but not for compressible gases or plasmas.

In cosmological codes, such as those used in the cluster comparison, physically motivated dissipation terms (turbulent or otherwise) are not included. This implies that any diffusion present is numerical in nature or is absent entirely. In Section 4, we demonstrate that false diffusion due to numerical truncation errors has undesirable properties.

### 3 ADVECTION: LAGRANGIAN VERSUS EULERIAN EXPRESSIONS

The Lagrangian representation of the partial-differential equation for energy evolution of a compressible fluid (without viscosity) may be expressed as

$$\frac{\partial u}{\partial t} + (v \cdot \nabla)u = -\frac{P}{\rho} \nabla \cdot v, \quad (1)$$

where $u$ is internal energy, $P$ is pressure, $\rho$ is density and $v$ is the fluid velocity. A mathematically equivalent form is given below using the full or comoving derivative:

$$\frac{du}{dt} = -\frac{P}{\rho} \nabla \cdot v. \quad (2)$$

In an Eulerian method, equation (1) is being modelled and advection terms explicitly move fluid between fixed volumes. For a purely Lagrangian method, the fluid control volumes move with the flow and no explicit advection terms are required. This provides automatic Galilean invariance but cannot support mixing between the control volumes. SPH is a purely Lagrangian method. Hybrid methods have been proposed, such as Softened Lagrangian Hydrodynamics (Gnedin 1995) which combines features of both approaches. PPM has two main forms, a commonly used purely Eulerian approach and the Lagrangian remap approach. In the remap approach, the control volumes move with the flow in each dimension and are then mapped back to the regular mesh which induces mixing. We will not consider this method in detail. For this work, we will be using SPH as a representative Lagrangian method and Eulerian PPM as a representative Eulerian method.

#### 3.1 Smoothed particle hydrodynamics

SPH (Gingold & Monaghan 1977; Lucy 1977) relies on expressions of the form of equation (3) to acquire smoothed local averages for
physical quantities:

\[ f_{i, \text{smoothed}} = \sum_{j=1}^{n} f_{j} W_{ij}(r_i - r_j, h_i, h_j), \]

where \( f_{i, \text{smoothed}} \) is a smoothed version of the quantity \( f \) at particle \( i \) given particles \( j \) at positions \( r_j \), \( W_{ij} \) is a kernel function and \( h_j \) is a smoothing length indicative of the range of interaction of particle \( j \). Locally adaptive smoothing \( h_j \) varying in time and space was introduced by Hernquist & Katz (1989) in the context of an astrophysical tree-code for computing gravity. Spatial derivatives are constructed through derivatives of the Kernel function (see the references for details).

SPH is attractive for its ease of implementation and spatial adaptivity (at fixed mass resolution), which makes it particularly well suited to astrophysical collapse problems. This is particularly true in cosmology where structural evolution is tied to the dominant dark mass which also has fixed mass resolution. In this case, SPH is efficient even when compared with adaptive mesh refinement (AMR) (O’shea et al. 2005).

SPH relies on smoothed averages of physical quantities stored on particles in disordered distributions that track fluid motions directly. Analysis on the irregular particle-set is more difficult, however, than for corresponding regular mesh methods. Constant readjustment of the particle distribution to accommodate motions and density changes adds inescapable low-level noise into the method. SPH relies on artificial viscosity both to capture shocks and to suppress the noise due to individual particle motions. These motions have been investigated previously (Lombardi et al. 1999) and occur at a few per cent of the sound speed in any non-uniform flow due to constant readjustment of the glass-like particle distribution to accommodate the flow geometry. General capabilities of SPH have also been examined in detail by Steinmetz & Müller (1993) and Hernquist (1993). It is also worth noting recent work by Trac et al. (2007) comparing SPH and grid codes for the mixing of polytropes. The differences they find are consistent with the results and underlying causes described here. For a modern, parallel SPH implementation for astrophysics and other fields that includes the key underlying causes described here, the reader is referred to the GASOLINE code (Wadsley et al. 2004). All SPH tests and results shown here were generated using GASOLINE.

