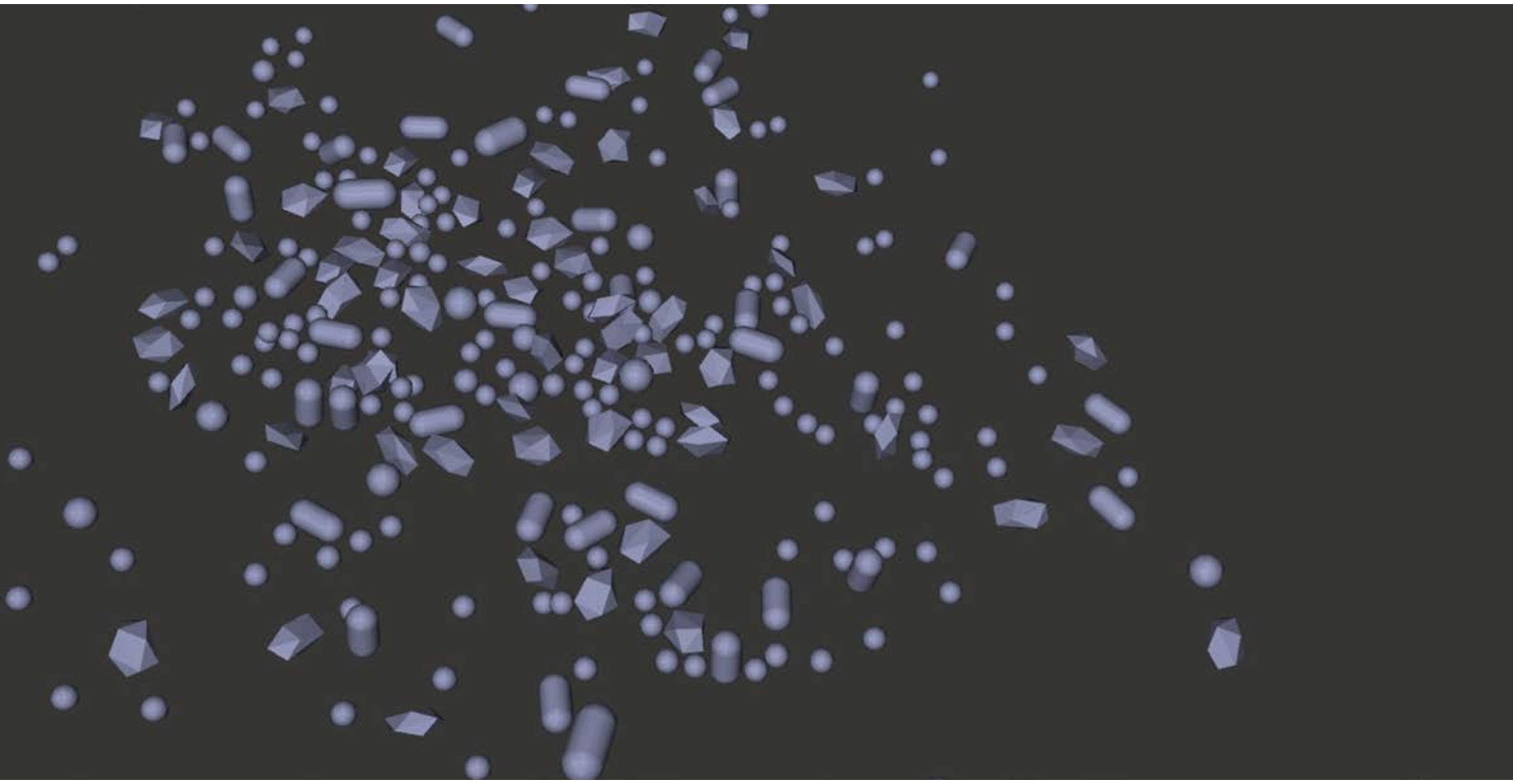
ROCKY

Mission: Possible - A Case Study of Cloud-based HPC for Discrete Element Modelling Computations

by CrunchYard, NVIDIA, Microsoft Azure, ESSS and Qfinsoft using ESSS Rocky DEM



HOW A SPECIALIST SIMULATED 300 MILLION PARTICLES AND GENERATED 1.2 TB OF DATA - REMOTELY

DEM, or Discrete Element Modelling, is a series of numerical methods for computing the motion of large amounts of small particles. DEM enables the complicated geometric behaviour and effects of granular materials, such as coal, ore, rocks, powders or tablets to be simulated. Used in everything from Agriculture to Pharmaceuticals, this specific case study involved the manufacturing of explosives.

