Projecting SPH Particles in Adaptive Environments

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Abstract—The reconstruction of a smooth field onto a fixed grid is a necessary step for direct comparisons to various real-world observations. Projecting SPH data onto a fixed grid becomes challenging in adaptive environments, where some particles may have smoothing lengths far below the grid size, whilst others are resolved by thousands of pixels. In this paper we show how the common approach of treating particles below the grid size as Monte Carlo tracers of the field leads to significant reconstruction errors, and despite good convergence properties is unacceptable for use in synthetic observations in astrophysics. We propose a new method, where particles smaller than the grid size are ‘blitted’ onto the grid using a high-resolution pre-calculated kernel, and those close to the grid size are subsampled, that allows for converged predictions for projected quantities at all grid sizes.

I. INTRODUCTION

SPH is well known for its adaptivity; by tracing mass rather than volume the method can accurately capture the large dynamic range (of a factor $10^{11}$ in density, and $10^4$ in smoothing length, in cosmological galaxy formation simulations, see [1]) present in astrophysical phenomena, and is hence a natural choice for such simulations. The post-processing of SPH data in adaptive environments, however, presents a challenge due to the unpredictable structure of the underlying particle fields.

One post-processing case of interest, particularly within the astrophysics community, is the projection of three dimensional data onto a fixed two-dimensional grid. In astrophysics, projected quantities naturally correspond to those that are observable; for instance, it is significantly easier to measure the gas column density of a galaxy than it is to probe the three dimensional density structure. With projected quantities being instrumental in the connection of simulated datasets and the real Universe, obtaining accurate projected reconstructions of density (and other, e.g. temperature) fields from SPH data is vital. In specialised post-processing fields such as radiative transfer convergence and accuracy are a subject of regular discussion (e.g. [2]), but for projected SPH quantities it is generally assumed that basic algorithms will suffice.

Typical solutions to the ‘projection problem’ do not guarantee converged results in highly adaptive situations, particularly in the case where the smoothing length is of a similar order to the cell size that is chosen for projection. In this context, convergence refers to producing a result at a given grid resolution that corresponds to a resolution where all particles are resolved by a large number of cells, down-sampled to the lower resolution. Past work (e.g. [3], [4]) introduced the concept of using a Voronoi decomposition to ensure that each pixel is assigned the correct fraction of each particle. This procedure, however, is computationally and conceptually complex.

We consider various methods to project SPH data to a fixed grid, from basic kernel interpolation, to ‘blitting’ kernels to the fixed grid, and subsampling the kernel. There are many software packages available to perform this deposition, including (but not limited to) those described in [5]–[7]. The open-source package used in this work is swiftsimio [8], used for reading and visualising data produced by the SWIFT code, and is the first package that we are aware of that makes subsampled techniques publicly available.

II. BASIC SPH PROJECTION

As noted in the introduction, there are many ways to project SPH data. The most common approach uses a pre-projected version of the kernel and for each particle loops over all pixels, calculating the kernel contribution from each particle to each pixel. It is important to ensure that the projected kernel corresponds directly to the same kernel used in the simulation, projected along one axis, to get the most accurate reconstruction. Here, for simplicity, we ignore the limb-brightening effects associated with this and simply use the two-dimensional version of the Wendland-C2 kernel,

$$W(r, h) = C \cdot \max \left(1 - \frac{r}{h}, 0\right)^4 \left(1 + 4 \frac{r}{h}\right).$$

with $r$ the inter-particle separation (or here the separation between the pixel sampling point and the particle), and $h$ the smoothing length of the particle. We take the ratio between the smoothing length and kernel extent $H/h = 1.897367$, and $C = 7/\pi$ in accordance with [10], [11].

Algorithmically, such a scheme (described below as ‘Original’) looks like:

1) Start with a pixel grid full of zeroes, with the pixels of size $d_2$ along one axis.
2) If the particle has a kernel extent $H < 0.5d_2$, add all of its contribution onto the nearest cell centre, as this particle is ‘unresolved’, otherwise:

a) Take all particle positions $r_{\text{part}}$ and particle smoothing lengths $h$, and find which pixels this cell overlaps.

\[1\]The specific implementation of the kernel used here is defined in swiftsimio.visualisation.projection_backends.kernels.
There is no excuse for the poor reconstruction of this smooth gradient; the problem demonstrated here is purely static. We have simply chosen to throw away everything we know about the smoothness of the field at a specific grid size and as a result have been penalised with significant reconstruction errors. This method, as we will demonstrate later, does converge to the correct answer when all particles are well resolved by the grid, but for some applications grids of that size are prohibitive and large pixel sizes (relative to the particle spacing) may be required for direct comparison to real-world observations.

