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ADVANCING DYNAMIC PROCESS MODELING OF COMMINUTION AND CLASSIFICATION CIRCUITS: A PARADIGM SHIFT WITH GPU-ENABLED DEM SOLVER

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Abstract: The minerals processing and aggregate industry have relied on steady-state population and mass balance simulators for decades. However, accurately modeling new processes remains a critical challenge that hinders innovation and decision-making in the industry. In recent years, time-dynamic simulators have been developed, which offer more accurate predictions of process variability and performance, as well as the ability to introduce regulators and control algorithms. Yet, these still require simplified process models of each unit in the system. The development of high-performance discrete element method (DEM) solvers with advanced particle physics models presents a new opportunity to model complete comminution and classification processes.

In this paper, we discuss the potential, challenges, and current limitations of using DEM for advanced dynamic process and equipment evaluation, exemplified by a coarse comminution crushing and screening case. We demonstrate the methodology using a GPU polyhedral DEM implementation with a boundary-volume hierarchy (BVH) collision search algorithm. The results show that the scale of a full-scale two-stage crushing process is possible to simulate. The transition from algebraic process models to DEM would make a significant advancement, bridging the current gap between overly simplified generalized process models and specific equipment design. This approach offers exciting opportunities for the mineral processing and aggregate industry to develop more innovative and efficient circuits.

Keywords. DEM, Simulation, Dynamic process simulation, Comminution, Screening, Crushing

Contents

1 Introduction

The resource extraction of metals and minerals from ore materials is increasingly important in light of market demand and global environmental challenges. To meet these demands, new mining sites are needed, and current operations have to increase production. Furthermore, mining operations have to tackle the difficulty of complex ore bodies with lower ore grade. These ore bodies are commonly more competent, requiring more energy for size reduction. The size reduction process, i.e. comminution, is currently estimated to stand for 1-3 % of the energy consumption in typical mining countries [5]. Current comminution machines are typically energy inefficient. Estimates vary depending on the choice of limiting energy base reference, but it is commonly claimed that about 2-5% of the energy is used to form new fractured surfaces [1, 5]. The energy efficiency problem has led to advancements in the last 30-40 years to find more energy-efficient comminution machine alternatives. Some examples of new devices are the High Pressure Grinding Roll, The Vertical Roller Mill, Tower Mills and several other technologies. Another key technology to improve circuit efficiency is pre-concentration with ore sorters. These devices are used to identify and separate single ore particles that contain valuable enough minerals. A problem for widespread adoption of ore sorters is the low capacity of single units and the consequences of complex bulk materials ore routing.

One of the essential approaches to tackle the challenges is different types of simulation techniques. Process simulation methods have been developed for decades and have evolved from relatively simple steady-state population balance models to more advanced time-dynamic process simulations with semi-mechanistic machine/unit models [16]. In parallel, particle simulations using the discrete element method and related methods have primarily been used to model single comminution and classification machines in detail or difficult problems related to e.g. transfer chutes, bins, and hoppers[6]. However, complete circuits are usually not simulated due to the lack of computational performance or a lack of value such simulation would produce since other vital aspects of the process are not included.

This paper aims to discuss and provide some examples of how accurate large particle system simulations based on GPU-parallelization could be utilised not only for single units but for process dynamics simulations.

First, the DEM method used for the study is presented, including a brief description of the particle fracture model. Further, a demonstration case is configured to provide a basis for discussion and exploration of the possibilities and challenges. Finally, the discussion is concluded with a set of statements regarding the approach's feasibility and potential future development.

2 Dilated polyhedron Discrete Element Method

For readers who are not specifically active in the area of DEM, a brief description of the method is provided as follows. In the discrete element method, each particle is represented and modelled as a geometrical shape with specified size and material properties. The contact interactions within the particle assembly and against geometry boundaries are calculated by solving physical equations based on Newton's laws for motion and rotation. These equations determine the movement of the particles. In their most general form, Zhou et al [4] write the governing equations for the translational and rotational motion of particle i with mass m_i and moment of inertia I_i as

$$m_i \frac{dv_i}{dt} = \sum_j \mathbf{F}_{ij}^c + \sum_k \mathbf{F}_{ik}^{mc} + \mathbf{F}_i^e + \mathbf{F}_i^g \tag{1}$$