The artificial viscosity approach (as opposed to using an explicit Riemann solver) allows SPH flexibility regarding equations of state and it is easy to incorporate phase changes, multiphase flows and sharp cooling and heating functions. Artificial viscosity has several drawbacks. First, it can result in spurious transport of angular momentum. Angular momentum is explicitly conserved in SPH but may be transported incorrectly in shear flows due to the artificial viscosity which is intended for highly compressive (shocking) flows. As part of his analysis of SPH, Balsara (1995) proposed an effective viscosity term that is intended for highly compressive but non-shocking flows. A recent investigation by O’shea et al. (2005) illustrates this to be the case for artificial viscosity when used in mesh codes as well. Lastly, the combined effect of the particle noise together with the minimum level of viscosity required to keep it at a reasonable level makes it difficult for standard SPH to handle gentle flows involving the growth of small instabilities. Of particular significance here is the standard KH instability test, where the sound speed is much larger than the typical flow velocities: the nearly incompressible regime. In astrophysics, this has not been an key issue because the flows are often supersonic or else the particle noise is thus a minor concern. It is possible to modify SPH to perform well in the incompressible regime for a variety of problems (Monaghan, private communication; Monaghan 1992).

SPH has two primary formulations for energy transport. It can be energy or entropy based, and this has been known for some time (Monaghan 1992; Hernquist 1993). With the original formulation, it was not possible to conserve both quantities equally well and most workers opted for the energy formulation and good energy conservation. Springel & Hernquist (2002) recently introduced a new approach that carefully controls error due to spatial adaptivity and makes the entropy approach highly effective. Both energy and entropy are well conserved for this method. It should be noted that for most tests the anisotropic energy formulation of equation (4) shown below and used in GASOLINE (Wadsley et al. 2004) performs comparably well:

\[ \frac{d u_i}{d t} = \frac{P_i}{\rho_i} \sum_{j=1}^{n} m_j (v_i - v_j) \cdot \nabla W_{ij}. \]

In the preceding equations \( u_i \) and \( \nu_i \) are the internal energy and velocity of particle \( i \), respectively, \( u_i = 1/\gamma - 1 \) \( P_i/\rho_i \) for an adiabatic gas where \( \gamma \) is the adiabatic index equal to 7/5 for diatomic gases such as air. This expression is a straightforward translation of the Lagrangian form of the energy equation (2) into an SPH summation. The artificial viscosity term is omitted for clarity.

3.2 The piecewise parabolic method

Mesh methods, such as PPM, are much more amenable to mathematical analysis, flux conservative approaches and explicit shock capturing techniques. PPM is a third-order extension of the Godunov method. It is based on piecewise parabolic reconstructions of the fluid quantities with additional monotonicity constraints (Woodward & Colella 1984). Fluxes are generated at cell boundaries using a Riemann solver for explicit shock capturing; it is also worth mentioning the characteristic-based Total Variation Diminishing scheme of Harten et al. (1987) and the characteristic-free scheme of Kurganov & Tadmor (2000) which achieve similar shock results without an explicit Riemann solver.

PPM excels at shock capturing. However, it uses fixed volume cells and requires AMR to handle large density contrasts. For our own experiments (reported here), we have used the FLASH code (Fryxell et al. 2000). FLASH is a highly adaptable parallel PPM AMR code using MPI and the PARAMESH library.

O’shea et al. (2005) performed tests in a cosmological context comparing different SPH implementations using the GADGET (Springel, Yoshida & White 2001) code to the ENZO (Bryan & Norman 1997) AMR PPM code. In this work, we focus on the transport of entropy rather than accurate adiabatic evolution or entropy production in shocks. It is important to note that standard AMR for compressible hydrodynamics, as originally proposed by Berger & Colella (1989), uses an accuracy criterion that selects the maximum refinement level at shocks. This is because the criterion is attempting to control the magnitude of the second derivatives which formally diverge at discontinuities. This is prohibitively expensive for astrophysical work where shocks occur throughout the medium, particularly in very low density regions, which may be of reduced interest. Most astrophysical AMR codes (including ENZO) primarily use mass-per-cell based refinement criteria in order to preferentially follow the collapse and formation of structures in a manner similar...
4 THE HOT BUBBLE PROBLEM