III. Constructing Converged Projections

In order to construct converged projections of the field, we must re-integrate our ability to assume that the particles are ordered regularly, and that the field is smooth. To do this, we introduce two new measures.

The first, for particles below the field grid size, is termed ‘blitting’. Here, we construct a pre-calculated high resolution image of the projected kernel (at \( N \times N \) pixels, where here \( N = 32 \)). If the kernel extent overlaps any pixel boundary, this pre-calculated kernel is overlaid on the pixel grid and each pixel is assigned the kernel contributions that overlap with the pixel.

The second, termed sub-pixel subsampling (or just ‘subsampling’) ensures that each kernel is well resolved by ensuring that at least \( N \times N \) sampling points are made available. If the particle overlaps fewer than \( N \) pixels in one dimension, sub-pixels are temporarily generated, which are aligned with the pixel boundaries. This ensures that the kernel gradient is well sampled for all particles. It also ensures that for cases where the kernel does not overlap with the pixel centre, but does overlap with some of the pixel area, that contributions are still made.

A demonstration of these two effects, compared to the standard projection scheme, is shown in Fig. 2. Algorithmically, the ‘Subsampled’ approach looks like:

1. Start with a pixel grid full of zeroes.
2. Pre-calculate an \( N \times N \) grid representing the kernel over a smoothing length, and store this.
3. Take all particle positions \( r_{\text{part}} \) and particle smoothing lengths \( h \). For each particle:
   a) Check for overlaps between this particle and neighbouring cells. If there are no overlaps, simply add \( m / A \) to the containing pixel with \( A \) the area of the pixel.
   b) If there are overlaps, use the pre-calculated kernel grid to spread the appropriate contribution from this particle over the relevant neighbouring cells.
5) Otherwise:
   a) If this is not the case, figure out how many pixels this kernel will overlap \( n \). If this is smaller than \( N \), sub-sample the pixels \( N/n \) times (rounded up) at positions \( r_{\text{sub}} \).
Fig. 2. Example cases where the size of the smoothing length (kernel extent shown with dashed lines) of a particle (black point) is smaller than a pixel size (top row) and approximately the size of a pixel (bottom row). The columns show the standard projection algorithm (left) and the sub-sampled, new, algorithm (right). The background black grid shows the pixels, with diamonds representing the kernel evaluation points at the centre of relevant pixels. These are omitted in the bottom right image for clarity, and are replaced with a representation of the sub-pixel grid. In the top left panel, the particle is treated as unresolved, and so its entire density contribution is given to the top left pixel, despite the particle overlapping with three other pixels. In the top right, the blitting grid (grey) is used to appropriately apportion the mass over the four pixels (coloured by their contributing sector of the grid). The bottom left panel shows how the particle usually contributes to each pixel using the evaluated value of the kernel at the pixel centre (with each evaluation point coloured by the appropriate projected density). The bottom right shows the subsampled grid, where the kernel is evaluated at each point to ensure a good reconstruction of the kernel gradient.
In the final column the original approach has visually converged to the subsampled result, with each particle being spread over many pixels. In Fig. 5 we show the numerical convergence, relative to a downsamped 81922 grid. This is used instead of the analytical solution to remove the impact of any shared systematics between the two approaches, such as the lack of limb brightening in our projected kernel. Percentage error $E\%$ is calculated as

$$E\% = 100 \cdot \frac{|\rho_{\text{test}} - \rho_{\text{ref}}|}{\rho_{\text{ref}}},$$  

with $\rho_{\text{test}}$ the calculated density reconstruction in that pixel and $\rho_{\text{ref}}$ the reference density. Each point shows the median absolute percentage error over all pixels, with the bar showing the 10-90 percentile range.

