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# Numerical Modelling and Imaging of Industrial-Scale Particulate Systems: A Review of Contemporary Challenges and Solutions †

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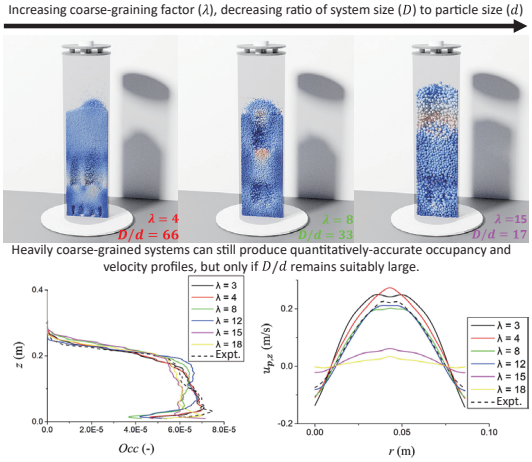
Numerical modelling offers the opportunity to better understand, predict, and optimise the behaviours of industrial systems, and thus provides a powerful means of improving efficiency, productivity and sustainability. However, the accurate modelling of industrial-scale particulate and particle–fluid systems is, due to the complex nature of such systems, highly challenging. This challenge arises primarily from three factors: the lack of a universally accepted continuum model for particulate media; the computational expense of discrete particle simulations; and the difficulty of imaging industrial-scale systems to obtain validation data. In recent years, however, advances in software, hardware, theoretical understanding, and imaging technology have all combined to the point where, in many cases, these challenges are now surmountable—though some distance remains to be travelled. In this review paper, we provide an overview of the most promising solutions to the issues highlighted above, discussing also the major strengths and limitations of each.

**Keywords:** discrete element method, two fluid model, kinetic theory of granular flows, coarse graining, particle tracking, tomography




## 1. Introduction

The handling and processing of particulate solids is of central importance to myriad processes in diverse industries, including (but by no means limited to) the chemical, defense, food, green energy, and pharmaceutical sectors (Seville et al., 2012). Indeed, particulate media are involved in the production of more than 50 % of all goods sold worldwide (Blais et al., 2019). Despite their ubiquity, however, the mechanics of particulate solids remain poorly understood compared to 'classical' solids, liquids and gases. This lack of understanding manifests itself in industry in many negative manners, spanning numerous unit operations, be it the woeful energy-efficiency of processes such as milling (Holmberg et al., 2017), the tendency of hoppers and feeders to become 'jammed' (Schulze, 2014), or the highly unpredictable nature of mixing and segregation between non-identical species of particles (Windows-Yule et al., 2015). If we wish to reduce waste, increase efficiency, and in general develop more robust and sustainable manufacturing methods, we must improve our understanding of particulate media. In industrial processes involving *fluids*, a digital, 'Industry 4.0' approach to the optimisation of industrial equipment has already been widely adopted thanks to the wide availability of user-friendly computational fluid dynamics (CFD) software, and the ability of CFD to efficiently numerically model the flow dynamics of large, pilot/industrial-scale systems. The adoption of such digital approaches has been significantly slower for particulate media, however. There are several reasons underlying this slow adoption, but most can be traced back to the complexity of particulate materials, meaning that—to date—there does not exist a universally accepted particulate equivalent to the Navier–Stokes equations, and thus few commercially available, generalisable, "plug and play" CFD equivalents capable of (accurately) modelling industrial scale systems.

There are currently two main approaches to the modelling of industrial particle-handling systems: the discrete element method (DEM), which models all particles within a system as individual, discrete objects, and the kinetic theory of granular flows (KTGF), which takes a continuum approach similar to CFD, but solves equations that have

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been modified to represent particulate or multiphase flows[1]. A brief overview of each technique is provided in **Sections 2 and 3**. Each of these techniques suffers from its own distinct limitations. DEM has been widely shown to facilitate the quantitatively accurate simulation of particulate systems (Coetzee, 2017), but in its standard form is highly computationally demanding (Golshan et al., 2023). KTGF simulations are significantly more efficient, but the modelling assumptions required to describe a discrete, particulate system as a continuous medium make calibration and (thus) quantitative accuracy much more challenging to achieve.

Nonetheless, in recent years, improvements in hardware, software, and the development of new theoretical models mean that the tractable, accurate modelling of industrial systems is achievable—albeit with some limitations and caveats. In this review article, we provide an overview of the most promising contemporary methods for modelling industrial-scale particulate systems, highlighting their individual strengths and weaknesses, and summarising important recent developments.

## 2. Discrete methods

### 2.1 Overview of the discrete element method (DEM)

The discrete element method is currently the most common method for the numerical modelling of particulate systems. Though its efficient implementation can be highly challenging, the underlying concept of DEM is exceedingly simple: each individual particle within a given system is modelled as a distinct computational object, and assigned all the relevant properties of a 'real' particle—i.e. a position in space, a mass, a size, a friction coefficient etc. Each simulated particle within a DEM simulation is also subject to the relevant forces one may expect in a 'real' system, most notably gravity, and relevant 'contact forces' experienced during collisions with other objects. By coupling DEM with CFD, drag and other fluid forces may also be simulated (El Geitani et al., 2023). The sum of these forces may be used to predict the net force acting on a given particle at a given point in time (see **Fig. 1**), and from this and the particle's known mass, the instantaneous acceleration acting upon it. This, in turn, may be used to predict the velocity, and thus position, of the particle at some future point in time (assuming that the 'timestep' between this future point and the present point in time is small enough that the particle experiences no significant change in acceleration).

By repeating the above process again and again—effectively stepping through time in pseudo-infinitesimal increments—one may thus simulate the motion of a system of particles. By tuning the relevant parameters (friction coefficients, restitution coefficients, cohesive properties...) used to represent the interactions between particles, this simulated motion can be brought into quantitative alignment with the dynamics of the real system being modelled (Windows-Yule et al., 2016; Windows-Yule and Neveu, 2022)[2]. A significant shortcoming of the discrete element method, however, is its computational expense. Unlike CFD, each individual particle within a system must be individually modelled, meaning that the time required to run a simulation increases sharply with the number, $N$, of particles being simulated. Indeed, even with a highly optimised DEM engine, computation time can be expected to scale as $N \log N$ (Thompson et al., 2022). This shortcoming typically hampers efforts to simulate industrial-scale systems. In the following sections, we discuss some of the main ways in which this issue may be circumvented. It should be noted that the above provides only a rather crude overview of DEM. A more detailed yet still accessible introduction to the discrete element method can be found in Chapter 4 of reference (Rosato and Windows-Yule, 2020), and a deeper dive in reference (Luding, 2008).

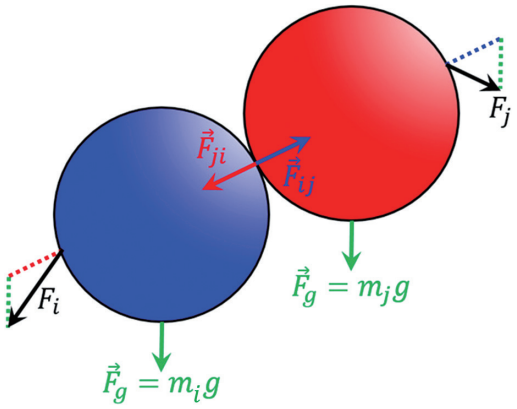


**Fig. 1** A schematic illustration of two interacting DEM particles. Particle $i$ is subject to a gravitational force $\vec{F}_g$ proportional to its mass $m_i$, and a contact force $F_{ji}$ due to contact with a second particle $j$. The net force $F_i$ acting on the particle is used to predict its position and velocity at the next point in time. Reproduced with permission from (Rosato and Windows-Yule, 2020).

### 2.2 Parallelisation and GPU acceleration

As discussed in the preceding section, the computational expense of a simulation—that is to say, the required number of CPU (central processing unit) operations required to simulate a system—increases monotonically with the number of particles, $N$, simulated. As each operation takes a finite time to perform, this means that, for simulations run on a single CPU core, the time required to run a simulation

[1] While these are certainly not the only available methods, they are decidedly the most commonly-applied, and thus will form the focus of this review.

[2] The calibration of numerical simulations is a complex field in its own right, and has been the subject of several recent review articles (Ketterhagen and Wassgren, 2022; Windows-Yule and Neveu, 2022) and as such will not be discussed in detail here.

increases with time. One of the simplest methods through which to reduce the time required is thus simply to split this effort across multiple CPUs—a process known as 'parallelisation' (Sawley and Cleary, 1999). Like DEM itself, the implementation of a parallelisation strategy may be complex, but the strategy itself is conceptually very simple: the computational volume is subdivided into two or more distinct regions (see e.g. **Fig. 2**) and each region is assigned its own CPU, which only performs operations for particles falling within said region. Thus, for a perfectly implemented parallelisation strategy, a simulation using two CPU cores might be expected to run in half the time of an equivalent 'serial' simulation, a simulation parallelised across 4 cores in a quarter of the time, and so on. With access to a suitable high-performance computing (HPC) system, one may hypothetically speed up a simulation hundreds or even thousands of times, and thus simulate numbers of particles which would be simply unfeasible using a single CPU.

