Visualization of Nanoparticle Formation in Turbulent Flows

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ABSTRACT

In this paper we offer methods for visualization of the formation of nanoparticles in turbulent flows. We present the use of pointillism as a technique to convey the distribution of nanoparticle sizes as texture in an area. We also demonstrate a method of producing and packing spot glyphs representative of the distribution of nanoparticle sizes at every point in the flow to produce an intuitive and extensible framework for the visualization.

1. INTRODUCTION

Nanoparticles play an integral role in a wide variety of physical/chemical phenomena and processes. An important goal of current research in the fluid-chemistry interactions of particle formation and growth is to provide a more through understanding of how to better control particle formation to facilitate the economical production of materials with unique and useful properties [1].

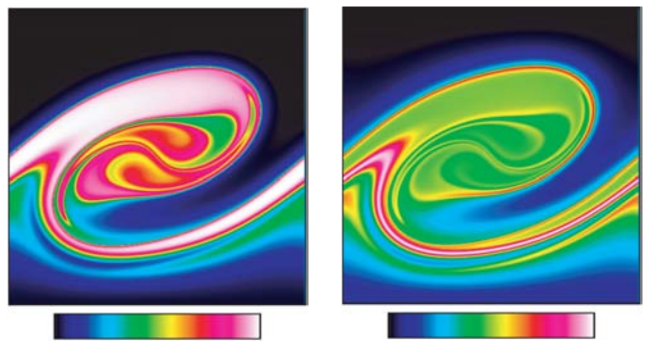
Traditional visualization of nanoparticle data has involved the display of pairs of images, color-coded to represent the values of the mean and standard deviation of the distribution of nanoparticle sizes over an infinitesimal area at each point in the flow [7]. In this application, we focus on developing visualization methods that allow a more complete, integrated and direct representation of the *full distribution* of particle sizes. Mental combination of multiple images is quite difficult [9]. There can also be problems with the rainbow color scale as even with a legend the ordering of colors is neither necessarily intuitive nor perceptually linear from a luminance perspective [8]. Our motivation is to improve on previous methods by visualizing both variables in a single, easy-to-understand image.

2. POINTILLISM AND RELATED WORK

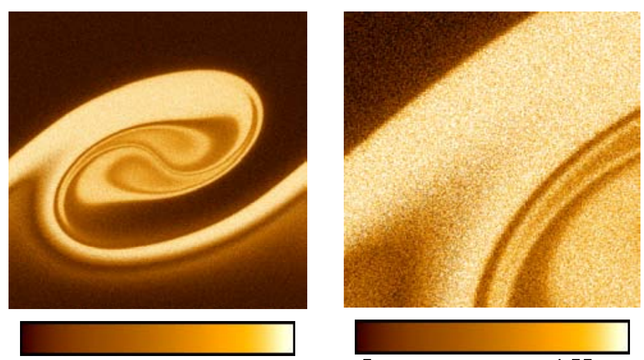
Painterly effects in data visualization have rich historical precedent. Laidlaw *et al.* [5] and Kirby *et al.* [4] have offered approaches to artistic rendering of data using layers and 'paint stroke' glyphs. *Pointillism* as a cartographic visualization method was suggested as early as 1953 [3]. We have found it also works well for our data.

Our pointillism visualizations represent a single data pair with a pixellated quadrant in the output image. For each pixel in a quadrant, we generate random normally distributed data values from a distribution defined by the underlying mean diameter and standard deviation data values computed in the simulation. We have utilized the Box-Muller Polar transform for generating normally distributed numbers from a pseudorandom uniform distribution.

In these figures, the random normal values have been mapped to the conventional heated-object color scale before output. The HOS was chosen to exploit human sensitivity to luminance in the yellow-orange hue [6]. At the macrocosmic level, our images (fig. 3, 4) convey the distribution of the data over the entire area, effectively showing large trends. On a smaller scale, our use of a pixellated quadrant for each mean diameter and standard deviation pair data point allows us to convey an individual data point's inherent distribution. The mean diameter manifests as the average color in a quadrant, the *graininess* of color expresses the standard deviation.



Figs.1 & 2. Standard visualizations of mean diameter and standard deviation of nanoparticles using the rainbow colorscale.