At all resolutions, the subsampled method ensures that the percentage error in the reconstruction is imperceptibly low, with a highest 90% value of roughly 0.05%. Notably, this
Fig. 4. A linear (diagonal) gradient in smoothing length from $10^{-3}$ to $10^{-2.5}$ (in units of the box-size) projected with three different methods (rows) at three different grid resolutions (columns). Here the top method is a simple histogram, where each particle is assigned to its nearest grid centre; this is to demonstrate the basic Moiré pattern generated when the grid resolution is close to the particle spacing. The centre row shows how this pattern is also present when using the original scheme for particles below the resolution limit, with the bottom row showing the same gradient for each resolution and demonstrating that the subsampled technique can remove all such patterns. These visualisations are used in Fig. 5 to demonstrate the convergence and costs (Fig. 6) of each method.
does not decrease with resolution, as the method is designed to produce converged results at all grid sizes. The original method, on the other hand, demonstrates a high level of error with almost all pixels having at least a 1% reconstruction error at $128^2$ resolution. This error does indeed converge at the expected rate ($1/dx^2$ as this corresponds to the number of pixels sampling each kernel), but even at the highest resolutions the subsampled approach still provides lower error due to its improved gradient reconstruction of particles with the smallest smoothing lengths (note that $10^{-3} \approx 5/4096$, so even at this high resolution the sub-pixel supersampling is still in effect for the highest densities).

The improved reconstruction using the subsampling technique hence provides a significant increase in accuracy relative to traditional methods in an adaptive environment. This, however, comes at the cost of increased computing cycles. Fig. 5 shows the scaling of the time to produce the projected density grid for points in Fig. 3. The red line shows, for comparison, the time taken to compute the 8192$^2$ reference grid, which could be downscaled to provide a high accuracy reconstruction. The subsampled technique is still roughly an order of magnitude faster than this, thanks to its efficient handling of particles that are already spread over enough pixels to be well sampled.

### V. Astrophysical Example

So far we have only considered the impact of the subsampling technique on simple problems, but have already demonstrated its ability to provide highly accurate, converged, solutions at all grid sizes. We now consider the astrophysical example of an isolated galaxy disk. The properties of galaxies are the key discriminator between galaxy formation models, as they host an abundance of readily observable properties which can be directly compared with projected quantities from SPH simulations.

This galaxy was simulated with the SWIFT code, using the SPHENIX [12] hydrodynamics model, and an analytical Hernquist [13] potential for the dark matter component with a mass of $M_{200} = 1.37 \times 10^{12}$ $M_\odot$ with $M_\odot = 2 \times 10^{30}$ kg, concentration $c = 9.0$, and a disk fraction of 4%. The simulation contains 123533 directly simulated gas particles (of mass $10^5$ $M_\odot$), which interact both through hydrodynamics and gravity, and 424467 star particles (of mass $10^5$ $M_\odot$) that only interact gravitationally. All particles are subject to a modified version of the EAGLE sub-grid model [14], which includes prescriptions for radiative cooling [15], star formation [16], and stellar feedback [17]. Here we use a snapshot after $t = 0.5$ Gyr, with 1 Gyr = $3.16 \times 10^{16}$ s. The initial conditions set-up is described in more detail as the fid galaxy in [16].

Fig. 7 shows the projected gas density of the galaxy in the left panel and the percentage error attained from such a projection if using the original scheme. The pixels are set to be 100 pc on a side, for comparison with typical observations of real galaxies (e.g. [18]). The dynamic range in smoothing length here is 300, with $h_{\text{min}} = 33$ pc. Here, the percentage error is calculated relative to the subsampled result for more consistent and simple visualisation in later figures, but the result is unchanged when comparing to a high resolution downscaled grid.