In reality, however, such 'linear' speed-up is not easy (or, in absolute terms, possible) to achieve for several reasons. Firstly, to achieve linear speed-up, the computational load must be balanced equally across all processors, meaning that the individual domains into which the computational volume is divided must be sensibly chosen. For example, in **Fig. 2**, the division shown in the top-most panel (which exploits the uniformity of the system along the axial direction) is significantly more efficient than that shown in the middle panel, where the lower domain contains many more particles than the upper domain. In the bottom panel, we see that one of the processors is entirely unused, making this an exceedingly inefficient configuration—yet one that is often accidentally used by DEM practitioners who leave their parallelisation schemes on default settings! In recent years, however, the use of 'dynamic load balancing' algorithms—which, as their name suggests, automatically optimise the spread of computational load across processors—have become increasingly common (Golshan and Blais, 2021; Yan and Regueiro, 2018). As such, in the future, this particular problem is likely to be less frequently encountered. Dynamic load balancing schemes, unlike 'manual' methods, also allow the distribution of processor power to be adjusted *during simulation*, allowing for even greater efficiency savings.

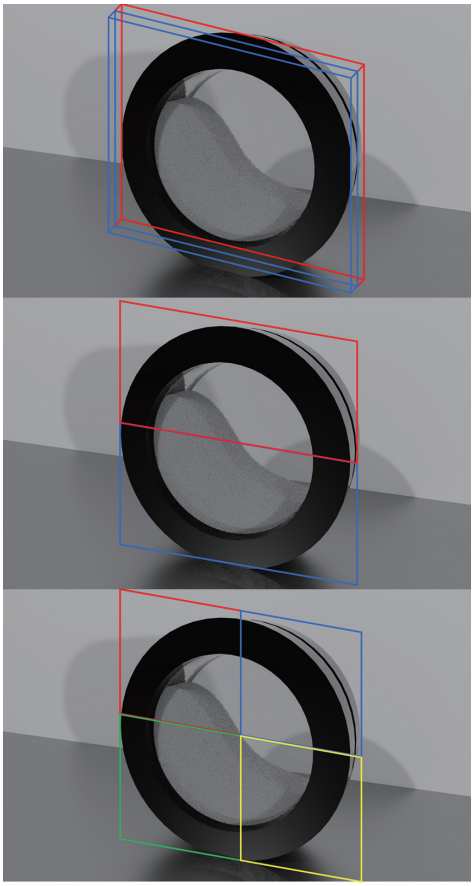

**Fig. 2** Examples of possible parallelisation schemes for a simulated rotating drum (Herald et al., 2022).

The second major issue to consider when parallelizing DEM is that a finite 'overlap' or 'communication region' must exist between all adjacent domains[3] allowing information (e.g. contacts between particles) from one domain to be passed to another. It is this restriction which ultimately provides an upper bound on the degree of speed-up which may be achieved through parallelisation: if a simulation is 'sliced too thinly'—for example if the width of a domain is smaller than the width of a particle—then no speed-up can be achieved (indeed the simulation may even become slower due to the increased overheads of such a scheme (Eibl and Rüde, 2019)).

In addition to CPU processing, the past decade has seen a considerable rise in interest in the use of GPU (graphics processing unit) computation in DEM (Fang et al., 2021; Govender et al., 2014; Lisjak et al., 2018; Lu, 2022; Spellings et al., 2017; Steuben et al., 2016; Wang et al., 2021). Though the development of GPUs has been largely driven by the desire for improved 3D graphics in the gaming and film industries (Das and Deka, 2016), their innate capability to efficiently perform highly-parallelised computations makes them well suited to the speed-up of DEM simulations (Govender et al., 2014).

The advent of GPU computing has not only helped to increase the number of particles that can realistically be simulated on a single PC (as opposed to the HPC clusters required for large-scale parallel CPU computations), but has also played a role in overcoming another major limitation of DEM—the difficulty of (efficiently) modelling aspherical particles (Govender et al., 2014; Spellings et al., 2017; Wang et al., 2021), which are all but ubiquitous in industry. The computational complexity of detecting

[3] It is for this reason that perfectly linear scaling is never fully possible in the parallelisation of DEM simulations, though for well-chosen schemes may come very close (Markauskas and Kačeniauskas, 2015).

collisions between simulated particles is significantly higher for aspherical particles than for simple spheres, meaning that historically a majority of DEM practitioners have preferentially used the latter, even when attempting to model the former. While under certain conditions the modelling of aspherical particles as spheres can produce quantitatively accurate results (Che et al., 2023a), this is not always the case, especially when considering denser packings and/or more elongated, 'needle-like' particles (Rhodes, 2008). Recently developed GPU-accelerated codes capable of modelling particles with arbitrary polyhedral geometries (Govender et al., 2014; 2015) thus represent a significant step toward the simulation of truly representative industrial systems.

It is important to note that, even with recent advances in both DEM software and computer hardware, DEM simulations are still typically limited to billions of particles (Kosaku et al., 2021), whereas in industrial systems the required numbers may easily reach the trillions or quadrillions. As such, the methods described here are often used in conjunction with other methods, notably the coarse-graining technique introduced in the next section.

For example, the MFIX-Exa Exascale Computing Project (ECP) (Musser et al., 2022) is currently developing a CFD–DEM architecture for future "exascale" supercomputers—i.e. capable of executing $10^{18}$ operations per second—for high-fidelity simulations of multiphase systems specifically targeted at carbon capture and storage. MFIX-Exa is based on the AMReX (Zhang et al., 2021b) software framework, which provides the data structures and iterators to enable massively parallel simulation, and allows simulations to be run using Nvidia, AMD, and Intel hardware. Using MFIX-Exa, a simulation of a pilot-scale 50 kW chemical looping reactor involving 5 billion particles and 2.5 billion fluid cells has been run on the Frontier supercomputer on 62,000 GPUs, with each GPU processing 14,080 stream processors and 128 GB of memory.

### 2.2.1 Pros and cons

The most notable benefit of accelerating DEM simulations through hardware and parallelisation alone is that—unlike for the coarse-graining method discussed in **Section 2.3** and the continuum methods described in **Section 3**—the system is still simulated at full resolution (i.e. all particles are directly, individually modelled). As such, this technique does not require the introduction of additional modelling assumptions, and in most cases the calibration parameters used to develop the system have real, physical meaning.

A major drawback to these methods is that significant speed-up requires access to significant computational resources. The inherent costs associated with acquiring and maintaining the necessary hardware are thus likely to price many smaller companies out of the market. That said, the rise of on-demand cloud computing platforms such as AWS, Microsoft Azure, Google Cloud Platform etc. has, to an extent, lowered this barrier, and will likely continue to do so over the coming years and decades.

A second issue with fully resolved DEM simulations is that, with current hardware, we can still 'only' simulate of the order of billions of particles, yet in industry one may easily reach the trillions or even quadrillions. While, in the long term, these numbers will inevitably improve in lockstep with the advancement of computer hardware, in the shorter term, if we wish to simulate such systems, then parallelisation and GPU acceleration can only form part of the solution, and must be used in combination with some of the other techniques discussed below.

## 2.3 Coarse-grained DEM (CG or CDEM)

As discussed in the preceding sections, the time—or, more specifically, the processor time—required to perform a given simulation increases monotonically with the number of particles to be simulated. As such, if we are able to represent multiple particles with a single 'pseudo-particle' then the computational expense of said simulation will naturally decrease. This is the underlying principle of the coarse-graining technique which lumps several distinct particles into a single 'coarse grain' or 'computational particle' (Patankar and Joseph, 2001).

All CG techniques available in the literature consider particles within a parcel to have the same properties and velocities—i.e. there can be no gradients within a parcel. In this way, CG is somewhat similar to continuum methods such as the two-fluid model (discussed in **Section 3**), where no gradients of particle properties (velocity, temperature et.) are allowed within a cell. Due to this similarity, the term 'coarse graining' is also widely employed to describe the post-processing of DEM data to represent continuum fields (Goldhirsch, 2010; Weinhart et al., 2012), or the smoothing of discrete data to be transferred to CFD for the calculation drag correlations in coupled CFD–DEM simulations (Che et al., 2021; Labra et al., 2013). As can be seen from **Fig. 3**, in recent years there has been a seemingly exponential increase in the number of papers published concerning coarse-graining, which is likely related to an increased interest in the use of DEM to simulate industrial systems (Di Renzo et al., 2021).

A coarse-grained pseudo-particle is typically characterised by the number, $W$, of particles represented by each cluster, and the coarse-graining ratio, $\lambda = d_{cg}/d$, where $d$ is the (linear) size of a 'normal' particle and $d_{cg}$ is that of a coarse-grained parcel of such particles, where $\lambda^3 = W$. It is typically assumed that the mass and volume of a coarse grain are equal to the sum of the masses and volumes of the constituent particles. Even in a publication where the parcel is assumed to have a non-zero void fraction for dilute flows (Lu et al., 2014), this void fraction is considered to

tend to zero at packing. Though the assumption of a particle packing with zero void fraction is obviously unphysical for all except a very small subset of particle geometries and system conditions, said assumption allows the user to keep the same initial bed weight and height in coarse-grained DEM (CDEM) that would be expected in conventional DEM.

