The BRIEF

Applications of Artificial Intelligence in Powder Technology

IFPRI wants to commission a review of recent developments in the field of artificial intelligence and their potential applications in the field of Powder Technology. The level of understanding in the IFPRI community of AI – what tools it is comprised of and what are their capabilities - is limited, hence this review would be simultaneously a tutorial and a state-of-the-art review. This review can be “a particle technologist’s guide to AI methods”. The review should begin with a definition of “artificial intelligence” and “machine learning” and other relevant terminology. It should describe the most applicable AI methods for particulate systems and discuss what types of problems they are designed to solve and what their strengths and weaknesses are. Of particular interest is the training/calibration problem: what types and volume of data are required? IFPRI members come from a broad range of industries, so the range of applications is correspondingly large, e.g., particle and powder characterization, product modeling, process modeling. Understanding how broad this scope is, we expect that the author(s) of the review will narrow its scope as needed to make it tractable.

Outline of the Report to IFPRI on Applications of Artificial Intelligence in Powder Technology

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1) Introduction of the report

a. Statement of the report's scope in context of IFPRI interest and experience in, and intent of use of artificial intelligence (AI).

b. What's in vs out?

   i. The report is an opinion piece on emerging trends in recent developments in AI and their potential applications in particulate science and technology (PST). The report is not a review of the literature on AI applications in PST. There are various reasons for this. First, such a review has just been published[1] and assessments of different AI methods for studies of particulate media are continuing to emerge[2]. More broadly, many reviews have also now appeared in various sectors of material science, which share common tasks and challenges with PST[3]. Second, providing a timely review of AI is challenging due to its rapid evolution[4], compounded by the fact that neither of us work in the field of powder technology. There is rapid growth in data sources from PST, which are fueling the deployment of AI in the sector, particularly due to synergies between AI-enabled data sources

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[1] **Thon et al. (2024)** Artificial Intelligence and Evolutionary Approaches in Particle Technology. KONA Powder and Particle Journal

[2] **Diaz et al. (2023)** Machine learning approaches to the prediction of powder flow behaviour of pharmaceutical materials from physical properties. Digital Discovery; **Chen et al. (2024)** An artificial intelligence approach for particle transport velocity prediction in horizontal flows, Particuology; **Ouyang et al. (2023)** Interpretable machine learning analysis and automated modeling to simulate fluid-particle flows, Particuology.

[3] The following are just a few examples from many in the literature: **Papadimitriou et al. (2024)** AI methods in materials design, discovery and manufacturing: A review, Computational Materials Science; **Mobarak et al. (2023)** Scope of machine learning in materials research—A review, Applied Surface Science Advances, **Sivan et al. (2024)** Advances in materials informatics: a review. J Mater Sci

[4] **Clinton (2024)** The Complete Obsolete Guide to Generative AI. https://www.manning.com/books/the-complete-obsolete-guide-to-generative-ai

(i.e., new instrumentation and measurement[5] and simulation[6]) and AI research[7] and software development[8].

ii. It is thus useful to frame our report around trends in AI applications in PST in the context of: (a) emerging instrumentation and simulation capabilities, and (b) the open challenges facing PST[9].

2) Structure of the rest of the report

a. Navigating the AI jargon and hype

i. AI still has no one authoritative, consistent and overarching definition.[10],[11] At best, this is our attempt at a "characterization of AI-today" from a PST perspective, mindful that AI is a complex system[12]. AI is dynamic, with feedback loops that constantly drive change.

ii. Basic glossary[13] and taxonomy of terms with references: AI (narrow vs general vs super), machine learning, deep learning, statistical learning, explainable AI etc

b. AI vs traditional analysis in PST (AI-PST vs TA-PST)

i. Key elements of scientific discovery and workflow[14] (including AI's way of discovering Hooke's law according to ChatGPT)

ii. Similarities and differences[15],[16]

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[5] **Graas et al. (2023)** Just-in-time deep learning for real-time X-ray computed tomography. Sci Rep; **Khanafer & Shirmohammadi (2020)** Applied AI in instrumentation and measurement: The deep learning revolution. IEEE Instrumentation & Measurement Magazine; **Elahi et al. (2023)** A comprehensive literature review of the applications of AI techniques through the lifecycle of industrial equipment. Discov Artif Intell; **Ferdoush et al. (2023)** Fast time-resolved micro-CT imaging of pharmaceutical tablets: Insights into water uptake and disintegration, International Journal of Pharmaceutics; **Machin et al. (2021)** In-line characterisation of continuous phase conductivity in slurry flows using artificial intelligence tomography. Minerals Engineering; **Madarász et al. (2023)** AI-based analysis of in-line process endoscope images for real-time particle size measurement in a continuous pharmaceutical milling process. International Journal of Pharmaceutics;

[6] **Kishida et al. (2023)** Development of ultra-fast computing method for powder mixing process. Chemical Engineering Journal, https://www.newswise.com/articles/ai-boosts-powder-engineering; **Lu et al. (2021)** Machine learning accelerated discrete element modeling of granular flows. Chemical Engineering Science

[7] **Ofosu-Ampong et al. (2024)** Artificial intelligence research: A review on dominant themes, methods, frameworks and future research directions, Telematics and Informatics Reports; JB will update this closer to submission of final report

[8] Depending on needs and interests, there are many sights that review the latest AI tools: e.g., Gartner Research: (https://www.gartner.com/en), Emerj: (https://emerj.com/). See also https://libguides.kcl.ac.uk/systematicreview/ai which reviews the various AI tools that can be harnessed to generate a systematic review of the literature on a given topic and their limitations.