In particular, Dr. René Heise was interested in the consolidation of explosive materials into shaped charges. The process of consolidation can lead to cracks and density variations in the material. This reduces performance. By simulating these processes, problems can be mitigated by defining improved process parameters.

As DEM simulations are computationally expensive, this involves the use of the correct software, hardware, tools and services. In addition, Dr. Heise wanted to evaluate the feasibility of using cloud computing to run ESSS Rocky DEM software.

OBJECTIVES

To evaluate the use of remote computing facilities, the tasks performed were the calibration of the material and the simulation of the actual consolidation process.

Two high explosive material powders were used for the evaluations, a commonly used RDX explosive in a fine powder form and an Insensitive Explosive composition in a coarse granular form.

The fine powder was approximated with spherical particle geometries less than 0.6 mm in diameter, as the real particles were relatively evenly shaped. For the coarse powder the approach was used of modelling the particles using non-spherical geometries. Three types of particle geometries and sizes were identified (see Figure 1) and modelled using default geometries available in Rocky 4.

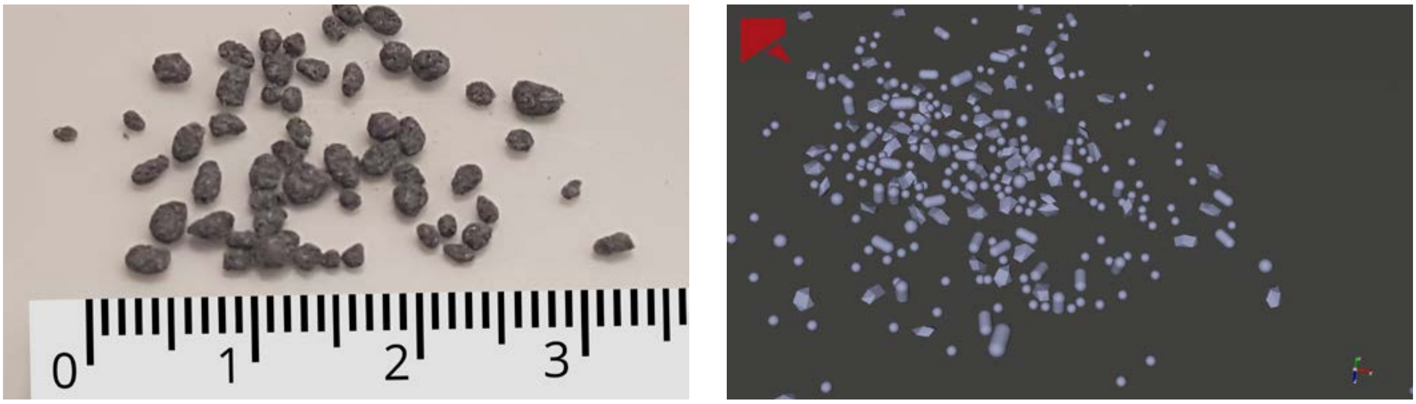


Figure 1: Particle geometry, a sample on the left and the Rocky approximation on the right.

With no "volume inlet" conditions available, if a volume inside a container needs to be filled, a simulation first has to be done of the filling process. These "setting up" simulations take a significant amount of time due to the high number of particles entering the domain. Such is the case for calibrating of the material; for an angle of repose test a box or cylinder of material needs to be filled with the material. So, the calibration tests, specifically the setting up of the test cases, was a natural choice for the simulations.

The test case for the angle of repose was formed by a 100 mm x 100 mm x 25 mm box. For the coarse HE granules the 2 Tesla K80 GPUs (Using the NC12 Azure virtual machine) used on the test filled the box after a run time of just over three days. Particle count was in the region of 1.2 million. In the case of using the fine HE powder, which had particle sizes of 0.1 mm to 0.04 mm.

This in itself is no small task: The processing time for an HP Z620 with 8 2.4GHz cores, was estimated in excess of 3 months. By comparison, the remote access solution filled the boxes in 7 days.

The actual calibration simulations, which model the process of removing the box and letting the material particles disperse and form the repose angle, could be done in 1 day for the coarse and 3 days for the fine powder.

While this may seem relatively slow for gaining just one numerical value, the calibration simulations are a "once-off" exercise; once completed with typically 3 to 4 runs of varying friction parameters for the material, the results can be used for all following simulations using that material.

The upper part of Figure 2 shows the results of the experimental repose trial and the lower part the results of the first Rocky simulation using the default friction coefficient values. Both images are to the same scale. Comparing the two parts of the figure it is noticeable that the static friction is too low, which results in the rounded edges at the top and a wider spread at the base. An iterative adjustment of both the static and rolling friction coefficient improved the results to the extent that even the "mesa" like features of the experiment were reproduced.

