

# IFPRI Round Robin: Toward a Best Practice for DEM Simulation

## Background and Goals of the Project

The discrete element method is a powerful numerical technique capable, if used correctly, of quantitatively reproducing the dynamics of diverse particulate systems – including those of relevance to the powder-handling industries. This is a big “if”, however, as quantitative accuracy is only possible when simulations are rigorously calibrated against detailed powder characterisation measurements and, at present, there exists no industry-wide Best Practice for the calibration of DEM simulations. In the IFPRI Round Robin, we intend to gain first-hand insight into current industry practices and, in doing so, establish what works well and what requires improvement, and thus develop, for the first time, a **standardised Best Practice for DEM simulation**.

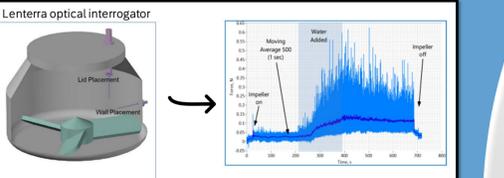
## Experimental Systems & Materials

In the previous Round Robin, we tested two experimental systems (rotating drum and high shear mixer) and three materials (1mm MCC, 2mm angular sand, and 300µm resins), encompassing:

- Both high- and low-shear dynamics
  - Spherical, aspherical, non-cohesive and cohesive materials
- However, there remain some missing pieces of key information
- Neither experimental system possesses a strong dependence on the coefficient of restitution
  - Materials chosen did not allow the isolation of size effects from cohesion effects

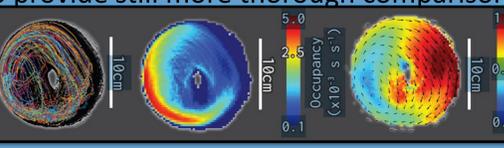
→ New systems (Resodyn RAM, Pascall mixer)  
→ New materials (elongated, lactose, binary...)

## PEPT Imaging and other experimentation

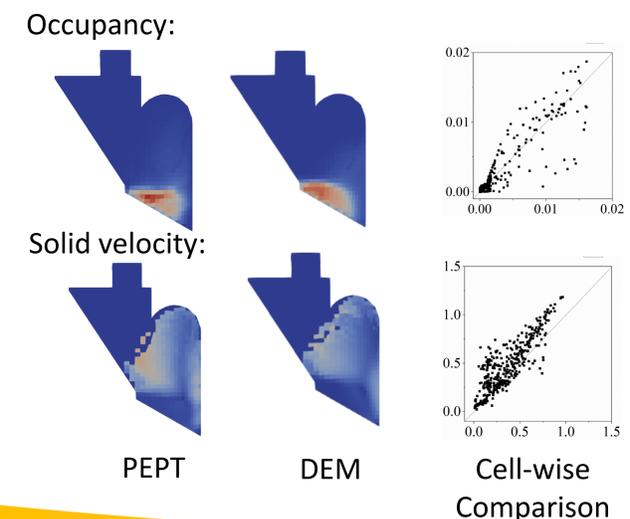


Lenterra optical interrogator

Positron Emission Particle is an imaging technique capable of extracting high-resolution, three-dimensional data from even the interior of large, opaque, three-dimensional systems. PEPT will be used to extract detailed information regarding the dynamics of our test systems, allowing one-to-one comparison with DEM data. This information will be complemented by force data extracted from an inline sensor to provide still more thorough comparison.



PEPT & DEM can *both* be used to produce High-resolution, 3D images of diverse fields, allowing highly rigorous comparison of the DEM simulations and “ground-truth” data



## Comparison and Analysis

## Industry Interviews

Interviews will be conducted with 9 industry participants spanning multiple industrial sectors in which DEM is utilised. The companies will detail their internal practices to the Round Robin team, who will then faithfully reproduce their methodologies during the “calibration” phase of the work.

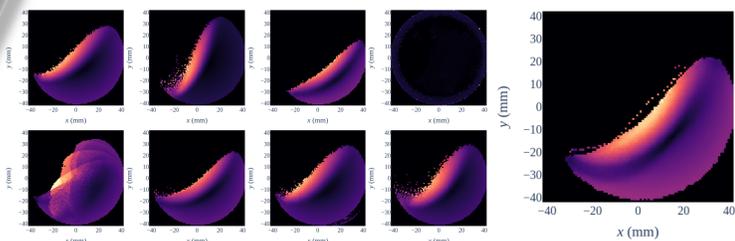


Characterisation performed as per participants’ instructions and data compared against “digital twins” of tools used to “back-compute” DEM parameters. Tools developed (or in development) include Granutools GranuDrum, GranuHeap, Granuflow & GranuPack; Freeman FT4 rheometer and shear cell; Schulze shear cells of various sizes. All models to be released, free and open-source

## Calibration

To ensure maximal accuracy, simulations will – as well as using the same methodologies for characterisation and calibration – be performed using the preferred simulation software of the participants, and using the shape models, time steps and other non-calibrated parameters as they would utilise in their own simulations.

## DEM Simulation



Having quantitatively compared DEM results to PEPT ground-truth data, **as well as force and torque data** acquired via conventional sensors and novel in-line force sensors produced by Lenterra Inc., we will perform detailed analysis attempting to link these outcomes to the quality of the calibration methods used to acquire them. We will also explore the application of alternative methodologies which may prove effective, including evolutionary-algorithm-based methods developed in our lab in Birmingham.