As discussed in the Introduction, the behaviour of hot bubbles is of interest in many circumstances in astrophysics and elsewhere. The response of a bubble that differs from its surroundings only through being warmer may be determined from its entropy relative to the background. For this purpose, a monotonic function of entropy, such as $A(s) = P/\rho^\gamma$, is equivalent. A bubble of higher entropy material in a hydrostatic background medium will rise until its entropy equals that of the surroundings. If the surroundings have an entropy gradient that increases upwards then the bubble must eventually stop. On the other hand, in a polytrope built on a single adiabat (entropy $s = $ constant) the bubble may rise arbitrarily far (expanding as it goes). Such a polytrope is also marginally stable to convection. This presupposes that the bubble does not mix with the surroundings. Once the bubble establishes velocity relative to the surrounding medium it is susceptible to KH instabilities at its margins. As shown in the following numerical experiments, the KH instabilities result in the bubble breaking up into symmetric vertical motions and cause the bubble material to be rapidly mixed with the ambient medium. This can prevent the material that originally formed the bubble from rising to the height of equal entropy previously discussed.

For our tests, we set up an initially isothermal hydrostatic distribution of an adiabatic gas ($\gamma = 5/3$) in a tube with periodic boundaries in the $x$, $z$ directions and reflecting boundary conditions in the vertical, $y$, direction. The vertical hydrostatic solution for density is an exponential function in $y$, and we chose parameters to give a scale-height of 0.25 starting from values of density and pressure of 1 at $y = 0$. The resulting entropy distribution increases vertically and is thus convectively stable. The box dimensions were $0.75 \times 1.0 \times 0.75$. A bubble was placed at $y = 0.375$ with a radius of 0.0625. This gives the bubble room to mix horizontally without being overly affected by the periodic horizontal boundaries. The density of the bubble was lowered by 0.670 at constant pressure. When compared to the background entropy gradient this implies the bubble would rise without mixing through one scaleheight to $y = 0.625$ before losing positive buoyancy. This limits the impact of the vertical boundaries. The sound speed in the unperturbed medium is uniform at $c = 1.3$. The fluid motions are limited by the potential energy available and 0.25 is a typical maximum vertical velocity. The fluid is thus only moderately compressible and shocks are unimportant.

4.1 PPM results

Fig. 2 shows FLASH AMR PPM results at fairly high resolution, equivalent to $192 \times 256 \times 192$, demonstrating the features described above. The figure shows a tracer of the original bubble fluid. This is advected in the same manner as all other fluid quantities using the PPM technique and thus should closely track the spread of intrinsic fluid properties such as entropy or passive contaminants. The rising bubble entrains colder fluid which is drawn up and later falls, resulting in a bobbing motion that creates an elongated well-mixed region in the centre. The outer regions curl up to give an initial mushroom-like shape which breaks up into smaller eddies that slowly dissipate as the fluid mixes. The fluid is well mixed and loses its buoyancy significantly before approaching the unmixed maximum height of 0.625 with a peak height averaged over the tracer fluid of 0.57. The PPM solution appears to model the fluid dynamics well.

PPM was able to directly model the KH instabilities and the resulting eddies advected the fluid to give mixing on coarse scales. Mixing on fine scales occurs through numerical diffusion that is attributable to the advection terms (e.g. in equation 1). This has long been known and the quality of fluid schemes is tested on advection problems to quantify the amount numerical diffusion. This numerical diffusion can be sensitive to the absolute motion of the fluid relative to the mesh. This is demonstrated in Fig. 3 which shows results for the same test with a uniform velocity of 0.25 to the right, with magnitude comparable to the maximum vertical fluid speed.

This has no effect on the fluid equations or their solutions from a mathematical standpoint but does adversely affect the numerical PPM result. The solution lost left-right symmetry and the bubble fluid evolved differently. In Fig. 10, we show the quantitative differences introduced. This illustrates that the intricate detail seen in the AMR solution is not correct or converged even though the
bulk properties do not vary substantially for a lower resolution case illustrated in Fig. 4. As shown in Section 4.4, the differences related to a lack of Galilean invariance also have a global impact.