$$I_i \frac{\omega_i}{dt} = \sum_j \mathbf{M}_{ij} \tag{2}$$

where v_i and ω_i are the translational and angular velocities of particle i, respectively, $\mathbf{F}_{ij}^c$ and $\mathbf{M}_{ij}$ are the contact force and torque acting on particle i by particle j or the walls, $\mathbf{F}_{ik}^{mc}$ is the non-contact force acting on particle i by particle k or other sources, F_i^e is the external interaction force from e.g. a fluid or field acting on particle i, and F_i^g is the gravitational force. The simulation cases used in this work do not have non-contact forces from external fields or particle fluid interactions, reducing the governing equations to

$$m_i \frac{dv_i}{dt} = \sum_j \mathbf{F}_{ij}^c + \mathbf{F}_i^g \tag{3}$$

$$I_i \frac{\omega_i}{dt} = \sum_j \mathbf{M}_{ij}. \tag{4}$$

To resolve the contact forces in the system, there are a wide range of contact models available in the literature for different types of granular material. In this work, the Hertz-Mindlin-Deresiewicz (HMD) model is applied to represent the interaction between dry non-cohesive rock materials.

In Demify® , the dilated polyhedron shape can be generated from any convex triangulation. In Figure 1, the geometrical state of four different example rock particles are presented. For a 3D laser-scanned rock particle with very high resolution, the triangulation is first decimated to a suitable number of triangles. A higher number of triangles per particle will have some impact on the computational load but will provide a more resolved particle population. In order to perform the Minkowski-sum operation between a sphere and the convex polyhedron, the convex hull of the non-convex shape is calculated. The final dilated polyhedron is, hence a result of the shape of the convex hull mesh and the radius of the sphere used for the dilation operation. It is important to consider the dilation radius in relation to the application and wanted stiffness and shear strength properties of the granular assembly.

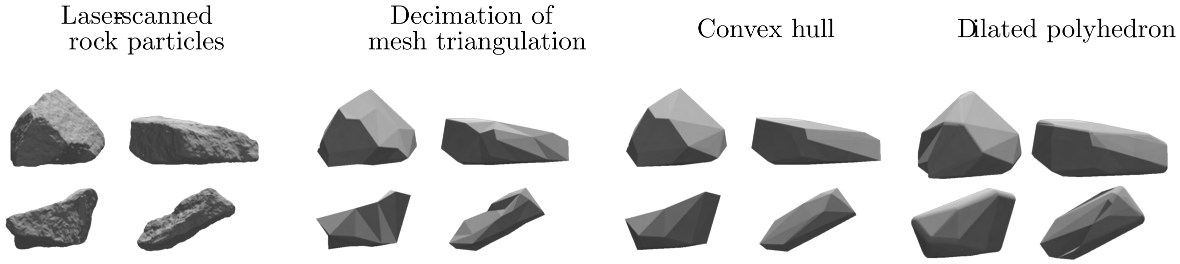
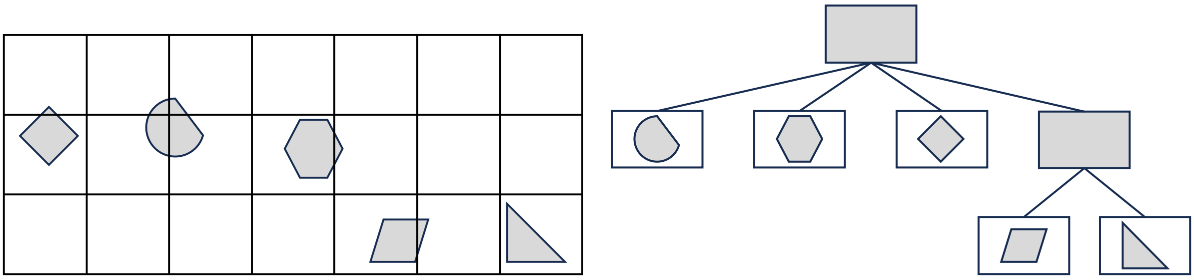


Figure 1: Particle shape representation from 3D laser scanned rock particle to the dilated polyhedron shape

2.1 Broad Phase Contact Detection

To calculate the interaction contact forces, the overlap between particles has to be computed. For spherical and multi-sphere particles, the calculation is relatively trivial. For non-convex general polyhedral shapes, the calculation of exact volumetric overlap is more complex [15]. In addition to the exact intersection of the particles, there's a need for a fast but approximate broad-phase collision detection method to filter potential particle and object collision pairs. This helps prevent a quadratic increase in computation as the number of particles grows. Typically, in GPU-based DEM literature, a Cartesian grid is employed for identifying collision pairs among particles. A schematic grid structure is depicted in Figure 2a. The advantage of using Cartesian grids lies in their straightforward implementation, well-suited for GPU parallelism. However, they suffer in scenarios with widely varying particle sizes, as all grid cells must have the same size and shape. This results in either oversized cells with excessive potential collision pairs or small cells leading to high memory usage (cubically scaling with smaller cell size). [2]. To address this, a GPU-based Bounding Volume Hierarchy (BVH), see Figure 2b, is employed in this work to create a versatile DEM solver capable of handling diverse particle shapes and size distributions. .