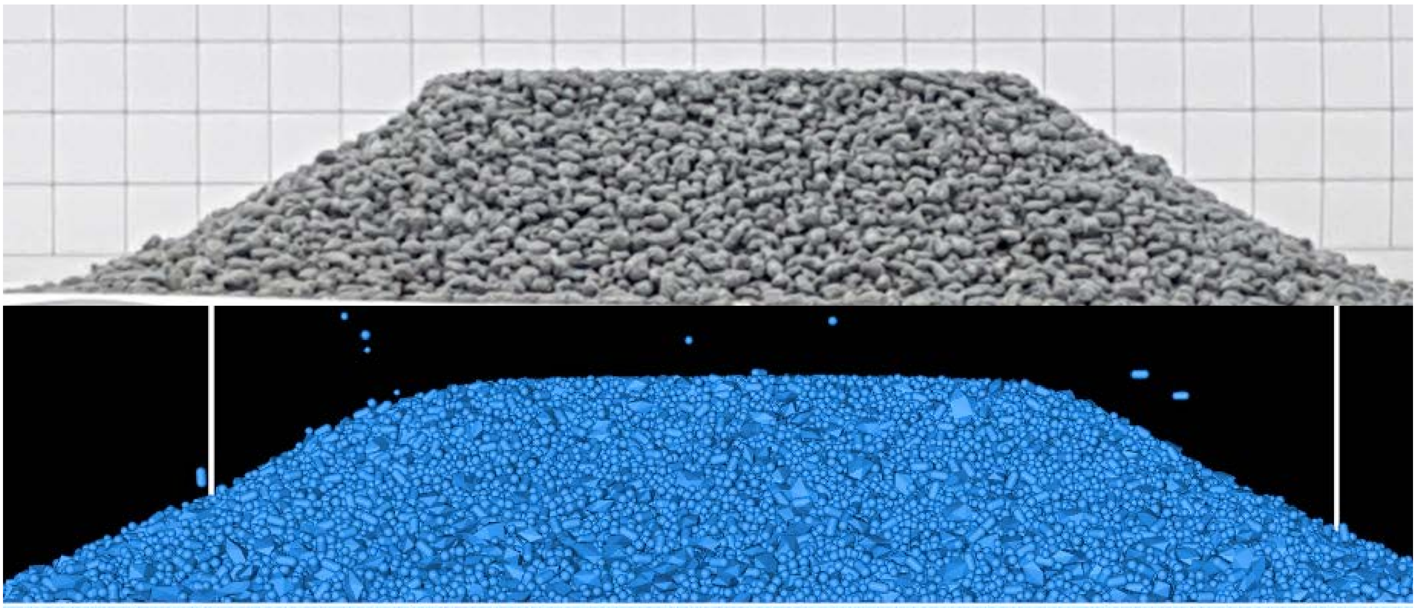


Figure 2: Comparison of experimental and Rocky simulations for an Angle of Repose Test

The consolidation simulations themselves are quick, once the holder into which the particles are to be pressed is filled. Simulation times on the GPUs, even with the fine powder, are completed in a matter of hours. Thus a few iterations can be done over a 24-hour period. By contrast, the CPU approach takes just over 48 hours to complete.

Shown here in Figure 3 is the typical process of consolidating a High Explosive charge. Particles are coloured by exerted force. The initial condition is an asymmetric filling of the holder cup, which leads to a non-uniform compression force on the particles, which can result in a non-uniform density of the final product.

