Artificial Intelligence in Comminution: From Predictive Models to Agentic Discovery

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Abstract. Artificial intelligence (AI) is reshaping how comminution and classification processes are modelled, optimised and understood. Early applications centred on narrow predictive models trained on experimental or numerical data, followed by surrogate models that emulate expensive simulations at a fraction of their computational cost. The current wave of transformer-based systems extends this spectrum considerably. As general-purpose reasoning and transfer-learning architectures, they enable domain-specific expert systems, agentic workflows to autonomously set up and analyse simulations, and the combination of language models with symbolic regression for data-driven discovery of interpretable, mechanistically meaningful equations. Beyond comminution, recent developments in frontier AI research, including autonomous coding agents that improve their own algorithms, AI co-scientists that generate and test hypotheses, and systems whose autonomous task-completion horizon doubles every couple of months, represent a rapid trajectory whose implications target every field. This contribution provides an overview that bridges classical and generative AI in the context of comminution, illustrates the state of the art through case studies on stirred media mills and DEM surrogate modelling, and contextualises current frontier capabilities.

1. AI in Comminution: From Data to Understanding

Artificial intelligence (AI) has moved from an external trend to an increasingly necessary complement in experimentation, mechanistic modelling and numerical simulation in comminution. The first broad wave of applications centred on narrow AI, predictive models trained on experimental or numerical data to estimate quantities such as product fineness, stressing conditions, collision energies or process performance [1–3]. These approaches already demonstrated major reductions in modelling effort and opened routes towards optimisation, control and scale-up. A next logical step was the move from predicting selected target variables to emulating entire simulations through surrogate models, for example for the discrete element method (DEM). In this mode, AI acts as a fast digital-twin layer above established tools, accurately emulating simulation outputs while reducing computational costs by several orders of magnitude. Similar trajectories in other scientific domains, most prominently AlphaFold in protein structure prediction [4], illustrate the broader potential of data-driven emulation whenever first-principles computation is expensive.

2. Transformers, Agents and Interpretable Discovery

Recent transformer-based models broaden this landscape considerably [5]. Unlike classical neural networks that map fixed inputs to fixed outputs, transformers are general-purpose architectures whose strength lies not only in language processing but in transfer and analogy learning across heterogeneous data, be it text, code, equations, images, sound, sensor-motor or measurement data, gene sequences and structured documents, or all of them combined. This generality makes them useful as reasoning engines and interfaces to scientific knowledge and engineering software. For comminution, this enables domain-specific expert systems for milling and classification knowledge, retrieval-enhanced access to literature and internal documentation, and agentic workflows that prepare simulation cases, operate software tools, execute analyses and summarise results with minimal human intervention.

In parallel, symbolic regression and related data-driven equation-discovery methods offer a complementary path towards interpretable, mechanistically meaningful relations rather than purely black-box predictions [6]. The combination is especially promising: language models can orchestrate data handling, hypothesis generation and workflow automation, while evolutionary symbolic or physics-guided methods identify compact equations with physical meaning. Applied to stirred media milling data, this hybrid approach converges on scaling-law families that are both predictively accurate and discussable by domain experts, opening a route towards automated assistance not only for reporting and knowledge access, but for model formulation itself.

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3. Where Frontier AI Stands Today

Beyond comminution-specific tools, the broader AI landscape is advancing at a pace the engineering community should be aware of. DeepMind's AlphaEvolve, an autonomous coding agent guided by evolutionary search, recently discovered the first improvement to Strassen's matrix multiplication algorithm in 56 years and optimised critical components of Google's data-centre infrastructure [7]. Sakana AI's AI Scientist produced a fully AI-generated research paper that passed blind peer review at an international machine-learning workshop [8]. Google's AI Co-Scientist and related multi-agent systems autonomously generate, test and refine scientific hypotheses, pointing towards a future in which AI contributes directly to the discovery process.

Benchmark data from METR quantifies this trajectory: the length of tasks that frontier AI agents can complete autonomously with 50 % reliability has been doubling approximately every couple of months over the past years [9]. Leading AI researchers estimate systems matching broad human-level cognitive capabilities within five to ten years, with some placing this horizon even sooner [10]. For comminution, where sparse data, changing feed materials and multiscale physics quickly expose modelling weaknesses, human validation remains essential for now. Yet the trajectory makes clear that the role of AI in engineering workflows is shifting from isolated prediction tools towards semi-autonomous collaborators.

4. Implications and Outlook for Comminution

The most immediate practical gains are likely to arise where general-purpose reasoning models are combined with fast, narrow digital twins. A frontier language model can formulate hypotheses, design parameter studies and interpret results, while surrogate models evaluate thousands of candidate configurations in seconds. With only the most promising solutions needing to be validated experimentally, a flywheel effect is established, massively accelerating iteration cycles. This paradigm applies across predictive models, DEM surrogates, transformer-based assistants, tool-using agents and interpretable equation discovery, each addressing different parts of the same workflow.

Longer term, the same trajectory points towards multimodal process understanding, closer integration with automated experimentation and laboratory robotics, and autonomous digital twins that continuously learn from operational data. At the same time, wider adoption requires clear guardrails, such as factual grounding, provenance of generated outputs, uncertainty awareness and expert review. The aim of the present contribution is to provide an overview of these developments and to outline where meaningful adoption for comminution can start today.

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