4.2 SPH results

In most SPH applications equal mass particles are used. In order to make initial conditions equal mass particles that vary in density it was necessary to vertically stretch an initially uniform particle distribution to give the desired run of densities. The uniform distribution was chosen to be a glass as this is more representative of conditions in an evolved SPH simulation. The top and bottom reflecting boundaries were modelled by extending the box with the direction of the imposed gravitational body force reversed to give a mirror image of the distribution from $y = [0, 1]$. Periodic boundary conditions were applied overall. In the standard SPH runs, 2597 particles were used to model the lower density bubble. For a constant particle mass of $5.96046 \times 10^{-8}$, 2300 000 particles would be needed to model a single copy of the box with the majority of the particles well below the bubble. The particle masses were instead increased by a factor of 8 far from the bubble to reduce the computational work and 1250 000 particles used. In the high resolution run with eight times as many particles, 20 647 particles were needed to model the bubble. For comparison, the grid would use 268, 2147 and 17 157 cells to model the bubble at $48 \times 64 \times 48$, $96 \times 128 \times 96$ and $192 \times 256 \times 192$ cells, respectively.

Fig. 5 demonstrates standard SPH results at $t = 0.3$ at the base resolution. Though SPH has more resolution elements in terms of particles, the higher order PPM scheme resolves flow structures with fewer cells and thus the SPH results are qualitatively similar to the $48 \times 64 \times 48$ AMR results shown in Fig. 4.

SPH with standard artificial viscosity performs very poorly as the viscosity rapidly redistributes the vorticity associated with the shear that drives the KH instabilities. The standard values of the artificial viscosity coefficients ($\alpha = 1, \beta = 2$, Monaghan 1992) are suited to high Mach number astrophysical flows but are excessive for this subsonic problem (Lombardi et al. 1999). SPH shows improved handling of instabilities and small-scale flow features when the artificial viscosity is lowered away from shocks Morris & Monaghan (1997). Given that no shocks are present in this flow, the coefficients were lowered by a factor of 10 to the minimum recommended by Morris & Monaghan (1997). The result is much improved as is shown in Fig. 6 and the characteristic mushroom shape develops. However, the SPH bubble fluid remains unmixed and thus buoyant. This is a result of SPH having no explicit advection terms (e.g. equation 2): individual particles retain their initial entropy and their buoyancy tends to re-assert itself as larger bulk motions die down. As a result, the fluid tends to rise higher in the SPH version as shown in the summary of Fig. 10.

4.3 Mixing in SPH

SPH models the motion of fluid parcels using the Lagrangian expression directly. This is strictly correct for an infinitesimally small fluid element with no intrinsic substructure. In practice, each SPH
particle is a coarse-grained representation of a volume of fluid that has internal motions and variation in its fluid properties. When the Navier–Stokes equations are subjected to a multiscale analysis and each fluid property is divided into a coarsely filtered or averaged quantity, and a fluctuating part, the resulting equations contain terms for momentum and heat transport whose coefficients are functions of unresolved fine-scale motions and gradients as discussed in Section 2. The leading order term in the momentum equation is the gradient of the Reynolds stress tensor. In the static, Large Eddy Simulations (LES) approach the two parts are identified as filtered fields and residual subgrid fields. These equations have been extensively modelled in engineering applications (Meneveau & Katz 2000), particularly for incompressible fluids ($\nabla \cdot v = 0$). The larger scale filtered fields are commonly identified directly with the numerical flow fields. The subgrid-scale contributions to the resolved flow are reconstructed using models. The Smagorinsky (1963) model assumes that the effects are primarily diffusive and can be modelled with a turbulent or eddy viscosity (for the momentum equation) and a turbulent or eddy diffusivity (for the energy equation). Both coefficients are assumed to be proportional to the magnitude of the strain tensor of the resolved flow and can be easily estimated. There are many more complex models that try to explicitly evolve the subgrid kinetic energy and its dissipation rate. The problem with all models of this type is that the unresolved motions are stochastic but have definite statistical properties and bear a complicated relationship to the resolved dynamics via an unclosed sequence of differential equations modelling the unresolved degrees of freedom. As shown in Meneveau & Katz (2000), every model has significant shortcomings and many models require problem-dependent coefficients. In the case of astrophysical turbulence, the physical dissipation occurs due to molecular motions on unresolvable scales. The crude properties of the turbulent cascade on scales much larger than this ultimate dissipation scale are largely insensitive to the details of the dissipation processes and thus, as a crude approximation, the presence or absence of dissipation on the smallest scale is qualitatively most important.