As one may intuitively expect, the physical properties of a coarse-grained pseudo particle do not necessarily have a one-to-one mapping to those of their constituent particles. Notably, one must typically lower the restitution coefficient as energy dissipation in a particulate system is a function of particle number density, which by definition decreased when the size of particles is increased (Benyahia and Galvin, 2010; Lu et al., 2014). There exist numerous scaling laws through which authors have attempted to relate the properties of individual particles to their CG equivalents. Perhaps the most commonly used is that of Sakai (Sakai, 2016) in which all forces are scaled by $\lambda^3$, thus providing the same overlap for the parcel and real particle, as well as the same spring constant, restitution coefficient, and friction coefficients. Where the Sakai method ensures a constant *absolute* overlap between parcel and particle, the approach of Queteschiner et al. (2018b) instead ensures the same *relative* overlap by scaling the spring constant by $\lambda$. There exist also a number of other scaling approaches, see for example (Che et al., 2023b; de Munck et al., 2023; Kishida et al., 2021; Kushimoto et al., 2021; Nasato et al., 2015; Sakai, 2016; Zhang et al., 2021a), including approaches for modelling cohesive particles (Chen and Elliott, 2020; Nasato et al., 2015; Sakai et al., 2012), systems in which liquid bridges are present (Chan and Washino, 2018; Zhang et al., 2021a), aspherical particles (Zhou et al., 2022) and even heat and mass transfer (Lu et al., 2017b)—matters of considerable importance in many industrial processes. Interestingly, recent comparative studies have found a surprising lack of differentiation between simulations employing different coarse-graining models (Che et al., 2023b; de Munck et al., 2023); however, both studies used fluidised beds as their benchmarking systems. Since, in these systems, particle dynamics are largely dominated by drag effects as opposed to particle–particle interactions, it is unclear whether the same degree of similarity could be expected in denser systems, and in particular single-phase particulate systems.

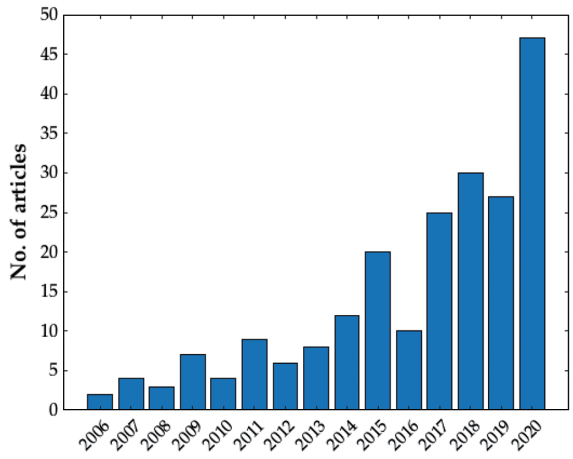


**Fig. 3** Number of indexed articles published per year concerning coarse-grained DEM. Image reproduced from reference (Di Renzo et al., 2021).

As alluded to at the start of this section, all particles forming a CG parcel must possess the same properties

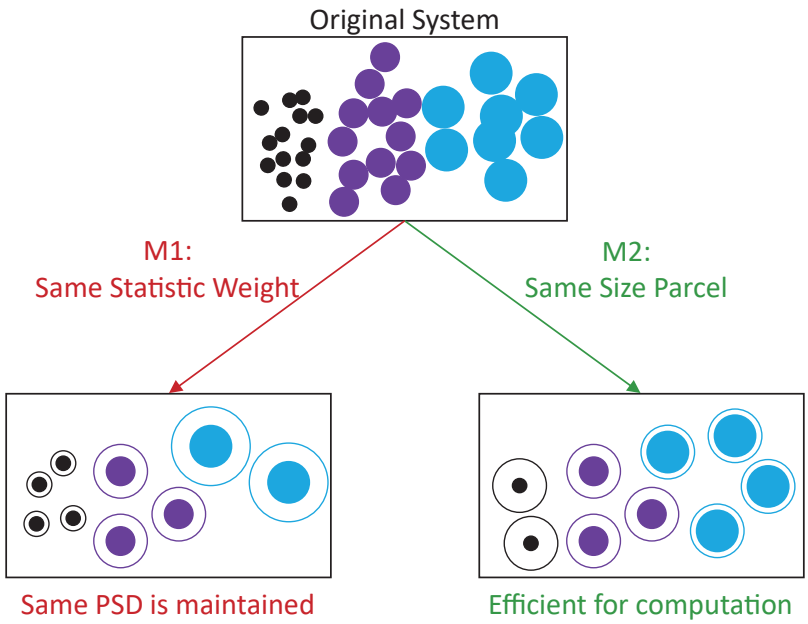


**Fig. 4** Simple schematic depicting the two methods for the coarse-graining of polydisperse systems described in the main text. Adapted with permission from Ref. (Lu et al., 2018). Copyright: (2018) Elsevier Ltd.

—including particle size. As such, when coarse-graining highly polydisperse systems (as are commonly found in industry) one must determine a suitable manner in which to represent the particle size distribution (PSD). There are two main ways to do so: the same statistical weight (SSW) method, in which the same number of particles are included in parcels corresponding to each size fraction, and the same size parcel (SSP) method in which (as the name implies) the size of the particles is instead kept constant. These methods are depicted schematically in **Fig. 4**. While the latter method is naturally more efficient, it is arguable that the former provides a more 'realistic' representation of the original PSD, and in some cases produces greater accuracy (Lu et al., 2018).

A notable limitation of the CG method is that in certain systems with heterogeneous geometries (e.g. hoppers (Coetzee, 2019)), coarsening cannot be conducted in the whole geometry due to flow restrictions. In such cases, it has been shown possible to locally refine CDEM back to DEM, or simply to a lower level of coarse-graining (De et al., 2022; Queteschiner et al., 2018a, 2018b).

Due to the different assumptions in CDEM, it is important to validate this method against data obtained with both finer DEM methods and experiments (discussed in further detail in **Section 4**). One can envision a series of validation studies by first comparing the simulation results of CDEM and DEM. Differences between the two simulation results can be quantified as uncertainties (UQ) due to the coarse-graining assumption. The UQ analysis can be extended to DEM simulation data through comparison with resolved DEM and/or DNS (dependent on the nature of the system studied) to quantify errors due to the assumed forms of fluid–particle interaction terms. Finally, the resolved DEM/DNS data can be compared with small-scale well-instrumented experimental setups where the experimental errors are carefully quantified. There exist limited examples of such a 'cascading series' of UQ missing in the literature due to the inherent complexity of conducting such numerical simulations and experiments for many different scenarios. Nevertheless, many attempts to validate CDEM with both finer DEM and experimental data are available in the literature.

Mori et al. (2019) compared bed height and pressure drop in a small-scale experimental dense fluidised bed of 0.05 m diameter using a factor $\lambda$ of between 5 and 10.

Oyedeji et al. (2022) validated CDEM for biomass (corn) pyrolysis reactions in a small-scale reactor of 0.15 m diameter with a coarsening factor $W = 10$ and 20, and at this low level of coarsening (real particles were already coarse), the results showed simulation data within a few percent of experimental pyrolysis reaction yields.

Zhou and Zhao (2021) conducted CDEM simulations of a small-scale fluidised bed with an immersed tube with $\lambda$ up to 3 which resulted in up to two orders of magnitude simulation speed-up for the discrete phase (the fluid solver required significant CPU effort and is not included in this comparison). Obvious agreement of bed expansion height and pressure drop reported as these are roughly equal to the weight of the bed, however noticeable disagreement was observed for the velocity profiles for different coarsening levels as compared with finer DEM results.

Wang and Shen (2022) studied biomass gasification in a small-scale dense fluidised bed reactor of 0.05 m diameter. CDEM results were validated against both finer DEM simulations and experimental data for CG ratios $\lambda = 2$, 3, with an order of magnitude speed-up of obtained by using CDEM.

A study of a small-scale gas-particle cyclone separator for monodisperse particles of 0.5 mm diameter using $\lambda = 4$ was conducted recently by Napolitano et al. (2022). The numerical results were observed to degrade with increasing $\lambda$, likely due to the small number of parcels used.

Sakai et al. (2014) validated CDEM in a small-scale fluidised bed where good agreement of bed height and pressure drop were obtained with for $\lambda = 5$. This study and many others in the literature compared only the bed height and pressure drop, commonly measured experimentally, indicating a good agreement because the weight of the bed and the drag laws are usually sufficiently accurate for fluidised beds. Less accuracy is usually observed for quantities that are affected by collisions, such as particle velocity and granular energy.

Lungu et al. (2022) conducted a validation study of CDEM in a small-scale fluidised bed containing large 3 mm particles with values of $\lambda$ up to 2. Their results showed little sensitivity of simulation time to $\lambda$ due to the small number of parcels used, which is usually an indication that the fluid solver is taking most of the CPU time. In fact, many cases in the literature that compare CDEM to finer DEM results use a small system with a relatively small number of particles so that a DEM simulation can be conducted. These simulations are not able to validate CDEM for a large parcel-to-particle ratio. Such results provide a useful cautionary tale for researchers—it is important to know whether the computational costs of your simulation are dominated by the particle phase or the fluid phase. If the latter, the application of coarse-graining may degrade one's results whilst not achieving any significant speed-up!

Takabatake et al. (2018) compared CDEM and DEM results in a small-scale spouted bed using $\lambda$ values of 2 and 3, achieving respectively a factor of 8- and 30-times speed-up, while maintaining similar mixing patterns to those obtained in resolved DEM simulations.

Coetzee (2017) found that while $\lambda$ values of up to 9 can be used to accurately model dynamic angles of repose in a medium-scale rotating drum as long as the drum-to-particle diameter ratio is above 25, hoppers showed a much

stronger dependence on the scaling factor, with hopper discharge only being reasonably predicted for $\lambda$ values up to 1.3. However, $\lambda = 1.3$ still provided a decrease in computational time by a factor of 3.2, showing both the usefulness and care required in using CDEM.

