ParticleSync: a program for simulating multiparticle interactions

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Abstract. A Windows application is presented that emulates a model previously developed. The model simulates the rotational disturbances of rigid ellipsoids subject to simple shear as a result of interactions between neighbours. A summary of the model along with instructions on how use the software are presented as well as results from simulations which reveal the particles’ preferred orientation at an angle to the shear direction.

1. Introduction
The interaction between two or more particles has been the subject of much research in the past with many different applications and approaches to solutions (cf. [1]). In this contribution, a software application is presented which implements a new model [1] that accounts for particle interactions. The model is an adaptation of the Kuramoto model [4] and treats particles in isolation as rigid inertialess ellipsoids immersed in a creeping shear flow of zero Reynolds number in the manner of Jeffery [3]. The effect of interaction is incorporated into the model via adjustments to the angular velocity of each particle, described below.

2. Interaction model
The model that is developed here (see [1] for a complete derivation) is inspired by the well known Kuramoto model:

\[ \dot{\theta}_i = \omega_i + \frac{K}{N} \sum_{j=1, j \neq i}^{N} \sin(\theta_j - \theta_i), \quad i = 1, \ldots, N, \]

(1)

which simulates the synchronisation between a set of \( N \) coupled oscillators, where \( K \) is the coupling constant. Here, \( \omega_i \) and \( \theta_i \) are the \( i^{th} \) oscillator’s natural frequency and phase respectively. Applied to a set of rigid ellipsoidal particles, we could assume that both \( \omega_i \) and \( \theta_i \) represent the angular velocity of the \( i^{th} \) particle in isolation and that \( \dot{\theta}_i \) would be the resultant coupled angular velocity. However, this model would suggest that particles tend to converge to a common rotation rate, which is dependent on the degree of coupling. What we would like is to simulate particle interactions, under simple shear, in a different, more natural way.

Consider the two-dimensional case (see Fig. 1a). Under simple shear, particles in isolation will rotate in the same direction. Therefore, the phase of a particle should be affected by the phases of all neighbouring particles in much the same way as a set of gear wheels would interact. In other words, neighbouring particles have an antithetic affect on each other. In three-dimensions the situation is a little more complex (see Fig. 1b-d). Here we suggest that particles only have an antithetical interaction if their angular velocity vectors are perpendicular to the line joining
their centers (Fig. 1c and d). If their angular velocity vectors are parallel to this line, then they should interact synthetically (Fig. 1b). As derived in [1], Eq. 7.12, the $i^{th}$ particle’s adjusted angular velocity, $\bar{\omega}_i$, as a result of interaction between neighbouring particles is

$$\bar{\omega}_i = \frac{1}{N-1} \sum_{i \neq j} \left( \omega_i - \kappa_{ij} \omega_j + \kappa_{ij} (1 + \delta) \frac{(x_j - x_i) \cdot \omega_j}{\|x_j - x_i\|^2} (x_j - x_i) \right), \quad (2)$$

where

$$\kappa_{ij} = \min \left( 1, \frac{K^2}{\|x_j' - x_i\|^2} \right) \quad (3)$$

such that $i = 1 \ldots N$, $x_i$ is the location of particle $i$, $\delta$ is the degree of synthetic interaction with respect to the line joining particle pairs, and $\kappa_{ij}$ is some coupling factor proportional to the distance between particle pairs. In what follows, a description of the software developed to simulate the above interaction model is described.

3. Software application: ParticleSync

ParticleSync is a simple point and click driven Windows application that implements the model described above. ParticleSync allows data to be instantly made visible through three-dimensional renderings and allows for more detailed analysis via porting to other applications (such as Mathematica). ParticleSync was written in Microsoft’s Common Language Runtime (CLR) using the integrated development environment (IDE) Visual Studio 2005. The graphical
user interface was written in C#. Visualisation of the data in 3D was achieved through the use of the open source libraries contained in the Visualisation Toolkit (VTK) found at http://www.vtk.org/ and VTK.NET which is a .NET wrapper of VTK for the .NET CLR (see http://vtkdotnet.sourceforge.net/). VTK uses the OpenGL graphics library to render the 3D images.