For SPH, the absence of any mixing of thermal energy is the chief problem. The artificial viscosity term in SPH provides dissipation for the kinetic energy. To investigate the role of fine mixing, we introduce a simple approximation to the turbulent heat flux (see e.g. Pope 2000). This term appears in the Lagrangian form of the energy equation with a coefficient modelled in a similar manner to the Smagorinsky (1963) approximation for the turbulent heat flux:

$$\frac{d u_i}{dt} = \frac{P_i}{\rho_i^2} \sum_j m_j (v_i - v_j) \cdot \nabla W_{ij}$$

$$+ \sum_j m_j Q_{ij} (u_i - u_j) \frac{(r_i - r_j) \cdot (r_i - r_j)}{|r_i - r_j|^2} \cdot \nabla W_{ij},$$

$$Q_{ij} = C \frac{|v_i - v_j| (b_i + h_j)}{\rho_i + \rho_j}.$$  (5)

This expression is constructed in the same manner as the thermal conduction term introduced to combat wall heating effects (Monaghan 1992), and is effectively an SPH approximation to $1/\rho \nabla \cdot (\kappa \nabla u)$ where $Q = \kappa/\rho$ as shown by Brookshaw (1985). The link to the Smagorinsky model is the use of local velocity differences and a characteristic length (e.g. a grid spacing) to construct the rate coefficient ($Q$) for what is essentially a diffusion term. It must be emphasized that this is not a consistent turbulence model because the corresponding turbulent viscosity is not modelled explicitly as the artificial viscosity already provides substantial dissipation in the momentum equation. The goal was primarily to add a physically

Figure 5. Standard SPH results at times 1.5, 3 and 6. The artificial viscosity inhibits the rise of the bubble and formation of instabilities at the surface. The particles stay clumped and do not disperse. The lack of mixing at the particle level allows individual particles to rise higher than in the grid run.

Figure 6. Standard SPH with reduced viscosity ($\alpha = 0.1, \beta = 0.2$) results at times 1.5, 3 and 6. Vorticity generated during the bubbles rise now creates the characteristic mushroom shape but individual particles still rise further than desired.
reasonable amount of heat diffusion comparable to that mediated by turbulence. Using the magnitude of the velocity difference, it is ensured that the term is always diffusive in nature and can only result in an overall increase in the entropy of the fluid as expected for any physical dissipative process. Porté-Agel, Meneveau & Parlange (1998) compared the performance of the Smagorinsky SGS heat flux model with one-dimensional atmospheric air flow past a sampling point at a fixed height. Values ranging from 0.01–0.02 to 0.1–0.2 were required to match the average temperature variance diffusion rate and heat flux, respectively. Lilly (1967) showed that for isotropic, homogeneous, incompressible turbulence, a value of $C \sim 0.02$ was compatible with a Kolmogorov spectrum. The exact value of the coefficient tends to be problem dependent. A common observation for both experimental and numerical turbulence is that the Prandtl number, relating the eddy viscosity and the eddy diffusion, is around 1 at high Reynolds numbers. To maintain the consistency with the lowered artificial viscosity coefficients (0.1), coefficients for the diffusion term of the order of 0.1 were employed for this test.

With the addition of these eddy transport terms, SPH is no longer a purely Lagrangian method: individual SPH particles no longer perfectly trace the current location of the original parcel of fluid associated with the particle. The terms have been applied assuming no net mass transfer so that the particle masses stay constant. In order to follow the motion of the original bubble fluid it was necessary to introduce a tracer that is transported using the same expression applied to the energy. Tracer methods for Eulerian mesh codes are well established and sharpening techniques have been developed to preserve strong contrasts. The SPH tracer we have used is crude by comparison.

The diffusion term in the energy equation has relatively little impact in standard test problems where buoyancy is not a driving factor. For example, on the standard Sod shock tube problem as reported in Wadsley et al. (2004), the maximum difference in the fluid properties between runs with and without the diffusion term was less than 0.5 per cent.

