Particle models in civil and environmental engineering

Report

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Particle Models in Civil and Environmental Engineering

We have built our world around phenomenological observations in our macro world. Today we can simulate most of these phenomena with many particle processes on much finer scales. Particle models allow a simplistic, yet fascinating glimpse into the mechanisms of the meso-, micro- or even nano worlds, and explain complex phenomena occurring in civil engineering materials.

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Over the last century continuum mechanics made a triumphal parade through basically all engineering disciplines, mainly due to its transformability into processible schemes and implementation on fast micro-processors. Unfortunately, many engineering problems are too complex for continuum descriptions. In this article we intend showing how this complexity emerges from models that consist of simple, dynamically interacting particles, and the multitude of important phenomena that can be understood by particle models. First, we describe the building blocks behind such models, before we demonstrate on several civil and environmental engineering examples how particle model simulations enable us to understand them.

Particles and Interactions

The elemental particles can be – like the problem itself – defined in one, two or three dimensions and can basically be of arbitrary shape. Restrictions are the computational cost, in particular for contact force calculations.

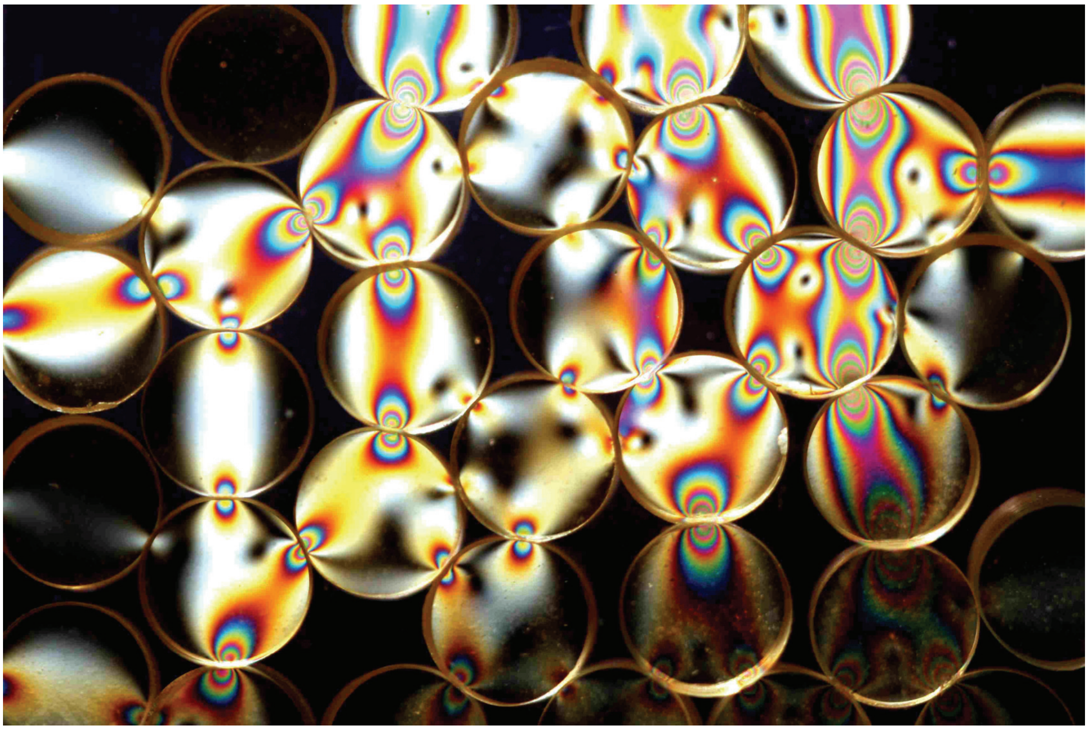

Figure 1: Force chains in a vertically loaded random packing of photo elastic discs. (FKW, HJH)

For many problems, the simplest particle shapes, like discs, spheres or polygons are the best choice. If necessary, these can be agglomerated by kinematical coupling to form more complex shapes. The way particles are allowed to interact is the key point when simulating with particle models. On the one hand, frictional contacts of colliding particles have to be defined. This is important particularly when granular materials are modelled. Additionally, particles can interact, for instance with their surrounding matter, if interaction with an embedding fluid is of interest. If cohesive frictional materials are addressed, additional cohesive elements like springs, beams or any other structural element can be employed that are attached to particle boundaries or the centre of mass. Before respective examples are shown, we need to look at different solving strategies. The simplest way is the static analysis, when equilibrium states are calculated. Dynamic processes, however, call for dynamic time stepping schemes when either Newton equations of motion are solved iteratively or collision event driven strategies are employed. With these tools at hand, we can model different classes of problems like the dynamics of granular materials, fracture and fragmentation of cohesive frictional materials or stability problems like the packing of particle chains or structural collapse of concrete structures.