(a) A Cartesian Grid broad phase data structure (b) A Bounding Volume Hierarchy (BVH) data structure

Figure 2: The two main collision detection schemes used in DEM

BVH-based broad-phase collision detection offers distinct advantages over Cartesian grids because its performance is less affected by complex particle shapes or wide particle size distributions. This resilience stems from the BVH's flexible tree structure and individually tailored bounding volumes for each particle. The implementation is rooted in binary BVH GPU research[7, 8, 9, 10], with adaptations for higher degree nodes. The use of the BVH broad phase collision detection scheme is relevant to mention in the context of this paper as it allows for large spatial domains. A typical grid-based search method would have difficulty dealing with case configurations as the demonstration simulation discussed in later sections.

2.2 Interfaces

There are three different interfaces worth mentioning in the context of the study. The first is the Graphical User Interface (GUI) of Demify® based on the IPS software platform. This is principally not needed to set up a DEM simulation; however, in practice, when dealing with very large CAD assemblies, it is nearly impossible to correctly configure and handle all geometries directly in the Advance Programming Interface (API) without visual feedback. When a base case model is configured, the case description is automatically translated to the Python API representation. The third interface of relevance is the Functional Mockup Interface (FMI). DEM cases can be packaged as a Functional Mockup Unit (FMU) and imported as a FMU block in third party software such as MATLAB Simulink. This allows for registration of input and out variables from the FMU that can interface to control modelling performed in Simulink.

3 The potential of dynamic process simulation with DEM

Historically, modelling and simulation of comminution systems have been done with a steady-state approach. Commonly used software are JKsimMet, Metso Bruno, AggFlow and ModSim. During the last two decades, time-dynamic simulations have been developed and performed using e.g. the MATLAB Simulink framework [3, 11]. While these solutions provide undisputed value to the industry, they inherently suffer from a lack of resolving the actual physical system. To fit unit model and process responses, extensive test work in the field and laboratory is typically required. The wide range of tests needed is both a cost and a feasibility problem.

In the initial phase of developing the time-dynamic framework for comminution processes, it was realised that at least the basics of interlocks and control loops had to be included. This realisation transformed into the approach of using the simulation framework for the development of control systems [13, 16]. The idea of integrating the Discrete Element Method (DEM) simulations with control algorithms, such as using Simulink and model predictive control (MPC), in minerals processing could open up a range of new possibilities for solving complex problems and optimizing various aspects of the process. A well-resolved DEM model includes a significant level of detail enabling new opportunities. In a conventional steady-state or time dynamic process models, the unit sub-models are general and usually based on population balance modelling with various levels of semi-mechanistic model structures. In many instances when troubleshooting a dry comminution circuit, it turns out that the main problem does not lie in the comminution or classification equipment but is rather related to problems in transfer points, bins, hoppers and so forth. These aspects are very difficult to include in a process model as they relate to the very precise geometrical representation of the process. A number of additional engineering use case scenarios for the idea are listed below,

- Equipment sizing and mass balancing
- Segregation and misalignment
- Equipment wear and life-time predictions
- Process stability and robustness
- Advanced control strategies and virtual sensor development
- Circuit expansion concept evaluation