The higher density regions of the galaxy (near to the centre) do not have the largest errors due to the stacking of particle layers; this simulation was performed in three dimensions, and as such the Monte Carlo-style sampling is less poor than

![Fig. 5. Compares the errors (in the 10%, 50%, 90% percentiles from bottom, point, to top) for the original and subsampled method. Note that each point is evaluated at the number of pixels given on the horizontal axis, with them offset for clarity when the range bars overlap.](image)

![Fig. 6. Time-to-solution (using four cores of an Intel i7-8559U) per pixel corresponding to the accuracy results in Fig. 5 for three strategies: the original method with no subsampling (blue); the subsampled method (orange); and using a downscaled pixel grid originally calculated at 8192$^2$ (red). Here we see that although there is significant computational cost associated with the use of the subsampling strategy (along with, of course, the accuracy gains), it still remains approximately 10 times faster than downsampling a large grid.](image)
Fig. 7. **Left:** Projected ('surface') density of a spiral galaxy from an SPH simulation performed with SNIF4. The projected density was calculated on a 512$^2$ grid, with each pixel corresponding to 100 pc of physical space, a common size in observations of real galaxies. **Right:** The error in the estimation of the surface density when not subsampling particles close to, or smaller than, the grid size (i.e. using the 'Original' algorithm). This correlates with medium-high density regions of the galaxy, where many particles have smoothing lengths below the grid size. Note that 1 pc = $3.09 \times 10^{16}$ m.

when only a single layer of particles is considered. In the intermediate density regions, where there is also a strong gradient in density, the error spikes as the kernel gradients are poorly resolved without subsampling. This is a particularly dangerous error structure, as it is typically assumed that the error in SPH simulations decreases as the density increases and the finite mass sampling of the field improves.

The density-dependent error findings are confirmed in Fig. 8, where the projected densities in individual pixels are compared between the two methods. The increase in error with density, except at the highest densities, is confirmed. Additionally, the error is not biased or systematic in any way; the errors inherent in using the poorly sampled projection method are random and as such impossible to offset with, for instance, a scaling factor.

Fig. 9 shows the convergence of the median error with image resolution. Because of the higher dynamic range in this image, relative to the gradient in Fig. 5, the error ranges for both methods are larger. Here we see that the subsampled method provides a lower than 0.1% error for all pixels, with the original method, as demonstrated in Fig. 8, leading to errors for individual pixels that are higher than 30%. The median error does converge at the expected rate, but as noted before as real-world observations are taken on coarse grids the convergence properties are not relevant to the accuracy of the method.
These final two figures demonstrate that the correct sampling of kernels in projection is not simply an academic exercise; for simulated observations of real-world problems in adaptive environments subsampling is necessary to produce accurate results.

VI. CONCLUSIONS

In this paper we have demonstrated the issues of using a basic kernel deposition strategy when projecting SPH data onto a fixed grid in adaptive scenarios. This strategy was shown to be unable to accurately reproduce a linear gradient in density at low grid resolutions, and also led to large errors when projecting an astrophysical example problem. In addition, these issues are also present (if not exacerbated by even poorer sampling) when constructing the smoothed 3D density at a plane through the field.

To resolve inaccuracies in the deposition of SPH data onto fixed grids, we introduced two techniques:

1) Using a pre-calculated kernel grid to ‘blit’ particles that are smaller than the pixel size to ensure that particles that overlap pixels even at this small scale have their contributions weighted accurately.

2) Using subsampling to ensure that gradients of kernels are always well resolved during the projection process.

With these two techniques we showed that it is possible to produce converged results with very low errors (less than 0.1%) even when using a low grid resolution. In adaptive scenarios, we hence recommend the use of subsampling techniques.

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REFERENCES

[1] J. Borrow, R. G. Bower, P. W. Draper, P. Gonnet, and M. Schaller, “SWIFT: Maintaining weak-scalability with a dynamic range of $10^4$ in time-step size to harness extreme adaptivity,” Proceedings of the 13th SPHERIC International Workshop, Galway, Ireland, June 26-28 2018, pp. 44–51, Jul. 2018.

[2] Y.-L. Yang, N. J. Evans, A. Smith, J.-E. Lee, J. J. Tobin, S. Terebey, H. Calcutt, J. K. Jorgensen, J. D. Green, and T. L. Bourke, “Constraining the Infalling Envelope Models of Embedded Protoplasts: BHR 71 and Its Hot Corino,” ApJ, vol. 891, no. 1, p. 61, Mar. 2020.

[3] C. M. Koepferl, T. P. Robitaille, E. Dale, and F. Biscani, “Insights from Synthetic Star-forming Regions. I. Reliable Mock Observations from SPH Simulations,” ApJ Supplement Series, vol. 233, no. 1, p. 1, Jun. 2020.

