

On the Estimation of Centre of Mass in Periodic Systems

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Calculation of the centre of mass of a group of particles in a periodically-repeating cell is an important aspect of chemical and physical simulation. One popular approach calculates the centre of mass via the projection of the individual particles' coordinates onto a circle [Bai & Breen, *J. Graph. Tools* **13**(4), 53, (2008)]. This approach, which is mathematically equivalent to finding the first moment of the Fourier series of the mass density, suffers from some numerical error. Here, we discuss this inaccuracy and propose an extension that overcomes it, enabling improved accuracy across computational simulation.

I. INTRODUCTION

The calculation of the centre of mass of a group of particles, such as in a molecule, is important across computational chemistry and physics.^{1–6} However, computing the centre of mass is non-trivial for systems with periodic boundary conditions. Any group of particles will have the same number of valid centres of mass—positions in the simulation cell where the weighted relative positions of the masses sum to zero—as the number of particles (Fig. 1a). In the physical sciences, we may be concerned with the centre of mass of a single bonded molecule or a defined group of particles. For such systems, there is only one correct answer for the centre of mass. Practically speaking, for most simulations, it is most desirable to compute the centre of mass that minimises the periodic distance to the measured particles.

In a non-periodic system, identifying the “correct” centre of mass of a group of particles, the average position weighted by the masses, is trivial. However, where the periodic boundary can intersect the particle group, this naive calculation may be “incorrect” (Fig. 1b). This problem can be resolved where bonding or other relational information is present, but this is not always the case for computational simulation trajectories.

Bai and Breen proposed an elegant algorithm to efficiently estimate the minimised periodic distance centre of mass,⁷ involving the projection of each orthogonal Cartesian dimension onto a circle to find the centre of mass in the periodic space (Fig. 1c). However, this approach is approximate and introduces numerical error, regardless of whether particles span the periodic boundary. For the original use case, to allow the recentering and visualisation of groups of aggregated particles, the method is effective, as numerical accuracy is less important. However, within the context of computational chemistry and physics, this is not the case. Here, we propose an extension to the Bai and Breen algorithm that removes this numerical error, allowing the correct centre of mass to be found in nearly all practical cases.

II. BAI AND BREEN APPROACH

To outline the approach of Bai and Breen and the source of the numerical error, we consider a simple one-dimensional periodic system, where the cell ranges from 0 to 1. This system is analogous to a fractional coordinate system. A group of N particles can be described with two vectors, one for the positions, \mathbf{x} , and another for the masses, \mathbf{m} . Each particle i is then projected onto the two dimensions of a unit circle, ξ and ζ , where,

$$\xi_i = \cos(2\pi x_i), \quad (1)$$

and

$$\zeta_i = \sin(2\pi x_i). \quad (2)$$

The average of the vectors ξ and ζ are then found, weighted by the masses of i ,

$$\bar{\xi} = \frac{1}{N} \sum_{i=1}^N m_i \xi_i, \quad (3)$$

and

$$\bar{\zeta} = \frac{1}{N} \sum_{i=1}^N m_i \zeta_i. \quad (4)$$

The projection process is then reversed for the weighted average circular coordinates. Practically, this is achieved using the 2-argument arctangent,

$$\bar{x} = \frac{\text{atan2}(-\bar{\zeta}, -\bar{\xi}) + \pi}{2\pi}, \quad (5)$$

to give the centre of mass position. In the case of an orthogonal multi-dimensional system, this method can be repeated independently for each dimension.

While not discussed in the original work, this method is equivalent to finding the first moment of the Fourier series of the mass density as a function of position (see

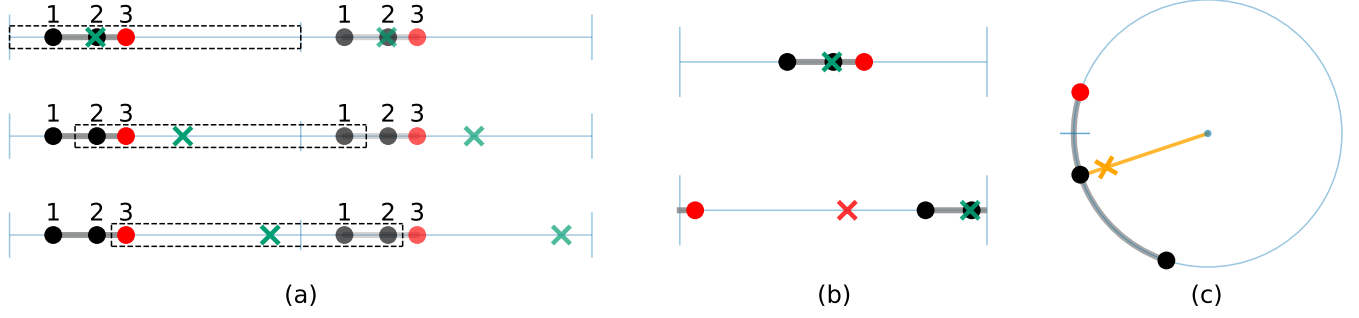


FIG. 1. (a) Demonstration of the N possible centres of mass in an N particle system, where two periodic cells are visible, and the dashed line indicates the particle grouping that leads to a given centre of mass (cross). (b) The problem with the naive centre of mass (red cross) calculation in periodic systems, where the particle group spans a periodic boundary. (c) The projection of the particles in the bottom diagram of (b) onto a circle to find the centre of mass, which minimises the weighted distance to all particles.