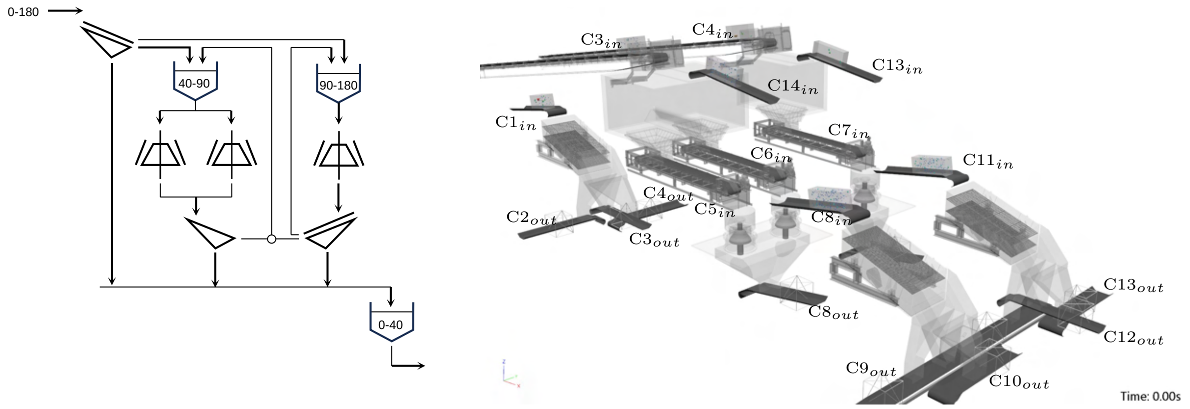
It should be emphasised that the vision described above is not fully implemented in this paper. Rather, the aim is to open up the discussion of the topic in the comminution and classification community. Still, to provide some insight into the potential of the approach, a two-stage crushing and screening circuit has been modelled using the existing capabilities in Demify® as described in the following section.

3.1 Demonstration of a complete process simulation

The circuit is an academic example and illustrated in Figure 3. The process is a two-stage crushing and screening circuit beginning with a primary screen that feeds a secondary crushing and screening stage with re-circulation, as well as a tertiary crushing and screening stage with recirculating load from both the tertiary and secondary screens. The product from the circuit could be e.g. a feed material to a HPGR circuit.

The case settings can be seen in Table 1. The system was simulated for 60 seconds of operation and a steady state condition between generators and destructors was achieved after 25-30 seconds, see Figure 4. A real physical circuit has to abide by the constraints of conveyor belt inclinations. Therefore, conveyors are typically very long in order to reach the top of storage bins. Long conveyors pose a practical problem in a DEM simulation. It is of low value to simulate the flow of particles on a 100 meter long conveyor belt. We therefore propose the solution of only considering the first and last sections of the conveyor. In Demify® , particle populations are created in objects called *generators* and removed using a modelling object called *destructors*.

A solution to the conveyor problem is to use the destructor to remove material but utilize the bulk flow information as input to the next generator. This could be seen as a portal generator object. In this demonstration case, this idea has not yet been implemented. Instead, a rough estimation of the circuit mass balance was done, and the generators were given static size distribution and mass flow input. Since the fracture in the crushers is not included yet either, a certain size reduction was assumed to define the product size distribution. To allow for the flow through the crushers the mantle liners were excluded from the simulation.



(a) Flow sheet diagram of a coarse comminution circuit

(b) Complete DEM simulation setup including notation for conveyor belts

Figure 3: Illustrations of the simulated flowsheet

Table 1: Simulation settings for demonstration case

Parameter	**Aspect**	**Value**	**Unit**
	Geometry		
Particles	Steady-state	110 900	[-]
Particle triangle elements	Steady-state	1 774 400	[-]
Geometry vertices		2 569 297	[-]
Geometry traiangles		856 399	[-]
No of particle shapes		3	[-]
Polyhedral resolution		16	[-]
Domain dimension	X	48	[m]
	Y	19.5	[m]
	Z	17	[m]
	Particle population		
Coefficient of static friction	particle-particle	0.55	[-]
	particle-part geometry	0.45	[-]
	particle-rubber	0.8	[-]
Coefficient of restitution	particle-particle	0.14	[-]
	particle-part geometry	0.12	[-]
	particle-rubber	0.1	[-]
Young' Modulus	particle	500	[MPa]
	part geometry	500	[MPa]
	rubber	1	[MPa]
Poisson's ratio	particle	0.28	[-]
	part geometry	0.3	[-]
	rubber belt	0.35	[-]
Density	particle	3200	[kg/m^3]
	part geometry	7800	[kg/m^3]
	rubber	1000	[kg/m^3]
Relative dilation radius		0.15	[m/m]
	Simulation Settings		
Time-step		2.00E-05	[s]
Computational rate	(Steady-state)	8	[min/s]
Hardware	GPU model	RTX3090	[-]
	CPU model	Ryzen 16 core	[-]
	Process settings		
Vibratory screen motion	Periodic translation amplitude	4	[mm]
	Periodic translation frequency	12	[Hz]
	Ocillating motion	Circular	[-]
Archard wear	Constant	2.00E-12	[m^2/N]
Feed	Mass flow	1500	[tph]
	PSD	30-280	[mm]

