Motivation
Magnetic resonance imaging is a common technique in the medical field. However, an emerging alternative, magnetic particle imaging (MPI), has shown promising initial results [1]. MPI uses the response of magnetic nanoparticles to an external magnetic field, showing results of a very clean signal. The reduced noise in the response, as compared to MRI, allows for faster imaging and better resolution with cheaper equipment.

While MPI has already shown good results, there is still room for improvement of this recent technique. There are simple analytic models. However, these fail to account for many of the complex interactions between particles in a large system. Simulations become necessary to model these large, realistic situations in order to optimize parameters for better imaging.

Methods
A body of simulation code was written for this specific purpose, giving freedom to control a wide variety of interactions and situations. Numerical integration was used to progress the simulation forward in discrete time intervals. A graphical interface complemented the simulation internals, playing an important role in discovery by actually showing the particles and allowing interactive control of parameters in real-time.

Surfactant Simulation
An early simulation involved looking for resonances in the motion of a system of two surfactant particles under the influence of an oscillating magnetic field. The force between the surfaces of the particles can be modeled as a spring.

The results of running simulations with different external magnetic field frequencies show clear resonance peaks at a regular interval for the RMS distance between the particles.

Results with and without 2D confinement
Running long simulations confined to different thicknesses yields different equilibrium results. For a thin, effectively 2D, volume, the results are qualitatively the same as from experiment, with single-core ring formations uniformly distributed. The 3D analog instead shows distinct, long chains of cores with ring particles distributed along them. It is of interest to see if these chains can be confirmed with future experiments.

Rotational Entrainment
An alternative technique uses a rotating magnetic field, rather than oscillating [3]. The effect is expected to depend on the magnitude of the field. For large fields, a particle will rotate at the same frequency, while small fields cause a slower overall rotation with additional harmonics.

An interesting result shown through simulation and confirmed analytically is the entrainment of a particle to the frequency of the field. The magnetic field strength is increased until the particle rotates with it, and then the strength is gradually decreased. The resulting hysteresis causes the particle to stay entrained at this frequency for lower field strengths.

2D Confinement
Another situation focused on is the experimental confinement of these particles to a 2D surface for viewing under a microscope. Simulations in 3D show a tendency for larger core particles to chain together, while experimental images show uniformly spaced ring formations. Results of simulations for ring formations in both 2D and 3D are shown below.

Conclusions
The various simulations have shown good promise for an accurate description of their experimental counterparts. This gives real potential for aiding in the prediction of new results and guiding new experiments.

References
[3] Thanks to Professor Mark Griswold for informing us of early work with this technique from the University of Würzburg