Agertz et al. (2007) have also compared grid and SPH codes on the related problem of a dense blob of material moving through a hotter medium. They found that the development of instabilities and the associated macroscopic mixing was suppressed in SPH as a result of large density gradients. They were able to demonstrate the role of density gradients by examining the development KH instabilities in SPH with and without a large density contrast. In Fig. 7, we present results from a shearing box with an imposed perturbation almost identical to that used by Agertz et al. (2007) ($\Delta v = 1/40 \times_\text{shear} \times_\text{shear} = 0.68 \times_\text{dense}/\text{flow}$) and a density contrast equal to the maximum contrast present in the bubble problem (2:3) with uniform pressure. A smaller box containing just one wavelength of the perturbation was used but the number of particles per wavelength (32) is very close to that used previously so that the resolution is the same. The results show that the density gradients present in the hot bubble problem are low enough not to suppress the growth of fluid instabilities. The second panel of Fig. 7 shows results for the same test with non-zero turbulent diffusion ($C = 0.1$). The instability grows similarly in both cases. More recently, Price (2008) has shown that diffusion of thermal energy dramatically improves KH results in high-density contrast cases similar to those presented by Agertz et al. In the work of Price, the diffusion coefficient was constructed differently, to depend primarily on pairwise particle pressure differences. This specifically targets pressure errors that arise for larger density contrasts. It raises the possibility that thermal diffusion, with an appropriately crafted coefficient, could address two substantial problems for SPH at once. We intend to investigate this in future studies.

Results for the bubble problem with diffusion term with a coefficient, $C = 0.1$, are shown in Fig. 8. This choice for $C$ gives results

![Figure 7](http://mnras.oxfordjournals.org/) A shearing box with an initial perturbation at a level of 1/40th of the shearing velocity shown after one characteristic time for the KH instability. Only particles initially below zero, vertically, are shown. The instability develops normally for standard SPH (first panel) and with diffusion applied (second panel). The diffusion coefficient $C = 0.1$ as for the bubble test problem.

![Figure 8](http://mnras.oxfordjournals.org/) SPH with turbulent diffusivity added (coefficient $C = 0.1$) results at times 1.5, 3 and 6. The addition of a diffusion term allows mixing at the particle level. The bubble height evolution is qualitatively similar to the grid results (cf. Fig. 4). Varying $C$ tends to smoothly move the solution further from the original SPH case, with $\alpha = 0.1$, $\beta = 0.2$ and $C = 0.1$ providing the best quantitative match to the PPM results.
most similar to the highest resolution PPM result. Selecting smaller values of $C$ smoothly varies the result between no-mixing $C = 0$ to 0.1. Higher values of $C$ are much more diffusive. Note that to facilitate comparison with the mesh results, we have interpolated the particle tracer values onto a regular grid. Though the fine structure is still poorly realized, the SPH result now displays the main features of the PPM solution, including both the outer ring of eddies and the central stem at time $t = 3$. These features are clearer at high resolution, as shown in Fig. 9.

The diffusion terms used here only mimic the effect of subgrid diffusion and the authors recognize that substantially greater effort would be required to properly treat subgrid, turbulent transport in SPH. Sophisticated models for subgrid momentum transport have been proposed, such as the alpha turbulence model recently derived in SPH compatible form by Monaghan (2002). Monaghan suggested that the alpha turbulence model could be extended to model heat transport.

4.4 Overview of hot bubble results

Fig. 10 summarizes the different results for the hot bubble problem with PPM and SPH. The upper curves in each panel show the bubble height weighted using the tracer of the original bubble fluid. The bubble rises and bobs around near $y = 0.57$. Without mixing, the SPH results allow the bubble to rise higher before getting to a point of equal entropy with the background. Both SPH and the stationary PPM runs result in the bubble oscillating with a half-period of the order of 2 time units. When the entire box is moving right, the bubble oscillates more rapidly in the PPM results but there is no effect for SPH. The lower curves in each panel show the $rms$ bubble size weighted by the tracer. This measures the spread of the bubble but is insensitive to whether the fluid is coarsely mixed (with a high contrast preserved between the original bubble fluid and interpenetrating background fluid) or finely mixed (with a relatively uniform distribution of the tracer). The horizontal spread of the bubble in SPH (independent of mixing) is sensitive to the amount of artificial viscosity.