Cai and Zhao (2020) conducted a validation study of CDEM in a small-scale drum and conical mixer with $\lambda = 3$ and obtained reasonable agreements for mixing time and power consumption whilst achieving a speed-up of almost two orders of magnitude.

Other small-scale CDEM simulations have demonstrated the validity of this technique in powder die-filling using $\lambda = 3$ (Widartiningsih et al., 2020), and for a dry powder inhaler where only fine particles were coarsened (Liu et al., 2021).

Most recently, Che et al. (2023b) applied values of $\lambda$ up to 30 to a laboratory-scale fluidised bed of Geldart group B particles, providing detailed comparison both to lower degrees of coarse graining (due to the number of particles in the system, fully resolved DEM was not computationally tractable) as well as experimental data obtained using positron emission particle tracking (Windows-Yule et al., 2020; 2022a). It was found that values of $\lambda$ up to ~20 still produced good agreement with experimental data, despite the comparatively small size of the system and the rigorous validation methods implemented.

As is evident from the above-discussed studies, the majority of existing studies have focused on smaller laboratory-scale systems, as opposed to larger-scale flow systems of greater interest to industry. One reason underlying the lack of industrial-scale studies may be the difficulty in obtaining accurate experimental data in large systems, which makes such data less available in the literature. This issue—and potential solutions to it—are discussed in **Section 4**. Nevertheless, some such studies do exist. Work by Lu et al. (2017a) and Lu and Benyahia (2018a) has included the simulation of pilot-scale catalytic crackers and regenerators, methanol to olefin reactors, and rare-earth elements solid-liquid extractors, none of which could feasibly have been simulated using resolved (non-coarse-grained) DEM.

Stroh et al. (2018) studied a pilot-scale circulating fluidised bed carbonator of approximately 0.6 m diameter and 9 m height during stable operation by CDEM, using a coarsening factor $\lambda = 60$. Reasonable comparison between simulation and the available experimental data of pressure drop and $CO_2$ absorption rate was obtained. The same group later studied a smaller (0.2 m diameter, 3 m height) cold-flow circulating fluidised bed, this time instrumenting the system with a capacitance probe to allow more detailed experimental validation.

Nikolopoulos et al. (2017) compared the performance of CDEM and two-fluid model (TFM—see **Section 3**) approaches for a 1 MWth pilot-scale fluidised bed carbonator of 0.6 m diameter and 8.7 m height. The CDEM approach compared well with experimental pressure-drop data, whilst also achieving a reasonable computation time, similar to the TFM simulation.

Hu et al. (2019) conducted CDEM simulations of a medium-scale (0.22 m width by 2 m height) fluidised bed coal gasifier in the bubbling regime with $\lambda = 5$. Their results were compared to both previously published TFM and experimental results, demonstrating a good degree of accuracy.

In 2019, a medium-scale biomass gasification reactor of 1.3 m height with a diameter varying from 0.08 to 0.2 m CDEM study was pursued by Ostermeier et al. (2019b) who also provided a nice summary of the different CFD approaches to model biomass gasification in fluidised bed reactors. Large values of $\lambda$ up to 50 were used to represent the finest particles due to consideration of the wide PSD of sand and biomass particles. This level of coarsening allowed the authors to validate the technique over a long range of operating hours, and found good agreement with available experimental data of bed pressure and temperature as well as chemical products of the gasification reactions.

Prior authors have already conducted CDEM simulations of industrial-scale gas–particle cyclone separators (Chu et al., 2016, 2022; Ji et al., 2018). In the 2022 work of Chu et al. (2022), the models used could accurately predict the cyclone efficiency and the formation of ribbons of particles in the cyclone.

## 2.4 Pros and cons

In summary, the past two decades of research have demonstrated the ability of CDEM to tackle complex, industrially relevant problems in chemical engineering. CDEM can provide solutions with almost any computer resources available to the engineer, ranging from a desktop computer to the most powerful supercomputers, and still produce a good representation of the systems being modelled. The main challenge at present regarding CDEM is the lack of consensus regarding the mapping of the properties of ‘true’ particles to those of coarse-grained ‘meso-particles’. More research is also necessary to evaluate the uncertainties associated with the coarsening assumption keeping in mind that DEM solutions are available for UQ analysis (Lu and Benyahia, 2018b).

## 2.5 Mapping-based extrapolation

Perhaps the most recent development in the speed-up of discrete particle simulations is the ‘mapping-based extrapolation’ technique, originally developed by Bednarek et al. (2019). Mapping-based extrapolation techniques exploit the pseudo-periodic behaviour of processes. The periodic time is a process-inherent variable and does not depend on any DEM parameters. The period is several orders of magnitude larger than the DEM integration time steps.

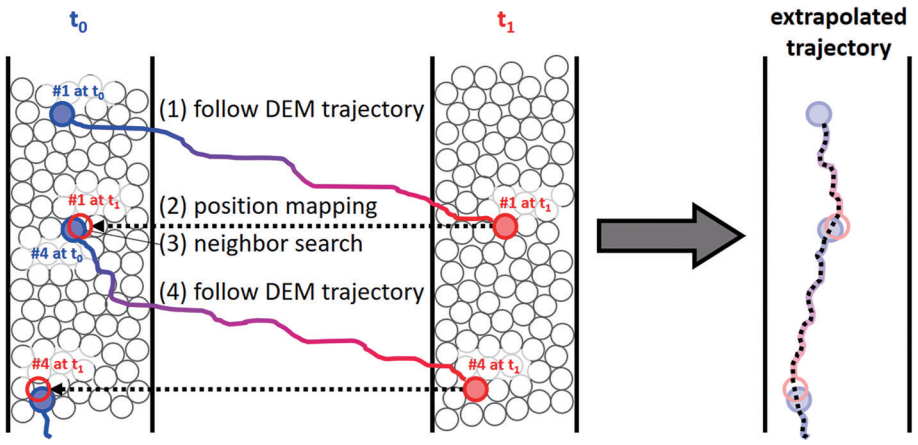


**Fig. 5** Schematic overview of a mapping-based extrapolation algorithm. Image reproduced from Ref. (Siegmann et al., 2021). Copyright: (2021) Elsevier B.V.

Examples of a process period could be one rotation of mixing blade, or the time between refills of a twin-screw feeder.

The method uses two simulation states taken at time points $t_0$ and $t_1$. These two points represent, respectively, the start and end points of the periodic time (or an integer multiple of periods). **Fig. 5** shows a sketch of the mapping-based extrapolation. The numbers in the figure pertain to the following key steps of the algorithm:

1. The trajectory of particle #1 from $t_0$ to $t_1$ is known from the simulation states. However, the particle did not leave the system at $t_1$ (continuous process) or the process has not ended at $t_1$ (batch process).
2. Although the exact trajectory of particle #1 after $t_1$ is not known, it makes intuitive sense that it will be very similar to a particle that started at a similar position at $t_0$.
3. A neighbour search finds that particle #4 has a similar starting position where particle #1 ended.
4. The extrapolated trajectory of particle #1 uses the data for particle #4. This process is repeated until the particle leaves the system (continuous process) or the process duration has been reached (batch process).

The exact mapping procedure depends on the application. If the goal is to only extrapolate the trajectories of a subset of particles (e.g. tracer particles for a virtual spike experiment to characterise the residence time distribution), the mapping procedure is a nearest-neighbour search (Siegmann et al., 2021). However, if the goal is to extrapolate all particle positions, it makes sense to invest computational time in a bijective[4] mapping function that minimises the average mapping error (i.e. the distance between the particles at $t_1$ and their mapping partners at $t_0$).

As a relatively young technique, mapping-based extrapolation does not have the same extensive back catalogue of example applications as coarse-graining, but nonetheless has demonstrated some success in the limited number of papers produced to date, accelerating DEM models of conical screw mixers (Jadidi et al., 2022), continuous blenders (Moreno-Benito et al., 2022), and tablet press feed frames (Forgber et al., 2022). The applications are not limited to DEM simulations, but can also be extended to other particle-based methods such as smoothed particle hydrodynamics (SPH), for example, in the accelerated modelling of twin screw extrusion processes (Bauer and Khinast, 2022; Bauer et al., 2022; Matić et al., 2023).

One hard requirement for mapping-based extrapolation is the existence of pseudo-periodic process behaviour. For example, the discharge of a twin-screw feeder from maximum to minimum fill level is an inherently transient process and will never reach some kind of pseudo-periodicity: the fill level in the hopper of the feeder is constantly decreasing and causes constantly changing flow patterns (Toson and Khinast, 2019). Thus, mapping-based extrapolation is not able to speed up the prediction of the discharge process. However, if periodic refills at the same fill level are considered, mapping-based extrapolation can predict, for example, the washout of old material over multiple refills (Toson and Khinast, 2019).

A soft requirement for the successful application of the technique is the presence of dense flows in the process, as such flows offer multiple (good) mapping partners for each particle. The mapping error is then in the order of one particle radius (Siegmann et al., 2021). It is speculated that mapping-based extrapolation could be applied to more dilute flows at the expense of accuracy (Bednarek et al., 2019), though there are currently no examples in literature to either support or disprove this. In addition, if the dilute particle flow is caused by interaction with air (e.g. in fluidised beds), it is generally a better idea to use the air flow field for extrapolation (Lichtenegger, 2020; Lichtenegger and Miethlinger, 2020; Lichtenegger and Pirker, 2020).