An overview of the simulation is provided in Figure 5a with particles colored according to particle characteristic size. In Figure 5b-5c the particle load on the tertiary screen deck is visualized with particles and with the wear pattern. The utilization of the screen deck surface is reasonable, however, there are unloaded areas in the top corners. The feeding to

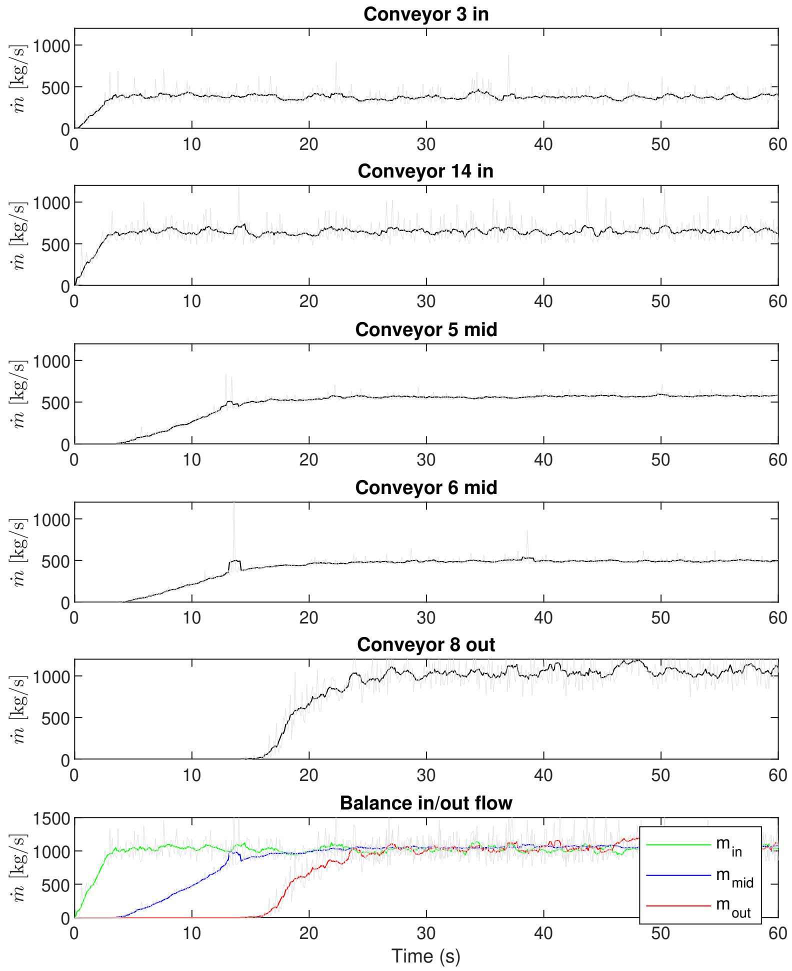
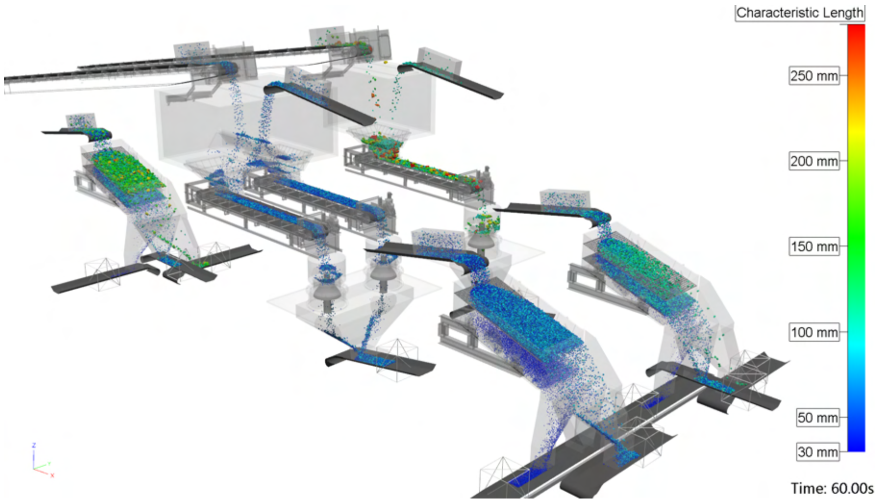
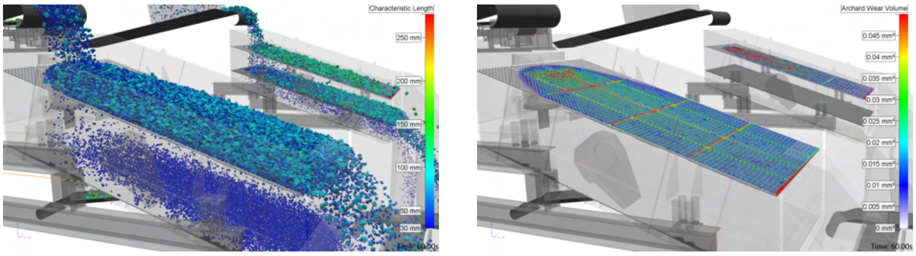