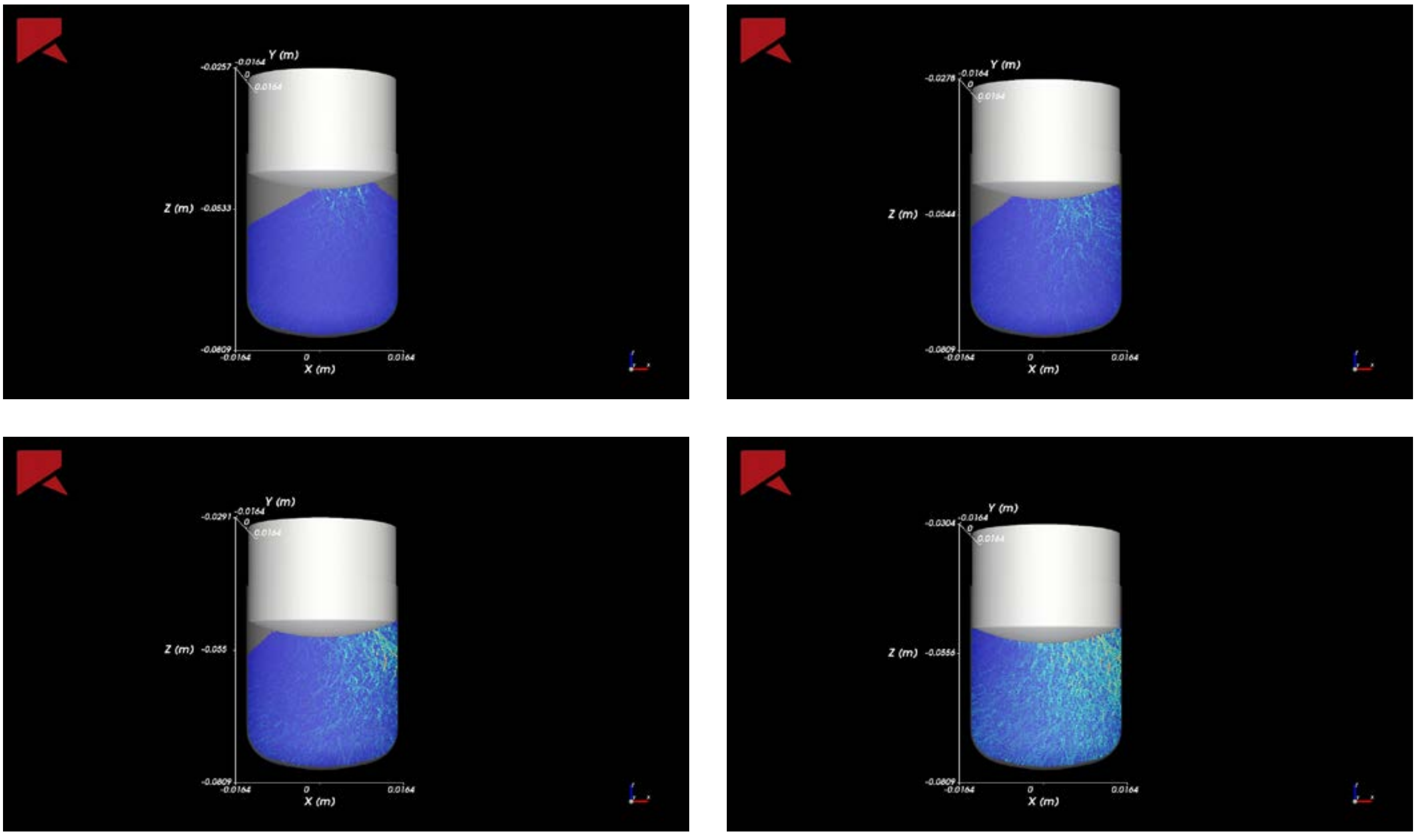


Figure 3: A section through the middle of the cup during the consolidation of the explosive powder, particles coloured by exerted force.

EXPERIENCES ALONG THE WAY

From a practical point of view, the use of GPUs is essential – specifically for the filling of the "set-up" simulations. The actual simulations of the consolidation process were found to not be markedly faster with the GPUs in terms of relative scaling.

From a practical point of view, the ability to complete several simulations in a day allows for a better mental picture of the results and requirements for follow-on simulations.

The business case speaks for itself: faster results mean less production losses in the end. Money and time saved.

Some of the challenges faced of using remote computing was the reliability of the network connections. For the case study, the network hosting the computers seemed to be slow. This caused a lagging response when working with Rocky using the user interface. The effect was even more amplified when trying to work with Rocky on a smart phone and a not-so-great cell phone network connection in the South African Bushveld....

The latency and reliability issues invariably impact performance. However, engineers and researchers should take note that Microsoft Azure is currently completing data centres in both Johannesburg and Cape Town, which will negate these issues. Issues like copying large output files and final results to local hard drives (during this 3-month evaluation, 1.2 TB of data was generated) will also be greatly reduced with the new centres.

CONCLUSION

Scaling HPC to this extent will always be a steep learning curve, with some lessons learned only in hindsight. However, provided engineers have the right tools for the job – in this case, Qfinsoft and their ANSYS Rocky DEM software, NVIDIA's Tesla GPUs, Microsoft Azure cloud facilities and CrunchYard's leading HPC know-how and capabilities, scaling HPC beyond what was previously possible is now very possible.

And it makes sense from time, cost and ease of use perspectives. Capital acquisitions that age and depreciate rapidly are no longer necessary – with the remote computing solution as an effective alternative solution.

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