[4] Bijective mapping means that each particle in time step $t_1$ has exactly one mapping target at $t_0$, and that each particle at $t_0$ is referenced by exactly one particle from $t_1$. This optimised mapping function can then be used for all mapping steps and does not need ad-hoc neighbor searches in each mapping step.

### 2.5.1 Pros and cons

The main benefit of the mapping-based extrapolation method is that it allows significant speed-up yet, unlike coarse-graining methods, is still 'fully resolved'—i.e. particles can be modelled at their true size, and calibrated using their 'real' properties. As such, for processes involving dense particle flows, the technique has been shown to facilitate high-accuracy simulations. It can also be applied to other particle-based methods such as SPH, thus allowing the acceleration of fluid simulations in a similar manner. The main drawbacks of the technique are that it is not suitable for transient (i.e. non-periodically-repeating) processes and is currently untested for more dilute flows.

### 2.5.2 Recurrence CFD

It is worth, at the end of this section, briefly mentioning the existence of another technique—recurrence CFD (rCFD)—which provides another approach not dissimilar to the technique discussed above, though for fluid-phase (as opposed to particle) simulations. As the main focus of this work is on the particulate phase, we will not discuss rCFD in detail here, but rather point the reviewer to some useful references, namely (Lichtenegger et al., 2017; Lichtenegger and Pirker, 2016).

## 3. Continuum methods

As has been made abundantly clear in the preceding sections, the main limitation of discrete methods for the simulation of industrial-scale particulate systems is the computational expense of modelling each distinct particle individually. This problem can be overcome by instead modelling particulate media as continua, much as CFD does not consider the individual molecules forming a fluid. There are two crucial differences between particulate media and 'classical' fluids, however, that make the construction of a continuum formulation more complex:

I. Particulate media do not possess a reference equilibrium state.
II. Their temporal and spatial scales are not well separated—that is to say the scales of the dynamics of the individual particles are comparable to those of the bulk medium.

As put succinctly by the great Isaac Goldhirsch at the turn of the millennium, "*the notion of a hydrodynamic or macroscopic description of granular materials is based on unsafe grounds and it requires further study*" (Goldhirsch, 1999). Since then, much 'further study' has indeed been conducted, to the point that accurate continuum models of diverse industrial systems can be found in the literature.

While continuum models exist for both pure particulate systems and multiphase particle–fluid systems, the vast majority of (successful) industrial-scale studies have been performed with the latter, and as such for the present review we focus on the two-phase case.

The Eulerian–Eulerian Two-Fluid Model (TFM) treats both the liquid and solid phases as continua that can fully interpenetrate one another. When it comes to simulating the flow of particulate media, the remaining challenge is to develop closure laws for determining solid flow parameters, such as dynamic/bulk viscosities, particle pressure, and interfacial momentum transfer in multi-sized systems. The Kinetic Theory of Granular Flow (KTGF) has been developed for this purpose. TFM has a lower computational cost compared to (CFD–)DEM and other frequently used approaches for granular flow modeling and, as a result, are better suited for simulating industrial-scale applications.

It is worth prefacing the remainder of this section with the warning that the TFM and the KTGF are unavoidably mathematical, and as such any description thereof which does not include the relevant equations is inevitably somewhat vague and 'hand-waving'. That said, a full understanding of the methods themselves is not necessary to the purposes of the present review article. As such, for brevity (and so as not to be off-putting to the casual reader) we will provide in the main text only the 'hand-waving' explanation, but include as supplementary material a more complete, mathematical description.

Key publications introducing the theories of TFM and KTGF can be found in references (Anderson and Jackson, 1967; Bishop, 1975; Ding and Gidaspow, 1990; Karlsson et al., 2009; Liu et al., 2017; Zhou et al., 2010) and (Brilliantov et al., 2004; Ding and Gidaspow, 1990; Iddir and Arastoopour, 2005; Jenkins and Savage, 1983; Karlsson et al., 2009; Lun et al., 1984; Rao et al., 2008; Savage and Jeffrey, 1981; Schaeffer, 1987), respectively. Although these theories are well-established, there are numerous variations in the formulations, taking into account factors such as elasticity (Lun et al., 1984), particle size distribution (Liu et al., 2022), and particle types (Iddir and Arastoopour, 2005), among others. Consequently, the descriptions of TFM and KTGF are not unique.

The role of the KTGF is to formulate the stresses associated with particulate-phase flow. It is an extension of the classical kinetic theory of gases (Fowler, 1939) adapted for dense particulate flows. Initially, the kinetic theory was developed by Chapman and Cowling (Fowler, 1939) for gases to predict the behaviour of mass point molecules with conserved interaction energies. About three decades ago, this theory was extended to particulate flow, where interactions between particles are not conserved. Savage and Jeffrey (1981) were among the first to apply the kinetic theory to rapidly deforming materials in the (relatively simple) form of smooth, hard, spherical particles. In this theory, the fluctuation energy of particles is described by introducing the concept of a 'granular temperature', analogous to thermodynamic temperature for gases. Though different researchers consider different definitions of the

granular temperature (Goldhirsch, 2008), in the current context we adopt the most common (and indeed literal) definition as the ensemble average of the square of particles' fluctuating velocities. Having introduced a granular analogue for temperature, one must also develop expressions for granular pressure, bulk viscosity, shear viscosity, frictional shear viscosity, and diverse other terms (Lun et al., 1984; Johnson and Jackson, 1987; Schaeffer, 1987). Examples of these expressions can be found in the Supplementary Material.

The granular pressure represents the particle phase normal force caused by the particle–particle interactions. Its description, based on the kinetic theory of granular flow, was developed by Jenkins and Savage (1983) and Lun et al. (1984). The bulk viscosity is a measure for the resistance of a fluid against compression. It is obvious that the importance of the bulk viscosity depends strongly on the velocity gradients. In a fluidised bed, the bulk viscosity and the shear viscosity are of the same order of magnitude, and hence the bulk viscosity should not be neglected, as can be done when simulating Newtonian fluids. While the granular pressure and bulk viscosity describe normal forces, the shear viscosity accounts for the tangential forces. It was shown by Lun et al. (1984) that it is possible to combine different inter-particle forces and use a momentum balance similar to that of a true continuous fluid. In similarity to the particle pressure, a particle shear viscosity can also be derived from the kinetic theory.

While continuum models have been shown capable of simulating various particulate systems, including rotating drums (Schlick et al., 2015) and free-surface flows (Chassagne et al., 2020), the majority of industry-relevant studies have concerned two-phase flows, and in particular fluidised beds—including circulating fluidised beds (Liu et al., 2021), tapered fluidised beds (Khodabandehlou et al., 2018; Liu H. et al., 2017; Liu X. et al., 2019), spray coaters (Shuyan et al., 2010; Srčič et al., 2013), spouted beds (Gryczka et al., 2009; Moliner et al., 2019) and bubbling beds (Lungu et al., 2021; Nikolopoulos et al., 2017; Ostermeier et al., 2019a; Xi et al., 2021), as well as being used to study jet behaviour (Chen and Wang, 2014).

A number of recent studies have also focused specifically on the comparison of CFD–DEM and TFM models (Chen and Wang, 2014; Moliner et al., 2019; Lungu et al., 2021; Ostermeier et al., 2019a). While in general—as one may expect—CFD–DEM models are generally found to provide stronger agreement with experimental baseline data than TFM, TFM models are found in many (though not all) cases to provide reasonable agreement with experiment. Perhaps surprisingly, some specific aspects of system behaviour are, in some cases, *better* captured by TFM than CFD–DEM (Chen and Wang, 2014; Lungu et al., 2021), though overall agreement in the cited cases remains stronger for CFD–DEM.

### 3.1 Pros and cons

TFM is typically—though (dependent on system size and other factors) not always (Moliner et al., 2019)—the most computationally efficient of all the methods discussed thus far. However, as is evident from the preceding section, TFM simulations are typically less accurate than equivalent CFD–DEM simulations, though in many cases can still provide reasonable agreement with experimental data. As is also evident from the above, the models require a significantly larger number of modelling assumptions than either fully resolved or coarse-grained DEM simulations, and the existence of many competing theories makes the choice of the correct model somewhat challenging.

## 4. Validation of models via industrial-scale imaging

As touched upon above, one of the most significant (and often-overlooked) problems with the application of numerical models of particulate systems is the lack of rigorous calibration and validation (Windows-Yule et al., 2016). While the matter of calibration has been addressed in detail in recent reviews (Ketterhagen and Wassgren, 2022; Windows-Yule and Neveu, 2022), the matter of validation—and in particular the validation of simulations concerning industrial-scale systems—has received less attention.

The most rigorous validation of particulate systems is typically performed through comparison with experimental imaging data. At the laboratory scale, simulation models can be rigorously and (relatively) easily validated through comparison with comparatively cheap and readily available, optical methods such as particle imaging velocimetry (PIV) and particle tracking velocimetry (PTV) (Marigo and Stitt, 2015; Shirsath et al., 2015; Weber et al., 2019; 2021), see e.g. **Fig. 6**. At the industrial scale, however, this becomes still more challenging due to the fact that in most cases industrial systems are a) large and b) optically opaque.