Appendix A). This approach is used in signal processing to find the spectral centroid of a signal,⁸ where it is known that it is affected by noise and asymmetry.⁹ Describing an asymmetric function with a single sine wave leads to an incorrect estimate of the spectral centroid, or centre of mass.

Considering the limiting case of a 3-particle system, where a central particle is moved between the 2 edge particles. The error in the centre of mass varies, reaching the maximum when the central particle is very close to the stationary particles, where the system is most asymmetrical (Fig. 2). At the point where the particles are equally distributed, the system is perfectly symmetric, and there is no numerical error in the centre of mass. Similarly, there is no error in one or two particle systems as these are inherently symmetrical.

III. PSEUDO-CENTRE OF MASS RECENTERING

We suggest an extension that removes the error introduced by asymmetry, which involves using the Bai and Breen estimate as a *pseudo*-centre of mass. The group of particles is repositioned to the middle of the simulation cell using the *pseudo*-centre of mass, such that there is no risk that the group spans a periodic boundary condition. Then, the standard weighted mean may be used to find the centre of mass before restoring this to the original space.

The use of this recentering assumes that the inaccurate Bai and Breen method finds a centre of mass close enough to the true centre of mass that the recentering will place all particles contiguously in the periodic cell. This assumption holds true for all systems where the particle group is less than half the size of the periodic cell and is often still true unless the system is very asymmetric. If a group of particles spans more than half the size of the periodic box, the only way to guarantee the centre of mass is found accurately is by including bonding or other relational information.

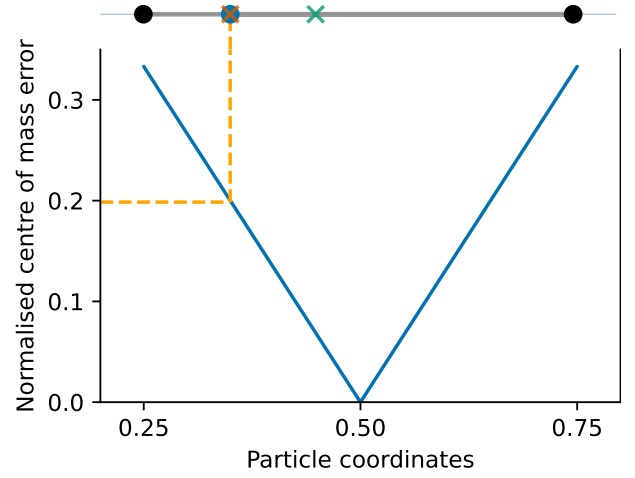


FIG. 2. Quantification of the limiting case (bottom), a 3-particle group spanning almost exactly half the periodic box, where the solid blue line shows the error in the estimate from the Bai and Breen approach normalised by the span (length) of the particle group. This error is shown visually for a single example (top), where the Bai and Breen estimate (orange cross) is not close to the true centre of mass (green cross).

IV. METHOD COMPARISON

To demonstrate the effectiveness of our *pseudo*-centre of mass recentering extension, Fig. 3 compares it to the Bai and Breen method. To achieve this, we compute the difference between the estimated centre of mass and the true value as a ratio of the span of the particle group. This error is compared with the asymmetry of the particle mass density in the periodic cell.¹⁰ In Fig. 3, as the asymmetry increases, so does the error in the Bai and Breen approach. However, the *pseudo*-centre of mass re-sampling is not affected in this way. Therefore, for most chemical simulations, this *pseudo*-center of mass recentering extension should be used to ensure accuracy in

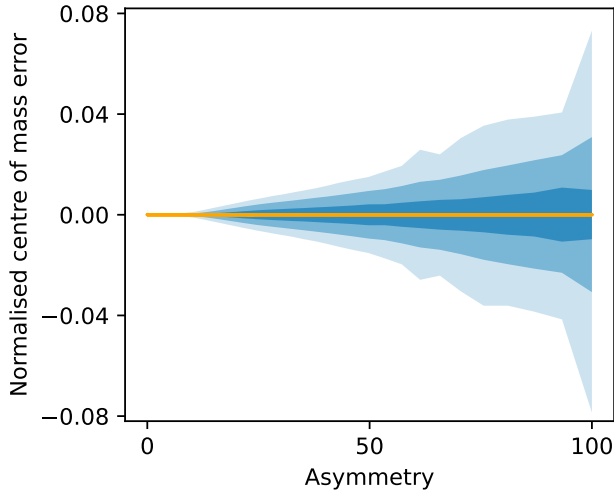


FIG. 3. Error in Bai and Breen method (blue shading representing 1, 2, and 3σ spreads) compared with the *pseudo*-centre of mass recentering approach (orange line). 2^{24} random configurations of one-dimensional periodic boundary-spanning particle groups were generated, with between 3 and 512 particles and a total length of less than half the box. For each configuration, the two approaches were used, and the asymmetry of the particle group¹⁰ is compared to the error in the estimate normalised by the span (length) of the particle group. The results were binned along the x -axis using 100 bins spaced evenly on a log scale.

the centre of mass calculation.

