Ansys

CASE STUDY /

Ansys Rocky + Bristol-Myers Squibb (BMS)

BMS Simulates Over 10 Million Particles using the Multi-GPU Capabilities of Ansys Rocky DEM

"The highlight of the Ansys Rocky software is certainly its speed and realistic particle shapes. For us, being able to simulate the exact number of particles in the exact same size distributions and shape representations that we have in our experimental studies is the primary benefit to using Ansys Rocky DEM."

Preetanshu Pandey, Ph.D.
Principal Scientist / Bristol-Myers Squibb

The pharmaceutical industry is known for its complicated manufacturing unit operations that involve complex physical processes. Because these processes are not well understood, scale-up during process development can be quite challenging as it is often done using large-scale Design of Experiments (DOEs), which can be difficult and expensive to accomplish.

To gain a better understanding of their processes and mitigate large-scale experimental costs during scale-up, some companies choose to study their material flow conditions with discrete element modeling (DEM) software.

Preetanshu Pandey, Principal Scientist at Bristol-Myers Squibb (BMS), says, “Some of our R&D processes involve DOEs going from one scale to another. With modeling support, we are able to perform smaller and fewer DOEs, which results in cost savings. Modeling helps in designing experiments better, and potentially reduces experimentation.”

“Due to the limitations of the software, we were restricted to short simulations using mostly sphere-based particle representations, which still took a really long time to process,” he says of their previous modeling experience. “In using Rocky DEM software, besides increasing the speed of the simulation, we are able to achieve a closer match to our experimental conditions in terms of the number of particles we are able to simulate at once.”

This increase in processing speed—made possible by Ansys Rocky’s powerful, multi-GPU solver—combined with Ansys Rocky’s unique non-spherical shape representation and integrated post-processing capabilities, are the features that most attracted BMS to the software. “With Ansys Rocky, in certain cases (e.g. tablet coating), we are able to use the exact number and particle shape that we have in an experimental setting,” explains Mr. Pandey. “Creating more of a one-to-one correlation of modeling-toexperiments is where I see the most benefit of using Ansys Rocky DEM.

/ HIGH-SHEAR WET GRANULATION STUDY

One of the studies BMS performed with Ansys Rocky was for a high-shear wet granulation process, which is used in the manufacturing of solids for oral-dose tablets. The challenge was to come up with the most effective scaleup rules by achieving a particle-level understanding of the process.

Granulators at various scales (1-L, 10-L, and 150-L) using both dry and wet placebo were simulated in Rocky and the results were compared with experimental data obtained via high-speed image analysis. According to BMS, the ability to simulate particle sizes and distributions relatively closer to reality was a standout advantage of Ansys Rocky over other DEM codes they had used in the past. These abilities, coupled with Rocky’s high-performance, mutli-GPU solver, enabled them to compute a large amount of particles in a single simulation—over 10 Million for the 150-L case (Figure 1). This was not possible with prior codes due to the restrictive memory requirements involved. The Ansys Rocky solver uses the combined power of the available GPUs to distribute this memory in the motherboard, thus allowing very large particle counts to be computed in a much more reasonable timeframe (Figure 2). By using Ansys Rocky’s multi-GPU processing, simulations were 20x faster than a 24 core CPU alone.

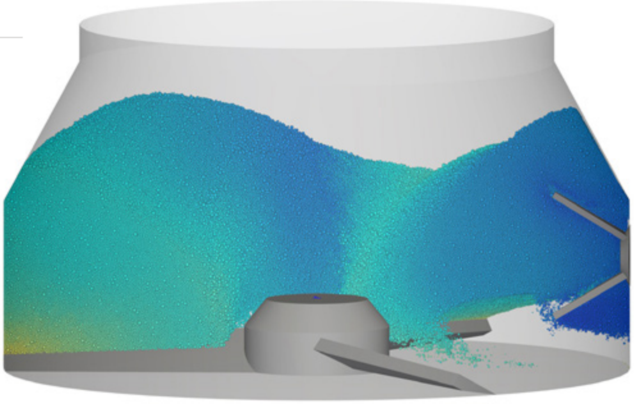

Figure 1: Ansys Rocky DEM simulation snapshot of the granulator showing 10 Million particles colored by their translational velocity.

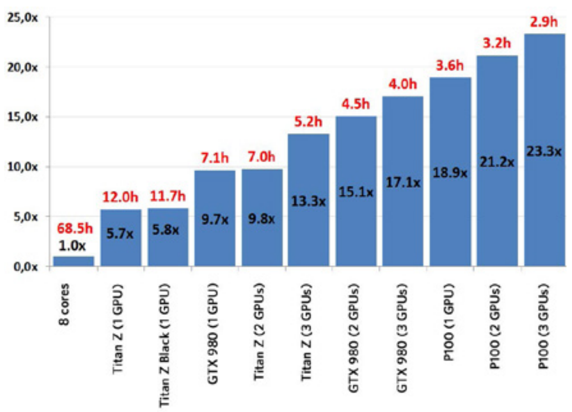

Figure 2: Speed-up and simulation run times (for 1 sec of real time) of a 10-L scale granulator (approx. 700,000 spherical shaped particles). Simulations were run on an 8-core CPU and also on various single and multi-GPU cards. By using Ansys Rocky’s multi-GPU processing, simulations were 20x faster than an 8-core CPU alone.