The issue of opacity can be overcome by a variety of techniques, including X-ray tomography (CT) (Wang et al., 2004; 2007), radioactive particle tracking (RPT) (Roy, 2017), positron emission particle tracking (PEPT) (Windows-Yule et al., 2020), magnetic resonance imaging (MRI) (Gladden and Alexander, 1996), electrical capacitance, impedance or resistivity tomography (ECT/EIT/ERT[5]) (Wang, 2015), or magnetic particle tracking (MPT) (Neuwirth et al., 2013). An introductory summary of each of these techniques can be found in Chapter 4 of (Windows-Yule et al., 2022b). However, of these imaging techniques, many are still not suitable for industrial imaging. The small bore size of MRI systems, for example,

[5] For the sake of this article, where the focus is not a deep analysis of the techniques discussed, we will refer to this group of techniques simply as 'EXT'.

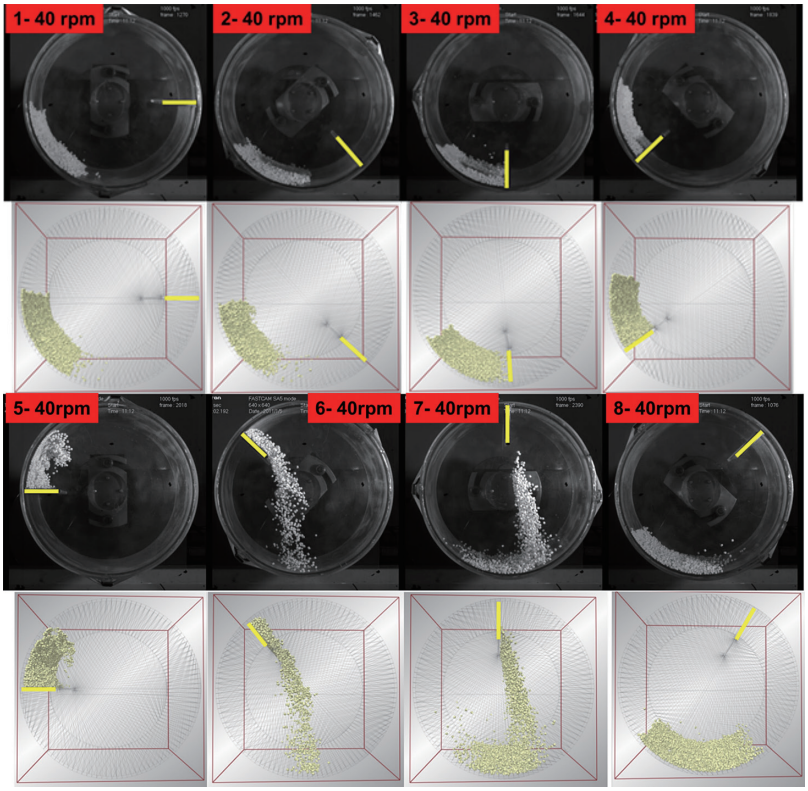


**Fig. 6** An example of the use of optical data for the validation of DEM simulations for a laboratory-scale rotating drum. Image reproduced from Ref. (Marigo and Stitt, 2015) under the terms of the CC-BY 4.0 license. Copyright: (2015) The Authors, published by Hosokawa Powder Technology Foundation.

combined with the fact that most industrial systems are metal-clad, makes this technique largely unsuitable (Elkins and Alley, 2007).

The requirement of MPT for strongly magnetic tracer particles (Buist et al., 2014) again means that it cannot be realistically used in systems containing (or constructed from) ferrous or other magnetic materials, thus again limiting its industrial value. Even in nonmagnetic systems, the tracers used for imaging are typically of millimetre size, making them unsuitable for representing a wide variety of industry-relevant particles, which (in the chemical and pharmaceutical sectors in particular) tend to be closer to the micron scale.

X-ray CT is widely used in industrial applications (De Chiffre et al., 2014) and, as commercially available systems become able to use higher-energy X-rays (Sun et al., 2022), it can be used to image increasingly thick, dense targets. However, its primary use in industry is for metrology, and the imaging of individual parts (Sun et al., 2012), as opposed to imaging the dynamics of active industrial systems—though that is not to say that it has not found certain valuable applications, for example studying fluid flow in porous media (Bultreys et al., 2016), or studying morphological changes in batteries (Finegan et al., 2016). However, despite significant recent improvements in the acquisition rate of X-ray CT systems (Withers et al., 2021), and in particular the very impressive capabilities of synchrotron systems (Dewanckele et al., 2020) and lab-scale systems (Maire and Withers, 2014), the temporal resolution offered by current, commercially-available industrial scanners still remains too low to meaningfully capture the rapid flows exhibited by many industrial particle-handling systems (Zwanenburg et al., 2021). The requirement for X-ray CT systems to be entirely shielded also means that their use for the in situ imaging of real industrial processes remains challenging.

Following from the above, we are left with three techniques which can realistically be applied to the in situ imaging of a reasonably wide range of industrial particle handling systems: EXT, RPT, and PEPT. All three techniques carry the advantages of being able to penetrate metal-walled systems, image comparatively large systems, and having suitably high temporal resolution to capture the dynamics of rapid granular flows. All three techniques can also be applied using a modular array of detector devices (Wang, 2015), allowing the imaging of large systems with complex geometries. Each technique, however, also carries its own distinct strengths and weaknesses. In the following paragraphs, we will briefly summarise these strengths and weaknesses in the specific context of industrial imaging and the validation of numerical models, provide an overview of the types of systems which can (and cannot) be successfully imaged, and highlight recent developments in the relevant fields.

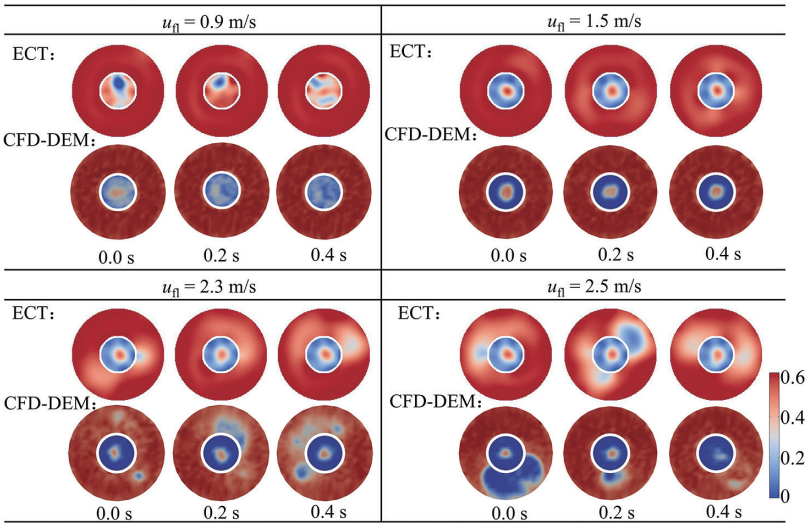


**Fig. 7** Example of the use of ECT data in the validation of a CFD–DEM model of a Wurster coater. Reproduced with permission from Ref. (Che et al., 2020). Copyright: (2020) Elsevier B.V.

## 4.1 Electrical tomography

EXT techniques operate, in simple terms, by transmitting an electrical signal through a given system of interest, which is then received by an array of detectors (electrodes) placed strategically around the system. By analysing the intensity of the signals received by each part of the sensor array, various system properties can be back-computed (Scott and McCann, 2005). A previous KONA review paper providing an more detailed yet still accessible introduction to electrical tomography techniques can be found in reference (Rasteiro et al., 2011). EXT is already widely used for the imaging of a wide range of industrial systems and unit operations, including pipes (Dong et al., 2003), storage vessels (Kowalski et al., 2010), mixers (Holden et al., 1998), reactors (Bolton and Primrose, 2005), cyclones (Meng et al., 2008). Indeed, EXT methods can realistically be applied to almost any system physically resembling a pipe or tank (Rasteiro et al., 2011; Sharifi and Young, 2013).

Key metrics which can potentially be used to validate numerical simulations include the flow rates and velocity distributions, the distributions of different materials and (thus) various mixing and mixing rate metrics, solids concentration, and solids hold-up (Sharifi and Young, 2013). **Fig. 7** shows an example in which ECT-derived cross-sectional images of solid distributions are used to validate CFD–DEM simulations of a Wurster coater (Che et al., 2020). This set of images, as well as those shown in **Fig. 8**, clearly illustrate the advantage gained in terms of the thoroughness and rigour when using two/three-dimensional imaging techniques (as opposed to simpler, lower-dimensional data such as pressure drop measurements) when validating simulations.

In terms of the relative advantages and disadvantages of the ECT technique, two particularly significant benefits for industrial applications are the low cost and easy installation of the technique (Eda et al., 2013). Compared to nuclear imaging techniques such as PEPT and RPT (which we discuss next), it also carries the advantage of not using ionising radiation, thus providing non-trivial benefits in terms of ease of use, as no permits etc. are required for its implementation. Electrical tomography systems can also be used as on-line, in-line sensors, offering access to real-time data from a system.

In terms of drawbacks, EXT techniques offer comparatively poor spatial resolution—typically of the order of 10 % of the diameter of the vessel being imaged when used in practice in industrial systems (Xie et al., 1995). While of course these figures fall well below what is hypothetically achievable with more carefully controlled conditions and cutting-edge algorithms, it is nonetheless well accepted that spatial resolution remains an Achilles heel of EXT techniques (Rymarczyk et al., 2019; York, 2001). Another disadvantage of electrical tomography compared to methods such as RPT and PEPT is that it provides only Eulerian information—that is, it can provide information regarding the bulk motion of a particulate medium (velocity distributions, solids distributions...), but provides no particle-level information (e.g. circulation time, dispersion rate, etc.).