[4] M. A. Potkova, G. Laibe, and I. A. Bonnell, “Fast and accurate Voronoi density gridding from Lagrangian hydrodynamics data,” Journal of Computational Physics, vol. 353, pp. 300–315, Jan. 2018.

[5] D. J. Price, “SPLASH : An Interactive Visualisation Tool for Smoothed Particle Hydrodynamics Simulations,” Publications of the Astronomical Society of Australia, vol. 24, no. 3, pp. 159–173, 2007.

[6] M. J. Turk, B. D. Smith, J. S. Oishi, S. Skory, S. W. Skillman, T. Abel, and M. L. Norman, “Yt: A MULTI-CODE ANALYSIS TOOLKIT FOR ASTROPHYSICAL SIMULATION DATA,” ApJ Supplement Series, vol. 192, no. 1, p. 9, Jan. 2011.

[7] A. Benitez-Llambay, “Py-sphviewer: Py-SPHViewer v1.0.0,” Jul. 2015.

[8] J. Borrow and A. Borrisov, “Swiftsimio: A Python library for reading SWIFT data,” Journal of Open Source Software, vol. 5, no. 52, p. 2430, Aug. 2020.

[9] M. Schaller, P. Gonnet, A. B. G. Chalk, and P. W. Draper, “SWIFT: Using task-based parallelism, fully asynchronous communication, and graph partition-based domain decomposition for strong scaling on more than 100,000 cores,” Proceedings of the Platform for Advanced Scientific Computing Conference on - PASC ’16, pp. 1–10, 2016.

[10] H. Wendland, “Piecewise polynomial, positive definite and compactly supported radial functions of minimal degree,” Advances in Computational Mathematics, vol. 4, no. 1, pp. 389–396, Dec. 1995.

[11] W. Dehnen and H. Aly, “Improving convergence in smoothed particle hydrodynamics simulations without pairing instability,” MNRAS, vol. 425, no. 2, pp. 1068–1082, Sep. 2012.

[12] J. Borrow, M. Schaller, R. G. Bower, and J. Schaye, “Sphexis: Smoothed Particle Hydrodynamics for the next generation of galaxy formation simulations,” arXiv:2012.03974 [astro-ph], Dec. 2020.

[13] L. Hernquist, “AN ANALYTICAL MODEL FOR SPHERICAL GALAXIES AND BULGES,” ApJ, vol. 356, no. 2, p. 6, 1990.

[14] L. Schaye, R. A. Crain, R. G. Bower, M. Furlong, M. Schaller, T. Theuns, C. Dalla Vecchia, C. S. Frenk, I. G. McCarthy, J. C. Helly, A. Jenkins, Y. M. Rosas-Guevara, S. D. M. White, M. Baes, C. M. Booth, P. Camps, J. F. Navarro, Y. Qi, A. Rahmati, T. Sawala, P. A. Thomas, and J. Trayford, “The EAGLE project: Simulating the evolution and assembly of galaxies and their environments,” MNRAS, vol. 446, no. 1, pp. 521–554, Jan. 2015.

[15] S. Plowacki and J. Schaye, “Radiative cooling rates, ion fractions, molecule abundances, and line emissivities including self-shielding and both local and metagalactic radiation fields,” MNRAS, vol. 497, pp. 4857–4883, Jul. 2020.

[16] J. Schaye and C. Dalla Vecchia, “On the relation between the Schmidt and Kennicutt-Schmidt star formation laws and its implications for numerical simulations,” MNRAS, vol. 383, no. 3, pp. 1210–1222, Jan. 2008.

[17] C. Dalla Vecchia and J. Schaye, “Simulating galactic outflows with thermal supernova feedback: Galactic outflows with thermal SN feedback,” MNRAS, vol. 426, no. 1, pp. 140–158, Oct. 2012.

[18] F. Bigiel, A. Leroy, F. Walter, E. Brinks, W. G. J. de Blok, B. Madore, and M. D. Thornley, “THE STAR FORMATION LAW IN NEARBY GALAXIES ON SUB-KPC SCALES,” The Astronomical Journal, vol. 136, no. 6, pp. 2846–2871, Dec. 2008.