/ TABLET COATING STUDY

Another unit operation BMS studied with Ansys Rocky was the tablet coater. Before Ansys Rocky, BMS was limited to spherebased particle representations and was thus unable to simulate realistic tablet shapes in their prior DEM models. By using Ansys Rocky, BMS was able to import a 3D polyhedral particle closely resembling the real-world tablet shape (Figure 3), which allowed for more accurate simulations of their commercial scale coater (250,000 tablets).

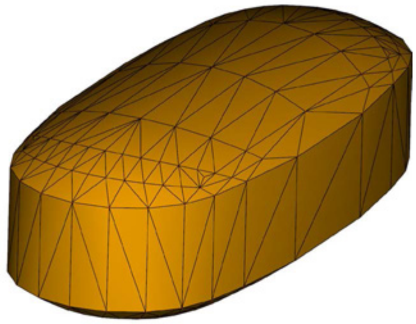

Figure 3: 3D Polyhedral tablet shape with 222 vertices imported into Ansys Rocky and used in BMS's tablet coater simulations.

In addition, Ansys Rocky's fast multi-GPU solver was able to predict the tablet movements within the coater in a reasonable amount of processing time. Figure 4 shows the relative speed-up of the tablet coating simulation using different GPU cards. The results showed that Ansys Rocky using multi-GPU capabilities was up to 86 times faster for this study than CPU processing alone.

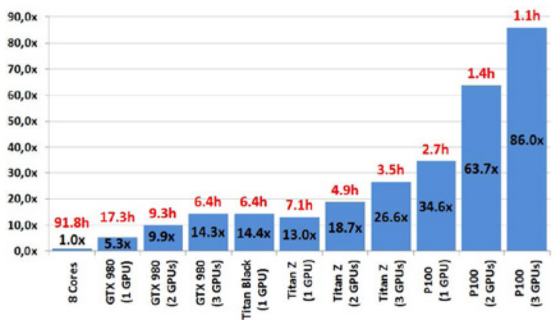

Figure 4: Speed-up and simulation run times (for 1 sec of real time) of a commercial scale (BFC-400) tablet coater (approx. 250,000 polyhedral-shaped particles with 222 vertices). Simulations were run on an 8-core CPU and also using various single and multi-GPU cards. By using Ansys Rocky's multi-GPU processing, simulations were 86x faster than an 8-core CPU alone.

The extensive post-processing tools available within Ansys Rocky's easy-to-use interface—such as discrete to continuum analysis of particle volume fractions, velocities and stress tensors, as well as streamwise velocity plots—enabled BMS to make direct comparisons with experimental data without needing to export data to third-party software (Figure 5). The comparisons proved that Ansys Rocky achieved remarkable accuracy in terms of its simulation predictions, and matched well with BMS'sexperimental data, as shown in Figure 6.

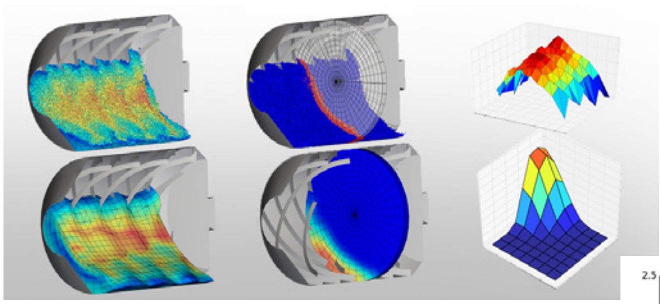

Figure 5: Examples of Ansys Rocky DEM's integrated post-processing results from the tablet coating study showing Lagrangian-Eulerian representations (left and center), and 3D surface plots (right).

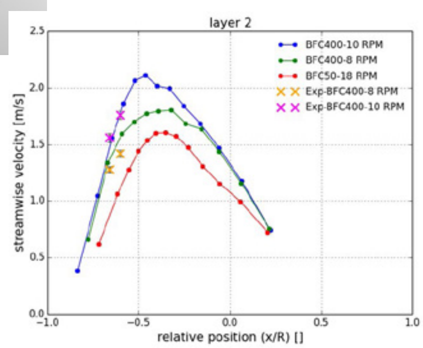

Figure 6: Stream-wise velocity profiles along bed surface for various coater scales. Predictions from Ansys Rocky DEM simulations show excellent match with experimental values.

/ CHALLENGE

BMS needed accurate and fast DEM models to predict flow behavior in their unit operations and reduce the need for expensive scale-up experiments.

/ SOLUTION

BMS used the processing speed of Ansys Rocky DEM's multi-GPU solver to create realistic simulations by matching the particle shape, size distributions, and quantities used in the experiments.

/ BENEFITS

By using Ansys Rocky DEM with multi-GPU processing, BMS not only acquired faster computing times and improved postprocessing capabilities, but was also able to perform more realistic simulations with 100 times more particles than they were able to simulate before.

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