## 4.2 Positron emission particle tracking

Positron emission particle tracking, as its name implies, tracks the motion of a 'tracer particle'[6] which is 'labelled' with a positron-emitting radioisotope.

When the positrons produced by said isotope annihilate with electrons within the tracer particle, they produce a pair

[6] PEPT may also be conducted using multiple such tracers (Nicuşan and Windows-Yule, 2020; Yang et al., 2006), but for the sake of simplicity in the present explanation of the technique we will only consider the case of a single tracer.

of 511 keV gamma photons whose trajectories are collinear and antiparallel, thus effectively 'drawing a straight line' (known as a line of response or LoR) through the tracer's position. If multiple such LoRs are detected by suitably-placed detectors surrounding a given system of interest, they can be used to triangulate the position of the tracer. For current detector systems and algorithms, tracers can be located with micron-scale spatial resolution and microsecond-scale temporal resolution (Windows-Yule et al., 2022b). Through suitable temporal averaging, the dynamics of the tracked particle(s) may be used to build up a picture of the full, three-dimensional dynamics of the system of interest. PEPT's use of high-energy gamma radiation means that it can be used to probe the interior dynamics of large, dense, optically-opaque, three-dimensional systems, making it well-suited to industrial imaging. The tracers used are also typically physically identical to those belonging to the system of interest, meaning that the technique is also non-invasive. A more complete but still accessible introduction to the PEPT technique can be found in reference (Windows-Yule et al., 2020), and a deeper dive into the algorithms used to track particles in reference (Windows-Yule et al., 2022a).

Like ECT, PEPT has been applied to the study of a wide range of industry-relevant processes and unit operations, including pipe flow (Fairhurst et al., 2001), diverse types of mixers (Jones and Bridgwater, 1998; Marigo et al., 2013; Mihailova et al., 2015), stirred tank reactors (Fangary et al., 2000), fluidized beds (Leadbeater et al., 2023), spouted beds (Al-Shemmeri et al., 2021), and vibrated beds (Windows-Yule et al., 2014), cyclones (Chan et al., 2009), drum roasters (Al-Shemmeri et al., 2023), mills (Conway-Baker et al., 2002), froth flotation devices (Cole et al., 2022), extruders (Diemer et al., 2011), and even household appliances such as washing machines, dishwashers and tumble dryers (Jones et al., 2022; Pérez-Mohedano et al., 2015).

Due to the rich, high-resolution, three-dimensional data provided by PEPT, the technique is also widely used in the validation of numerical models of particulate and particle-fluid systems, including industry-relevant systems. **Fig. 8** shows a comparison of PEPT and CFD–DEM data for a

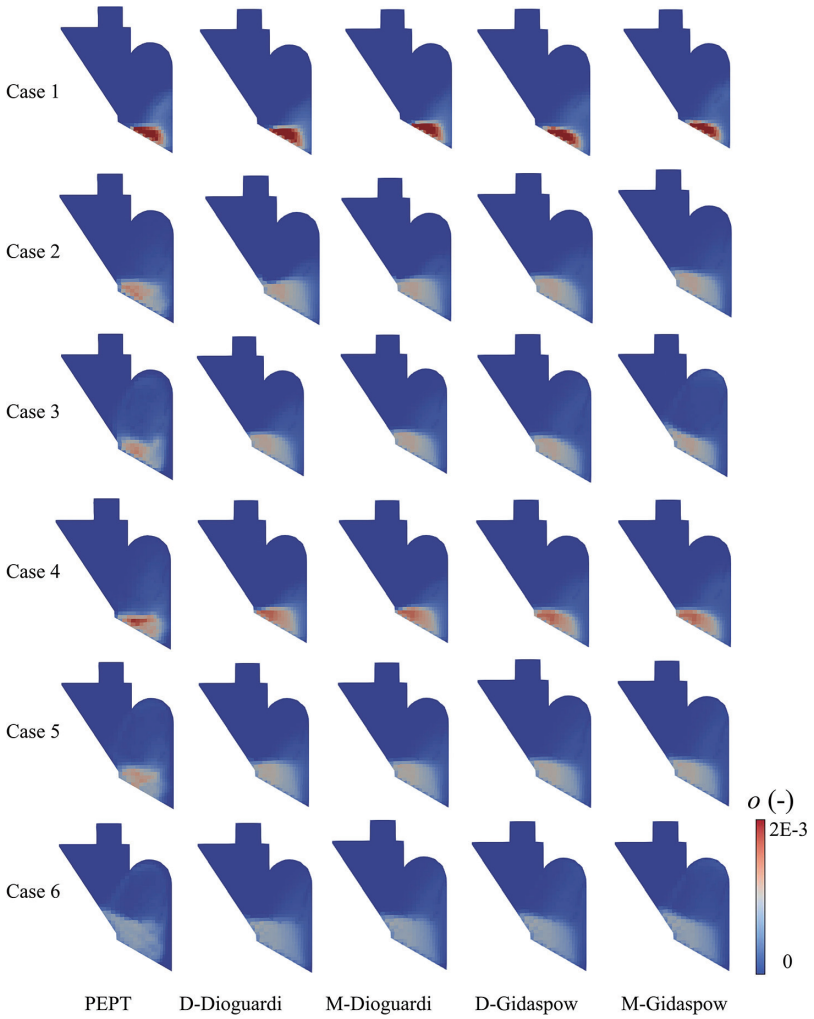


**Fig. 8** Comparison of PEPT and CFD–DEM derived solid occupancy distributions for a variety of different system conditions (rows) and drag models (columns). Reproduced with permission from Ref. (Che et al., 2023a). Copyright: (2023) Elsevier B.V.

NEUHAUS NEOTEC spouted-bed coffee roaster (Che et al., 2023a). By post-processing both PEPT and CFD–DEM data on the same Eulerian grid, it is possible to conduct a cell-by-cell comparison of experimental and numerical data for a variety of physical fields, and thus provide a fully quantitative assessment of the degree of accuracy exhibited by a given simulation. Full details of the process through which this may be achieved may be found in reference (Che et al., 2023a).

To date, however, while PEPT has been used to image a number of 'real' industrial systems, including pilot-scale systems, in the laboratory (Windows-Yule et al., 2022b), its use for the in situ imaging on active industrial sites has been comparatively limited as compared to techniques such as EXT.

In 2007, using a portable, modular detector system developed at the University of Birmingham, PEPT was successfully used to extract information from a large (750 mm diameter) fluidised bed at BP's site in Hull, operating at pressure and under industry-relevant conditions (Ingram et al., 2007). Data obtained included velocity vector fields indicating the flow regime of the system, and circulation rate data, both providing valuable insight into mass transport within the system and the variation thereof with changes to key system parameters.

In 2022, an upgraded modular camera system (Herald et al., 2023; Parker et al., 2022) was used to image particle motion within an active fluidised-bed pyrolysis reactor used for the chemical recycling of waste plastics (Ingenia, 2022). In this instance, not only were particles corresponding to the bed material used to image the flow dynamics of the system, radioactively labelled plastic pellets were also used to assess crucial aspects of system performance including the residence time of the particle (i.e. the time required for its complete volatilisation), as well as indicating whether or not the plastics injected into the system were subject to adequate mass transport to ensure temperature uniformity (and thus product quality).

The lack (to date) of PEPT's wider use in on-site imaging can likely be ascribed to one (or both) of two major factors: firstly, the current lack of widespread availability of the relevant expertise or equipment (there presently only exists one portable, modular PEPT camera). Secondly, the fact of the use of ionising radiation means there exists a considerable amount of 'red tape' as compared to techniques such as ECT. However, there do not exist any specific *technological* barriers to the wider adoption of industrial PEPT.

The above represents perhaps the most significant 'con' regarding the industrial application of PEPT imaging. Another notable drawback, however, is that while PEPT can provide real-time information regarding the motion of individual particles, the requirement of the time-averaging of multiple tracer passes to produce full, Eulerian data means that, unlike EXT, PEPT cannot provide direct information regarding transient bulk phenomena (e.g. bubble dynamics in fluidised beds)—though some indirect and/or statistical information regarding such processes can still be obtained (Windows-Yule et al., 2022b).

In terms of PEPT's advantages, as noted above, it facilitates the extraction of both Lagrangian and Eulerian data, providing a depth of information that can be extremely valuable for the rigorous calibration and validation of numerical models, as forms the focus of this section. It also offers the highest spatial resolution of all techniques discussed which can be crucial, for example, when investigating the mixing of micron-scale particles in the pharmaceutical industry.