5 CLUSTER COMPARISON

The simulation differences seen in the Frenk et al. cluster comparison may be well related to numerical mixing effects. Galaxy clusters are highly turbulent and thus potentially strongly mixed. Individual standard SPH particles do not mix entropy at all which allows particles to remain at lower entropy in the cluster core. Entropy production via shocks regulates the temperature of the central gas to the point where infalling substructure is not sufficiently supersonic to generate more entropy. This is consistent with the relatively

Figure 9. SPH with turbulent diffusivity added (coefficient $C = 0.1$) results at times 1.5, 3 and 6 with eight times as many particles. The results are quantitatively similar to the standard resolution case shown in Fig. 8.

Figure 10. The evolution of statistical properties of the bubble. The top curves starting at $y = 0.375$ indicate the mean bubble height weighted by the tracer for the original bubble fluid. The lower curves indicate the $rms$ bubble radius, again weighted by the tracer. The left-hand panel demonstrates the sensitivity of the PPM results to the fluid motion because the diffusion is numerical in nature. The right-hand panel demonstrates overshooting by SPH without explicit diffusion and a general tendency of artificial viscosity to limit the spread of the tracer.
uniform temperature cores seen for SPH in the initial cluster comparison. With high viscosity it may be hard for particles to physically intermix. Recent results by Dolag et al. (2005) show that using the (Morris & Monaghan 1997) approach to lower the artificial viscosity (to $\alpha \sim 0.01$) results in higher average gas entropy values in the centres of galaxy clusters in SPH simulations. This appears to be due to high entropy particles entering the cluster cores which is a coarse kind of mixing. However, in this case individual particle retains their entropy values and systematic segregation of high entropy particles out of the core is still likely. For this reason, we might expect that the Dolag et al. (2005) results are lower bound on the true mixing. However, the (Morris & Monaghan 1997) switch was not intended for flows that converge over broad regions of space without necessarily shocking and there are some indications of pre-shock heating in the Dolag et al. results. On the other hand, Agertz et al. (2007) have shown that very low viscosity can lead to noisy results with SPH for similar problems to those studied here. When the bubble problem was attempted with these very low viscosities, it led to large velocity noise and unabated mixing that was not related to the flow evolution.

For mesh codes, with intrinsic numerical mixing, the tendency is to generate uniform entropy cores in situations like the cluster comparison. It remains unclear how much mixing is appropriate and how large the cores should be. The ENZO mesh code of Bryan et al. gives the smallest entropy core (around 1/10th the virial radius) and it is the only grid code where the core is spatially well resolved. The core size is comparable to the radius where the averaged radial inflow velocity drops to zero which may indicate the extent of the well-mixed zone. A zoom on to the inner mixed region is shown in Fig. 11. The plot includes raw data inside the simulator’s chosen resolution cut-off which reinforces the trend in the SPH results towards no core, independent of resolution.

The cluster comparison was resimulated using GASOLINE with and without the new diffusion terms. The set up is the same as that used in Wadsley et al. (2004). The entropy profiles are shown in Fig. 12. At $64^3$ resolution, the same as most SPH codes in the original paper, Wadsley et al. (2004), the gas infall is strongly filtered, both by choice and due to the PM nature of the gravity solution. This makes the effective wave resolution similar to that specified.

![Figure 11](http://example.com/figure11.png)

**Figure 11.** Here, we zoom on in the inner region of the cluster comparison showing the Bryan AMR results against three SPH results. The thin curves show the extension of the entropy profiles inside the resolution cut-off specified by the code author (from the raw data). The vertical error bars at the base of the plot indicate the variation in a single GASOLINE run over an interval of $\Delta z = 0.025$ in redshift to give a sense of the time variability in the measurements.

Of using higher viscosity coefficients so as to model shocks. The results are not all that sensitive to the value of the coefficient if it is in the range expected for a turbulent Prandtl number of the order of $1$, $C = 0.1$–1. Though the prescription chosen is simple, the qualitative agreement is encouraging. Following the results of Dolag et al. (2005), it would be interesting to try using the variable artificial viscosity parameter, with appropriately matched diffusion terms.

There is still the question of numerical convergence. To address it, GASOLINE was used to simulate the cluster at $64^3$ and $128^3$. An issue often overlooked in cosmology is that increasing resolution typically adds small-scale waves in the initial condition. We chose to resimulate at $128^3$ with the original $64^3$ waves, denoted $128^3 (64^3)$ in Fig. 13 and with the added waves, denoted $128^3$. It is important to keep in mind that the mesh results are also filtered and though the Bryan results used a $128^3$ initial mesh, the gravitational forces were strongly filtered, both by choice and due to the PM nature of the gravity solution. This makes the effective wave resolution similar to that specified.