Figure 4: Illustration of mass flow rates on the conveyor belts around the tertiary crushing section demonstrating mass balance and evaluation of material residence time

the crushers are shown in Figure 5d indicating poor feeding conditions with misalignement. Such feeding conditions would likely result in non-optimal crushing performance and liner wear issues. In Figure 5e-5g the range filter feature in Demify® is demonstrated to visualize only the particles in size ranges +30/-40 mm, +40/-90 mm and +90/-280 mm respectively.

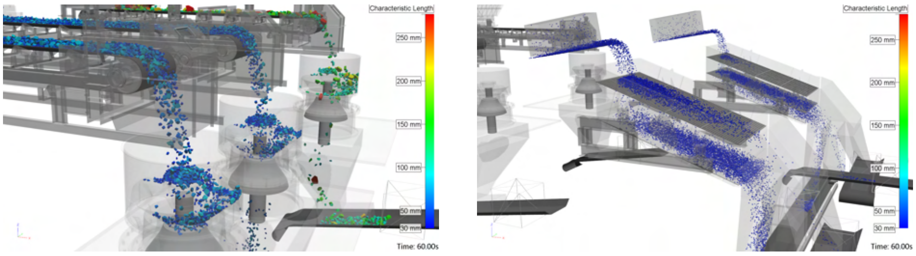


(a) Overview of the complete simulation at T=60s



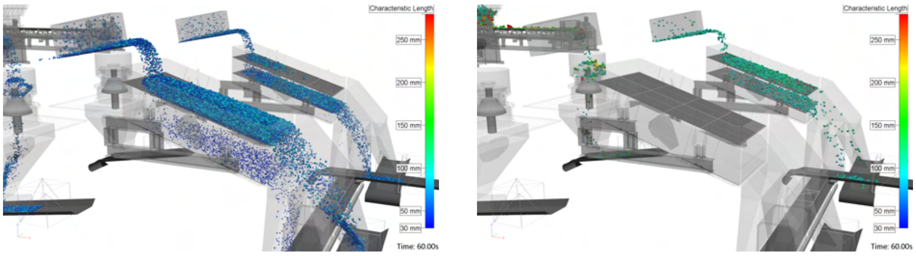
(b) Image of the material flow on the tertiary screen

(c) Image of the wear pattern on the tertiary screen deck



(d) Flow behaviour into the crushers showing a typical misaligned feeding condition

(e) Screening sections with a range filter visualizing only +30/-40mm sizes



(f) Screening sections with a range filter visualizing only +40/-90mm sizes

(g) Screening sections with a range filter visualizing only +90mm sizes

Figure 5: Detail visualisations of the performed DEM process simulation

An important aspect of the process is the residence time and live capacity of bins and conveyors. In this simulation, all the conveyors are active from the start of the simulation. However, if a time-delay would be introduced for e.g. C5 and C6 feeding the tertiary crushers, the feed bin would build up material. This allows for bin flow analysis and live capacity predictions. As seen in Figure 4 the residence time from the initial flow on the feed conveyors to the bin, to the stable flow of material on the crusher product conveyor can be analysed.

The performance of vibratory screens are critical to overall circuit performence. Screens are often overlooked and there is commonly large gains to be made from making sure they operate optimally. In Figure 6 an analysis example is shown for the convergence of the size distribution on the second screen deck on the primary screen. Geometric filters have been used to create 10 selection domains where the size distribution can be evaluated over time. This can be used to evaluate the process robustness and classification efficiency of the screen for different loading scenarios.