3.1. Installing ParticleSync
First, download ParticleSync from [2]. Install ParticleSync by running setup.exe and choose an appropriate location for the installation. Depending on your system configuration, you may be prompted to download Microsoft’s .NET Framework. When the installation is complete a shortcut to ParticleSync will be placed on your desktop. Upon running, press the F1 key to get further information on how to use the application.

[Image: Screenshot of ParticleSync]

Figure 2. Screenshot of ParticleSync.

3.2. Using ParticleSync
The results presented here were obtained from output from ParticleSync. Data obtained from ParticleSync was graphed using Mathematica. Shown in Fig 2 is a screenshot of ParticleSync upon first running. The system may be initialised as shown in Fig 3a given:

a/b: Ratio of the long to intermediate axes.
b/c: Ratio of the intermediate to short axes.
vol: Volume of each ellipsoid.
ph(0): The initial value of the Euler angle $\phi_0$.
th(0): The initial value of the Euler angle $\theta_0$. 
Figure 3. (a): Controls for system initial conditions. (b): Switches for the 3D display. (c): Playback controls.

Figure 4. Output from ParticleSync at the end of the simulation. The initial conditions are those in Fig. 3a. Plots of this simulation can be seen in Fig. 5.

\( ps(0) \): The initial value of the Euler angle \( \psi_0 \).
\( dx \): The distance between adjacent particles.
\( N \): Number of particles.
\( K \): The coupling, \( K \), as in Eq. (3).
\( sx \): The synthetic coupling, \( \delta \), acting along the line joining particle pairs. E.g., in Fig 3a, \( sx = -1 \times 10^0 = -1 \).

Selecting the items shown in Fig 3b has the following effects:

**Inclusions**: Show/hide ellipsoids.
Axes: Show/hide the axes and average ellipsoid as displayed on the bottom left of the screen. Zoom: If set, the camera will automatically zoom to ensure all objects are visible.

The items shown in Fig 3c control the numerical integrator time step and end time.

3.3. Example: fully coupled system

As an example, take the initial conditions as shown in Fig 3a and run the simulation until \( t = 50 \) progressing in steps of \( t = 0.01 \) as shown in Fig 3c. All particles have the same axial ratios and volumes but are initially randomly oriented (as shown in Fig 2). The output from ParticleSync at the end of the simulation is shown in Fig 4. The long axis of each particle points toward the shear direction at an angle of 45° above the shear plane.

**Figure 5.** (a): Stereographic plot of the average ellipsoid long axis over time. (b): Stereographic plot of the average ellipsoid short axis over time. Also shown is the short axis of each ellipsoid at \( t = 50 \). Since the ellipsoid is biaxial, the short and intermediate axes are equal and therefore the points are distributed on the plane inclined 45° away from the shear sense. (c): The angle above the shear plane made by the long axis of the average ellipsoid over time. (d): The shape of the average ellipsoid over time.

These results may be graphed in Mathematica by clicking the "View data in Mathematica" button. The plots from this simulation are shown in Fig 5. The stereographic plot in Fig 5a
shows the progression of the average ellipsoid long axis over time so that, as \( t \to 50 \), the long axis points toward the shear direction at an angle of 45° above the shear plane. Fig 5b shows the evolution of the short axis of the average ellipsoid over time. The dotted line denotes that the path is below the horizontal plane. In both Fig 5a and b the final position of the long and short axes of the individual ellipsoids is marked by points. In Fig 5a these points are not visible as they have accumulated at the same location at 45°. Due to the fact that the ellipsoids are biaxial the short and intermediate axes are the same length and so the points in 5b are distributed on the plane inclined at 45° above the shear plane away from the shear direction.

Fig 5c shows the angle above the shear plane made by the long axis of the average ellipsoid over time. It is clear to see from this plot that the preferred angle of the set of ellipsoids is 45°. Finally, in Fig 5d is shown the shape of the average ellipsoid which becomes prolate-biaxial with an axial ratio of 2 : 1 : 1 as \( t \to 50 \). This is to be expected as all the ellipsoids have the same axial ratio and eventually align themselves in the same direction.

4. Conclusions
The development of a Windows application, ParticleSync, for simulating particle interactions has been the subject of this manuscript. A brief overview of the model [1] which is simulated was also presented. ParticleSync aids in the calculation, visualisation and interpretation of results from large sets of interacting particles. It was shown that ParticleSync makes it easy to port data to other applications, such as Mathematica, for further analysis.

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