![Figure 12](http://example.com/figure12.png)

**Figure 12.** The cluster comparison calculated with SPH (GASOLINE) with different values of the diffusion coefficient at $64^3$ resolution. The points are labelled with value of the coefficient, $C$. An entropy core forms for values in the range of $C = 0.1$–1.0.

![Figure 13](http://example.com/figure13.png)

**Figure 13.** The cluster comparison calculated with SPH (GASOLINE) at $64^3$ and $128^3$ resolution with and without the diffusion term ($C = 1$). For lines labelled $128^3 (64^3)$, the initial waves were set equal to the $64^3$ run for a numerical convergence study. The $128^3$ results with more waves create a smaller entropy core.
the $64^3$ or $128^3$ ($64^3$) cases in the figure. This aspect of grid-based cosmological simulations has been investigated in detail by O’Shea et al. (2005).

As shown in Fig. 13, the SPH results without diffusion differ from the AMR results in a manner consistent with the original cluster comparison. However, with turbulence-related diffusion turned on with $C = 1$ the SPH results with $64^3$ waves produce an entropy core similar to the AMR result where we have argued the wave resolution is similar. It is noteworthy, however, that adding more waves as in the $128^3$ case shrinks the entropy core established with the turbulent diffusion term. It seems likely that additional non-turbulent processes will be required to establish a minimum scale for the entropy core in the case of real galaxy clusters as investigated in the studies by Reynolds et al. (2005) and Sijacki & Springel (2006).

For the ideal non-radiative case studied here, there are promising indications of numerical convergence between the Eulerian and Lagrangian codes if cosmological structures are filtered at a consistent scale. As discussed for the bubble problem, the numerical diffusion associated with advection terms in the grid methods is not Galilean invariant. However, for this problem, the velocities relative to the mesh are predominantly physical, related to the cluster formation process, and thus the resulting numerical diffusion is probably of the right order to mimic the expected turbulent diffusion. Overall, these results are a promising indication that full agreement between the methods will be achieved with careful attention to subgrid, turbulent processes.

6 CONCLUSIONS

The primary conclusions of this work are as follows.

(i) Simulating fluid flows without explicit dissipation are poorly motivated. A lack of physically motivated dissipation results in leading terms which are numerical in nature. These exhibit undesirable effects such as sensitivity to the absolute velocity of the flow (a lack of Galilean invariance). Without physical dissipation (i.e. viscosity) it is difficult to characterize the Reynolds number of the simulated flow and to relate the behaviour to real flows. In astrophysics, in particular, the true Reynolds numbers could be exceedingly high. SPH has a Galilean invariant viscous term but no diffusive term to mix entropy or tracers such as metals in cosmology. Grid methods typically have numerical viscosity and diffusion that is not Galilean invariant, so that the mixing occurs even if its qualitative correctness is unclear. These differences are apparent in the cluster comparison results of Frenk et al. (1999).

(ii) Results using a simple model for diffusion in SPH, with coefficients chosen to mimic the level of diffusion due to turbulence, were presented. This diffusion greatly modifies the SPH results for two test problems: a buoyant bubble and the galaxy cluster test of Frenk at al. (1999). Qualitatively, the SPH results are significantly changed and the model is able to bring the grid and SPH results into much better agreement. These results suggest that a flatter entropy core is to be expected for an idealized (non-radiative, non-magnetized) galaxy cluster. This result should be viewed in the context of interpreting the outcome of numerical simulations using different cosmological codes. The presence of detailed substructure and additional physics such as magnetic fields and radiative cooling will strongly impact the outcome for real galaxy clusters.

(iii) Based on these results it is still not possible to assess the quantitative correctness of either the grid models or SPH for problems like galaxy clusters where small-scale transport is important. The basic diffusion used here is not sophisticated enough to act as a consistent model of subgrid turbulence. It is the expectation of the authors that more rigorously derived models, such as an SPH implementation of the alpha turbulence model (Monaghan 2002), will ultimately provide a robust turbulent modelling capability for SPH.

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