V. CONCLUSIONS

We have presented the *pseudo*-centre of mass recentering extension to the Bai and Breen approach for determining the centre of mass of a group of particles in a periodic cell. Unlike the existing approach, this method has no error, even at very large asymmetry values. To enable the use of this approach, we have implemented it in the open-source Python package KINISI¹¹ and hope that others will consider its use in future.

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CONFLICT OF INTEREST STATEMENT

The authors have no conflicts to disclose.

AUTHOR CONTRIBUTIONS

CRedit author statement: H.R.: Formal analysis, Investigation, Methodology, Software, Visualisation, Writing – original draft. J.D.: Conceptualization, Investigation, Methodology, Supervision, Writing – review & editing. A.R.M.: Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Supervision, Writing – review & editing.

DATA AVAILABILITY

The data that support the findings of this study are openly available in a GitHub repository¹², under an MIT license, including a complete set of analysis/plotting scripts allowing for a fully reproducible and automated analysis workflow, using SHOWYOURWORK¹³.



Appendix A: Mathematical Equivalency of Bai and Breen and First Moment Methods

This appendix presents the mathematical equivalency between the Bai and Breen method for calculating the centre of mass, and finding the maximum of the first term of the Fourier series of the mass density as a function of position, known as the first moment method.⁹

For a real-valued function, the Fourier series can be described as

$$s_N(x) = a_0 + \sum_{n=1}^N \left[a_n \cos\left(2\pi \frac{n}{P}x\right) + b_n \sin\left(2\pi \frac{n}{P}x\right) \right], \quad (\text{A1})$$

where N is some finite number of terms that are computed, and P is the period of the function. Eqn. A1 is equivalent to

$$s_N(x) = A_0 + \sum_{n=1}^N A_n \cos\left(2\pi \frac{n}{P}x - \varphi_n\right), \quad (\text{A2})$$

by the identity,

$$\begin{aligned} \cos\left(2\pi \frac{n}{P}x - \varphi_n\right) &= \cos(\varphi_n) \cos\left(2\pi \frac{n}{P}x\right) \\ &\quad + \sin(\varphi_n) \sin\left(2\pi \frac{n}{P}x\right), \end{aligned} \quad (\text{A3})$$

where φ_n is the phase shift of the n -th harmonic. If we write,

$$a_n = A_n \cos(\varphi_n), \quad (\text{A4})$$

and

$$b_n = A_n \sin(\varphi_n). \quad (\text{A5})$$

Then a_n and b_n can be considered to be constants that “weight” the relative contributions of $\sin\left(2\pi\frac{n}{P}x\right)$ and $\cos\left(2\pi\frac{n}{P}x\right)$, akin to the weighted average of ξ and ζ carried out within the B&B method.

As stated in the main text, the Bai and Breen method is equivalent to finding the maxima of the first function of the Fourier series, f_1 ,

$$f_1(x) = a_1 \cos\left(2\pi\frac{1}{P}x\right) + b_1 \sin\left(2\pi\frac{1}{P}x\right), \quad (\text{A6})$$

where P is 1 as the Bai and Breen method projects the full box size onto a single unit circle. To maximise the value of $f_1(x)$ a stationary point is found where,

$$\frac{\partial f_1(x)}{\partial x} = 0, \quad (\text{A7})$$

which is

$$\frac{\partial f_1}{\partial x} = -2\pi a_1 \sin(2\pi x) + 2\pi b_1 \cos(2\pi x) = 0. \quad (\text{A8})$$

Eqn. A8 can be rearranged to give,

$$\frac{\sin(2\pi x)}{\cos(2\pi x)} = \frac{b_1}{a_1} \quad (\text{A9})$$

and from the trigonometric identity, $\tan(x) = \sin(x)/\cos(x)$,

$$\tan(2\pi x) = \frac{b_1}{a_1}. \quad (\text{A10})$$

Therefore the position at which the first function of the Fourier series is maximised, x , can be calculated as,

$$x = \frac{\text{atan2}(b_1, a_1)}{2\pi}. \quad (\text{A11})$$

In terms of periodic position,

$$\frac{\text{atan2}(b_1, a_1)}{2\pi} \equiv \frac{\text{atan2}(-b_1, -a_1) + \pi}{2\pi}. \quad (\text{A12})$$

The negative b_1 and a_1 in the Bai and Breen method ensure that the centre of mass is always in the correct periodic box with no additional wrapping.

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