[9] **Windows-Yule et al. (2023)** A multidisciplinary perspective on the present and future of particle imaging. Particuology

[10] Section 238(g) of the John S. McCain National Defense Authorization Act for Fiscal Year 2019 offers five definitions for artificial intelligence. See https://law.stanford.edu/2019/05/14/mapping-artificial-intelligence-taxonomy/

[11] John McCarthy ('the father of AI') coined the term and defined it as "the science and engineering of making intelligent machines" in 1956: see **McCarthy (2007)** in https://www-formal.stanford.edu/jmc/whatisai.pdf. Over decades in the 20th century, AI has progressively evolved, resulting in the development of intelligent machines and algorithms capable of reasoning and adapting based on sets of rules and environments that mimic human intelligence. **Wang (2019)** On Defining Artificial Intelligence. Journal of Artificial General Intelligence: expanded the definition of AI to include its ability to perform cognitive tasks, particularly learning and problem-solving, fueled by technological innovations in machine learning, computer vision, natural language processing, robotics etc.

[12] Chapter 5 Introduction to AI Safety, Ethics, and Society by Dan Hendrycks. ". .. the deployment of AI within society represents a case of nested complexity, where complex systems are embedded within one another. This vastly increases the range of potential interactions and the number of ways in which the systems can co-evolve. As a result, it is difficult to predict all the ways in which AI might be used and what its eventual impact will be." https://www.aisafetybook.com/textbook/5-2

[13] https://www.expert.ai/glossary-of-ai-terms/

[14] https://news.microsoft.com/source/features/ai/how-ai-and-hpc-are-speeding-up-scientific-discovery/

[15] We will each address IFPRI's question on: *Is AI a new species or an evolution of existing species of traditional analytical techniques? What is new or different about AI?*

[16] We will each address IFPRI's question on: *What types and volume of data are required?*

iii. Strengths and weaknesses[17]

c. Case studies: AI-PST[18] and other fields that share common tasks and challenges with AI-PST[19]
   i. Injecting physics in AI (recent review[20])
   ii. Making AI transparent and explainable
   iii. Getting real with fakes: relevance of DeepFake (generative) AI techniques for PST
   iv. Use of AI in the characterisation of particulate systems from imaging data[21],[22] including in real-time monitoring (e.g., Xray computed tomography[23],[24] , Dynamic Image Analysis (DIA), laser diffraction[25], direct analysis in real-time high-resolution mass spectrometry (DART-HRMS)[26],[27] Near-Infrared Spectroscopy (NIR)[28]
   v. Use of AI for forecasting in particulate systems from multivariate, high-dimensional, spatiotemporal time series data with nonstationary dynamics
   vi. Brief statement on adopting AI at speed and at scale for continuous monitoring

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[17] We will each address IFPRI's question on: *What types of problems they are designed to solve and what their strengths and weaknesses are?*

[18] AT will highlight applications in the broader context of granular media science from her research with connections to other AI-applications in the field (from granular physics & mechanics).

[19] JB will highlight other AI-applications in the medical field where imaging technologies are prevalently used.

[20] **Chen et al. (2024)** Physics-Informed neural network solver for numerical analysis in geoengineering. Georisk: Assessment and Management of Risk for Engineered Systems and Geohazards; **Chen & Koohy (2024)** GPT-PINN: Generative Pre-Trained Physics-Informed Neural Networks toward non-intrusive Meta-learning of parametric PDEs, Finite Elements in Analysis and Design; **Sutar et al. (2022)** "Physics Informed Neural Networks – A Methodology Review," 6th International Conference On Computing, Communication, Control And Automation; **Cai et al. (2021)** Physics-informed neural networks (PINNs) for fluid mechanics: a review. Acta Mech. Sin.

[21] **Farkas et al. (2021)** Image Analysis: A Versatile Tool in the Manufacturing and Quality Control of Pharmaceutical Dosage Forms. Pharmaceutics; **Taseva et al. (2023)** Application of an AI image analysis and classification approach to characterise dissolution and precipitation events in the flow through apparatus, European Journal of Pharmaceutics and Biopharmaceutics,

[22] **Larmuseau et al. (2021)** "Race against the Machine: can deep learning recognize microstructures as well as the trained human eye?" Scripta Materialia

[23] "The past 30 years have seen a dramatic increase in spatial resolution, a shortening of the time and a lowering of the dose needed to acquire CT scans through a combination of improved sources (both synchrotron and laboratory tube sources), detectors and reconstruction algorithms. There is little reason to believe that this progress will stall." **Withers et al.. (2021)** X-ray computed tomography. Nat Rev Methods Primers

[24] **Hunter L, Dewanckele J (2021)** Evolution of Micro-CT: Moving from 3D to 4D. Microscopy Today.

[25] Mastersizer 3000+ is an AI-enabled laser diffraction instrument released in April 2024

[26] **Tata (2022)** Authentication of Edible Insects' Powders by the Combination of DART-HRMS Signatures: The First Application of Ambient Mass Spectrometry to Screening of Novel Food. Foods

[27] **Busch (2000)** "Mass spectrometry has evolved from an art practiced by a few to a widely used analytical science that produces a billion individual mass spectra daily" Spectroscopy (quote from 14 years ago).

[28] **Ozturk et al. (2023)** Near-infrared spectroscopy and machine learning for classification of food powders during a continuous process. Journal of Food Engineering