### 4.3 Radioactive particle tracking

The fundamental approach of radioactive particle tracking (RPT)[7] is not dissimilar to that of PEPT, in that a single[8] radioactively-labelled tracer particle is followed through a given system of interest, and the time-averaged dynamics thereof are used to provide three-dimensional Eulerian information. Unlike PEPT, however, RPT does not require the use of positron-emitting tracers (though such tracers can be used for RPT if desired), but can feasibly be applied using any gamma-emitting radioisotope. Rather than finding the intersection of multiple LoRs produced by back-to-back gamma rays, in RPT the location of the tracer is determined by measuring the relative intensity of the radiation emitted by the tracer across a series of detectors placed around the system. In an entirely homogeneous system, the intensity received by a given detector will be proportional to the square of its distance from the tracer. As such, with multiple such detectors placed strategically around the system of interest, one could hypothetically determine the position of the tracer through triangulation. In reality, however, since the vast majority of particulate systems are heterogeneous to some degree, correction factors must be applied to account for the differing degrees of attenuation experienced by gamma rays taking different paths through the system. For this reason, unlike PEPT, RPT must be specifically calibrated for each new system and set of materials to which it is applied (Roy et al., 2002). The fact that local densities (and thus their ability to attenuate gamma rays) may, in many systems, undergo non-negligible fluctuations means that RPT measurements are typically subject to a larger degree of uncertainty than PEPT measurements, and thus correspondingly offer lower temporal resolution.

Like PEPT, RPT has been applied to a diverse range of

[7] RPT is also commonly referred to as *computer aided* radioactive particle tracking (CARPT). The two terms can, at least in the context of the present work, be used interchangeably.

[8] As with PEPT, RPT may also be conducted using multiple such tracers (Rasouli et al., 2015), but for the sake of simplicity in the present explanation of the technique we will only consider the case of a single tracer.

industry-relevant systems and applications including fluidised beds (Fraguío et al., 2007), packed beds (Chen et al., 2001), stirred tanks (Rammohan et al., 2001), bubble columns (Devanathan et al., 1990), and rotating drums (Rasouli et al., 2016). The advantages and disadvantages of RPT compared to ECT are also largely similar to those of PEPT, and as such will not be repeated here. Of greater interest in the current section are RPT's strengths and weaknesses compared to PEPT. One of the most notable differences between PEPT and RPT—as indeed has been explicitly noted by one of the most prominent practitioners of the RPT technique (Roy et al., 2002)—PEPT can in many ways be considered an 'off-the-shelf' or 'plug-and-play' technique, whereas for RPT "*a laborious trial and error experimental procedure has to be undergone before a good experimental run can be implemented*" (Roy et al., 2002). As alluded to above, the assumptions required for the calibration of RPT systems also mean that the spatial resolution achievable with this technique is typically lower than that achievable with PEPT—though sub-millimetre accuracy is still possible to achieve under suitable conditions.

In the context of industrial imaging, however, RPT does offer one significant advantage: PEPT's requirement for the use of back-to-back gamma rays produced by positron-electron annihilation events inherently fixes the energy of usable gamma rays at 511 keV. As RPT is free of such restrictions, radioisotopes producing higher energy gamma rays may be used, thus—due to their increased characteristic penetration lengths—allowing the imaging of larger systems.

### 4.4 Summary

**Table 1** provides a brief summary of the relative strengths and weaknesses of the techniques discussed in the previous sections. Though perhaps the weakest of the three in terms of its actual imaging capabilities, considering the reduced red tape, lower costs, and fewer health and safety concerns associated with electrical tomography techniques, it is perhaps unsurprising that, in the general context of commercial, industrial imaging, it remains by far the most popular technique. However, in the specific context of the calibration and validation of numerical models, it can be argued that the depth of data which can be extracted from PEPT and RPT (and the precision of said data) makes them more suitable choices: the calibration and validation of simulation models can (and, in the authors' view, should) be seen as a numerical optimisation problem, with a number of free parameters equal to the number of tunable variables in the simulation (Windows-Yule and Neveu, 2022). Even a simple, single-phase, one material simulation has in excess of 10 such free parameters, and a simulation involving a fluid phase and/or multiple distinct materials many more still. If we wish to provide closures for each of these parameters, then a greater range of data (as is available from the aforementioned particle tracking methods) is required.

**Table 1** Summary of the comparative strengths and weaknesses of electrical tomography (EXT), positron emission particle tracking (PEPT) and radioactive particle tracking (RPT) techniques.

| | EXT | PEPT | RPT |
|---|---|---|---|
| Spatial resolution | × | ✓ | ✓ |
| Capable of imaging large systems | ✓ | ✓ | ✓✓ |
| Cost | ✓ | × | × |
| Eulerian information | ✓ | ✓ | ✓ |
| Lagrangian information | × | ✓ | ✓ |
| Transient information | ✓ | × | × |
| Plug-and-play | × | ✓ | × |
| Non-ionising radiation | ✓ | × | × |

In the 'factory of the future', then, one might imagine that there exists an important role for both electrical tomography *and* particle tracking methods, the latter being used more occasionally for the development of new models (i.e. digital twins of process equipment), and the former for regular, day-to-day process monitoring, and informing the models created.

## 5. Summary and conclusion

In this review, we have provided an overview of several leading techniques for the numerical modelling of industrial-scale particulate and particle-fluid systems, as well as the experimental imaging techniques which may be used for the validation thereof. In both cases, it is evident that, with currently available technologies, there does not exist 'one technique to rule them all'; rather, different techniques are more suitable for different systems and situations, with clear tradeoffs to be considered. In terms of simulation models, the trade-off is typically between accuracy, ease of calibration/implementation, and computational cost. In terms of experimental imaging, the tradeoff is typically between accuracy, ease of calibration/implementation, and financial cost.

In keeping with the title of the review, it is perhaps of value to end by providing a brief summary of the main challenges associated with the methods discussed, and the potential solutions thereto. The main challenges can be broadly distilled down as follows:

(i) The use of fully resolved DEM can provide quantitatively accurate numerical models of experimental systems, created with relatively few simplifying assumptions, but even with state-of-the-art hardware and parallelisation techniques, is currently limited to the simulation of billions of particles, whereas industrial systems may contain trillions or even

quadrillions.

(ii) Coarse-grained DEM models can seemingly facilitate the meaningful simulation of systems containing arbitrarily large numbers of particles, but there is at present no consensus on the mapping of individual particle properties to meso-particle properties.

(iii) Mapping-based extrapolation methods also allow further acceleration of DEM simulations, but unlike CG methods remain fully resolved, thus allowing direct calibration; however, these methods are unsuitable for transient processes, and may not be viable for dilute systems.

(iv) Simulations based on the kinetic theory of granular flow are potentially (though not necessarily) capable of increasing simulation speed further still, but introduce still more extreme simplifying assumptions than CG, most notably by treating discrete systems as continuous.

(v) Experimental methods such as electrical tomography, radioactive particle tracking and positron emission particle tracking are capable of imaging industrial-scale systems, and thus providing validation data for numerical simulations, yet those techniques which offer greatest accuracy often involve the highest financial costs and most red tape, and vice versa.

In terms of a solution, the most effective route—and one increasingly being adopted by researchers—is not to use any one method in isolation, but to take a 'multi-scale' or 'bootstrapping' approach involving several (if not all) of the above-described methodologies. For example, one may begin by considering the largest (e.g. pilot scale) model of the system of interest that can both a) be simulated using fully resolved (CFD-)DEM, and b) be imaged with a desired imaging method (the ultimate size of the system being determined by whichever of a) and b) is the limiting factor). Once fully calibrated and validated against suitable experimental data, this resolved model may be used either to develop suitable closure relations for a KTGF/TFM model, or to determine suitable coarse-grained DEM properties. Since the models developed should be dependent only on the materials involved, one may reasonably expect—if they have been suitably rigorously calibrated—that they may then be used to efficiently model larger-scale systems[9]. Though convoluted, this process—as evidenced by the literature discussed in the preceding sections—provides a viable route to the accurate simulation of industrial-scale systems.

[9] The results of these full-scale simulations may then be pseudo-validated using more crude methods applicable to larger systems than may be imaged using EXT, PEPT or RPT (e.g. measurements of pressure fluctuations for a bubbling fluidised bed, or torque measurements for a bladed mixer).

## Supplementary Information

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**Dr. Sofiane Benyahia** currently works as a research engineer at the National Energy Technology Laboratory in Albany, Oregon. Dr. Benyahia has more than 20 years' experience conducting computational fluid dynamics (CFD) simulations of multiphase flows resulting in more than 40 peer-reviewed publications. He focuses on developing computationally efficient and physically accurate numerical tools to better understand, predict, and troubleshoot fluidized bed systems at the heart of most energy and chemical industries. Dr. Benyahia earned a bachelor's in chemical engineering from Polytechnic School in Algiers (Algeria) and a doctorate in chemical engineering from Illinois Institute of Technology in Chicago.

**Dr. Peter Toson** studied computer science and physics and received his PhD from the Vienna University of Technology in 2015. From 2016 to 2023, he worked at the Research Center Pharmaceutical Engineering in Graz as a principal scientist. His research focused on the discrete element method, modeling the flow of cohesive powders in pharmaceutical production equipment, especially the unit operations present in continuous direct compression.

**Dr. Hanqiao Che** holds a PhD from the Institute of Engineering Thermophysics, Chinese Academy of Sciences (2018). He was a Research Fellow at the University of Birmingham, specializing in multi-phase flow mechanics, particularly experimental measurement and numerical simulation of gas-solid fluidization. He has co-authored 16+ peer-reviewed papers in renowned journals.

**Dr. Andrei Leonard Nicusan** is a researcher at the University of Birmingham focusing on data-driven engineering across scales. He published featured articles and Scientific Highlights on machine learning-based positron emission particle tracking algorithms. His work on evolutionary algorithms for simulation calibration, optimisation and physics discovery has raised more than £260,000 from research and industrial funding bodies. His frameworks are actively being used in projects with Johnson Matthey, GranuTools, Jacobs Douwe Egberts and Unilever.