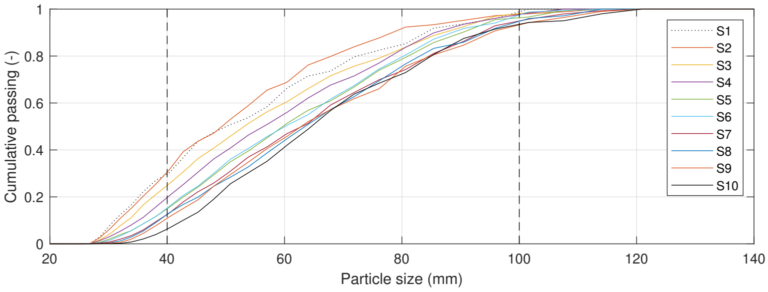


Figure 6: Particle size distribution for 10 filter boxes on the second screen deck of the primary screen showing the capability to review screening efficiency convergence along the deck length

4 Discussion

In Figure 7 a schematic illustration of the next level of envisioned integration is shown. A control layer can be modelled in e.g. Simulink and either the complete process DEM simulation can be packaged as a FMU to allow for simulation via Simulink as a FMI master. This approach would also allow for single units to be run as FMU units on separate nodes. This would open the challenge of performing the process simulation with asynchronous parallel computations.

The most critical limitation of performing process simulation with DEM has probably been the lack of computational performance to handle the system scale. The findings in this paper suggest that this limitation is at least sufficiently tackled to provide interesting insights. However, some process aspects require a much longer time-scale, hence it is likely that DEM based process simulations will be realistically limited to time windows that are below 10 min. An additional approach would be to couple the conventional dynamic process simulation method to the DEM. This would open up for cross-verification and optimization on different time-scales.

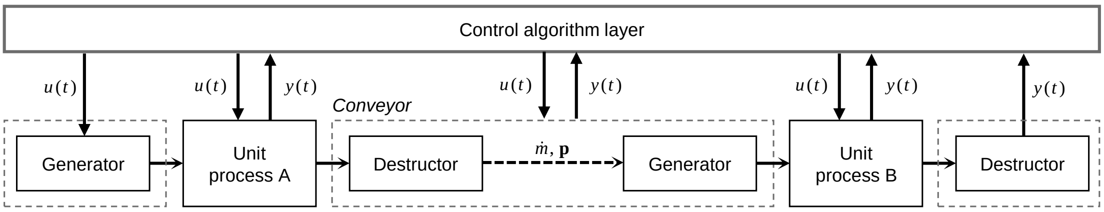


Figure 7: Schematic illustration of connecting destructor and generator objects to transfer the particle state, and how the units interface with a control layer in e.g. Simulink via FMI

5 Conclusions

The main conclusion of this paper is that a complete dry coarse comminution and classification process can be simulated in one simulation domain. As discussed the concept can be expanded to include relevant features to allow for more realistic connection between the generator and destructor objects. Even though the simulation is large in terms of spatial dimensions, the limit for the number of particles have not been reached and the computational load is still reasonable low. It would hence be of interest to include the particle fracture model for the crushers to investigate optimal crusher operation, choice of crusher liners.

The following aspects are instrumental in reaching these results:

- An efficient broad-phase collision detection algorithm based on a Boundary Volume Hierarchy algorithm on the GPU
- A complex shape dilated polyhedron GPU DEM solver
- Efficient handling of large geometry assemblies in the IPS Demify® GUI
- Flexible use of particle generator and destructor objects

There are several aspects to further develop to realise the vision presented in this paper:

- Evaluate FMU-coupling to e.g. Simulink and test different levels of control strategies
- Implement portal generator concept
- Utilize the recently implemented cohesive crack fracture model based on work by [12, 14] for resolved cone crusher breakage simulation
- Further evaluate a framework for simulation of parallel sub-systems on distributed nodes as an asynchronous parallel co-simulation with external FMI master.
- Investigate and verify the dynamics of existing plant operations

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References

[1] D. Fuerstenau and A.-Z. Abouzeid. “The energy efficiency of ball milling in comminution”. In: *International Journal of Mineral Processing* 67.1 (2002), pages 161–185. ISSN: 0301-7516. DOI: `https://doi.org/10.1016/S0301-7516(02)00039-X`.

[2] C. Ericson. *Real-Time Collision Detection*. USA: CRC Press, Inc., 2004. ISBN: 1558607323.

[3] Y. Liu and S. Spencer. “Dynamic simulation of grinding circuits”. In: *Minerals Engineering* 17.11 (2004). Communition ’04, pages 1189–1198. ISSN: 0892-6875. DOI: `https://doi.org/10.1016/j.mineng.2004.05.018`. URL: `https://www.sciencedirect.com/science/article/pii/S0892687504001864`.