Figs.3 & 4, 5x5 Grid pointillist rendering of mean diameter and standard deviation with enlarged detail

This visualization is quite effective for showing us the standard deviation of particles in a given area. One issue is that the user must interpret particle size from color intensity. This suggests an extension on the method that shows the size of particles in a more straightforward fashion through generation of spot voxels whose perceptual size is representative of the mean diameter of nanoparticles.

3. SPATIAL FREQUENCY AND SPOT PACKING

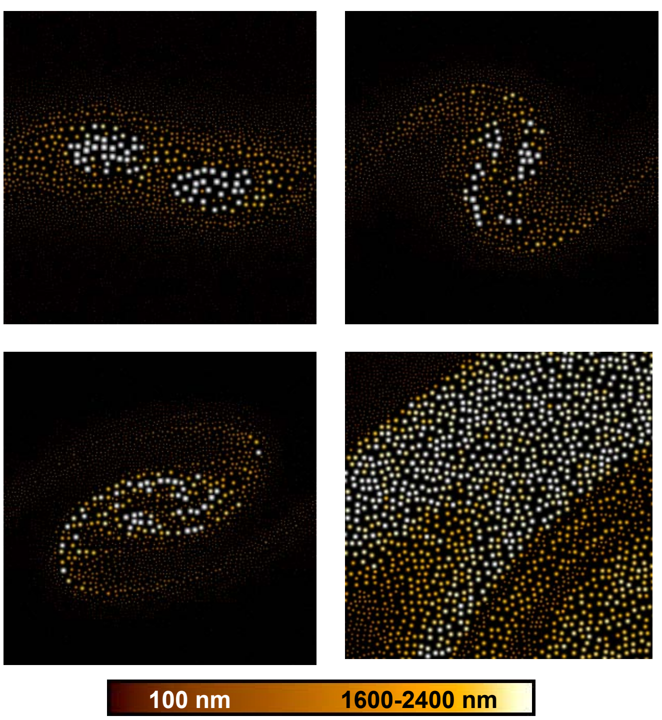
Healey and Enns have shown glyph density to be an effectively detectible artifact [2]; therefore, when we generate the various spots we must take care to maintain a perceptually similar spatial frequency so we do not imply false information about density in the underlying nanoparticle distribution.

A conventional Poisson method of distributing spots is not optimal from a performance perspective- the algorithm takes an unpredictable amount of time and there is no efficient way to determine when it has achieved "good enough" results. We have reasonably approximated a full Poisson packing through more deterministic methods. We generate a regular grid of potential locations to place the center of a spot then jitter these locations by a random small amount to avoid potential artifacts due to regularity of spacing [2].

Calculating the footprint of a would-be spot allows us to check for overlapping spots, in which case the spot is simply discarded; otherwise, we place the spot and move on. High spatial frequency in the underlying jittered grid ensures that in most cases spots will appear in a well-packed manner without covering each other unless we so desire. This algorithm cannot guarantee an optimal packing, but we believe the results are quite sufficient for avoiding visual artifacts due regularity or spatial frequency and it runs its course in a predictable amount of time.

4. Spot Sizing and Shading

The perceptual size of our spots is mapped to the mean diameter at a point. Our method utilizes Gaussian gradient shading based on mean diameter to perceptually convey the correct size to spot footprints of a few sizes; thereby, we achieve sufficiently fine gradations in the perceptual size of a spot without accruing prohibitively large overall size in the output image. We express standard deviation by randomly varying spot sizes in an area according to the underlying deviation. Figures 5, 6, and 7 show this technique in use to display the relative sizes of nanoparticles in formation at several time steps in the turbulent flow. Figure 8 shows a detail from a larger scaled image.



Figs. 5,6,7,8. Diameter of nanoparticles in formation at multiple timesteps and detail of enlarged rendering of spot glyphs.

5. Conclusions and Further work

The intent of our visualization method is to effectively convey the mean and standard deviation of the distribution of nanoparticle sizes within computed two-dimensional slices of multi-dimensional, incompressible, particle-laden flows through production of spot glyphs intuitively representative of these nanoparticles in terms of the spots' diameter and variation over space. Our pointillist method aims to effectively show distributions underlying each single data point and across the complete data space. Spot glyph methods are promising not only for their intuitive qualities, but also for the facility for expansion inherent in the representation. Negative space, color, and/or spot shape are being investigated for displaying additional variables useful in studying nanoparticle formation, such as temperature and chemical concentration. The pointillist method is being expanded with random grid partitioning for additional color variables.

Acknowledgements

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