[4] H. Zhu, Z. Zhou, R. Yang, and A. Yu. “Discrete particle simulation of particulate systems: Theoretical developments”. In: *Chemical Engineering Science* 62.13 (2007). Frontier of Chemical Engineering - Multi-scale Bridge between Reductionism and Holism, pages 3378–3396. ISSN: 0009-2509. DOI: `https://doi.org/10.1016/j.ces.2006.12.089`. URL: `https://www.sciencedirect.com/science/article/pii/S000925090700262X`.

[5] D. Tromans. “Mineral comminution: Energy efficiency considerations”. In: *Minerals Engineering* 21.8 (2008). Cited by: 139, pages 613–620. DOI: `10.1016/j.mineng.2007.12.003`.

[6] P. W. Cleary. “Industrial particle flow modelling using discrete element method”. In: *Engineering Computations* 26.6 (2009). Edited by A. Munjiza, pages 698–743. ISSN: 0264-4401. DOI: `10.1108/02644400910975487`. URL: `https://doi.org/10.1108/02644400910975487`.

[7] C. Lauterbach, M. Garland, S. Sengupta, D. Luebke, and D. Manocha. “Fast BVH construction on gpus”. In: *Computer Graphics Forum* 28 (2009), pages 375–384. DOI: `10.1111/j.1467-8659.2009.01377.x`.

[8] J. Pantaleoni and D. Luebke. “HLBVH: Hierarchical LBVH Construction for Real-time Ray Tracing of Dynamic Geometry”. In: *Proceedings of the Conference on High Performance Graphics*. HPG ’10. Saarbrucken, Germany: Eurographics Association, 2010, pages 87–95. URL: `http://dl.acm.org/citation.cfm?id=1921479.1921493`.

[9] K. Garanzha, J. Pantaleoni, and D. McAllister. “Simpler and Faster HLBVH with Work Queues”. In: *Proceedings of the ACM SIGGRAPH Symposium on High Performance Graphics*. HPG ’11. Vancouver, British Columbia, Canada: ACM, 2011, pages 59–64. ISBN: 978-1-4503-0896-0. DOI: `10.1145/2018323.2018333`. URL: `http://doi.acm.org/10.1145/2018323.2018333`.

[10] T. Karras. “Maximizing Parallelism in the Construction of BVHs, Octrees, and K-d Trees”. In: *Proceedings of the Fourth ACM SIGGRAPH / Eurographics Conference on High-Performance Graphics*. EGGH-HPG’12. Paris, France: Eurographics Association, 2012, pages 33–37. ISBN: 978-3-905674-41-5. DOI: `10.2312/EGGH/HPG12/033-037`. URL: `https://doi.org/10.2312/EGGH/HPG12/033-037`.

[11] G. Asbjörnsson, E. Hulthén, and M. Evertsson. "Modelling and simulation of dynamic crushing plant behavior with MATLAB/Simulink". In: *Minerals Engineering* 43-44 (2013). SI: Comminution, pages 112–120. ISSN: 0892-6875. DOI: `https://doi.org/10.1016/j.mineng.2012.09.006`. URL: `https://www.sciencedirect.com/science/article/pii/S0892687512003044`.

[12] G. Ma, W. Zhou, and X.-L. Chang. "Modeling the particle breakage of rockfill materials with the cohesive crack model". In: *Computers and Geotechnics* 61 (2014), pages 132–143. ISSN: 0266-352X. DOI: `https://doi.org/10.1016/j.compgeo.2014.05.006`. URL: `https://www.sciencedirect.com/science/article/pii/S0266352X14000950`.

[13] M. Johansson and M. Evertsson. "Applying linear model predictive control to crushing circuit simulations". In: 2019, pages 3423–3432. URL: `https://www.scopus.com/inward/record.uri?eid=2-s2.0-85059363442&partnerID=40&md5=1230d816aeeb69f40b1f7d5231f76000`.

[14] L. Liu and S. Ji. "Bond and fracture model in dilated polyhedral DEM and its application to simulate breakage of brittle materials". In: *Granular Matter* 21.3 (2019), page 41. ISSN: 1434-7636. URL: `https://doi.org/10.1007/s10035-019-0896-4`.

[15] A. Bilock. "A GPU Polyhedral Discrete Element Method". Master's thesis. Chalmers University of Technology, 2020.

[16] G. Asbjörnsson, L. M. Tavares, A. Mainza, and M. Yahyaei. "Different perspectives of dynamics in comminution processes". In: *Minerals Engineering* 176 (2022), page 107326. ISSN: 0892-6875. DOI: `https://doi.org/10.1016/j.mineng.2021.107326`. URL: `https://www.sciencedirect.com/science/article/pii/S0892687521005550`.