From Granular Matter to Complex Fluids

Granulates are ubiquitous in all engineering disciplines. They are basically conglomerations of discrete, solid particles. Their mechanical behaviour defies continuum mechanical descriptions, since single particle interactions form force chains and networks that span the entire assembly as illustrated in Fig. 1. Particle models contribute to the understanding of granular matter by using modern tools from statistical mechanics and powerful computers. Depending on particle size, property and the surrounding medium, a multitude of different important problems can be addressed. Here we only exemplify three problems, namely collapsing suspensions, particles with fluid interactions and charged particles.

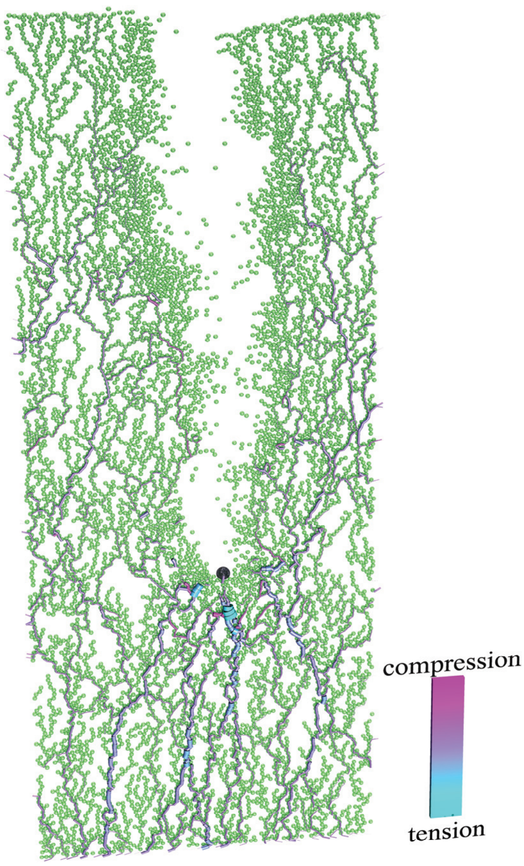

Figure 2: Collapsing particle suspension due to a falling intruder. Force chains are displayed by their magnitude (thickness and colour). (D. Kadau, HJH)

Inspired by quicksand, a substance that is shrouded in mystery by adventure books and legends, we create a particle model for collapsing suspensions or soils. It has been repeatedly argued that since the density of sludge is typically larger than that of water, a person cannot fully submerge and therefore cannot be really "swallowed up" by any quicksand. We study this using a 2D particle model with contact dynamics. The starting point is a suspended structure generated by ballistic deposition of cohesive discs. In the next step, an intruder is dropped into the suspension, leading to partial destruction of the structure along its trajectory. By using this approach, we capture the microscopic description of the essential physical processes underlying the dynamics of collapse of the system that exhibits the behaviour of a complex fluid. The direct comparison of the model with natural quicksand gives identical shear strength both in the unperturbed and collapsed states. Interestingly, our intruder can be trapped by the collapsing suspension that deposits on top, even though its density is smaller than that of the sludge.

The example for suspended soil did not consider fluid-particle interaction. In contrast, a model for fluid flow through layers of densely packed grains cannot neglect fluid-particle interactions. Such systems are characterized by a strong hydrodynamic interaction between the grains and the ambient fluid. To further complicate matters, we introduce two fluids: a liquid and a gaseous one that is separated by a liquid-gas interface which has a strong impact on the dynamics of the system. Our system consists of three phases: solid grains, water and air. The simulations start with a densely packed layer of grains completely submerged in water. Pressurized air is then injected at a fixed position leading to a growing air bubble. The bubble grows by displacing both the liquid and the grains (see Fig. 3). Liquid is pushed back into the capillary pores defined by the neighbouring grains. Since grains move, capillary pores continuously rearrange. The air first invades the largest pores. Since the grains also move, these invaded pores open even more due to the forces exerted by the advancing air.

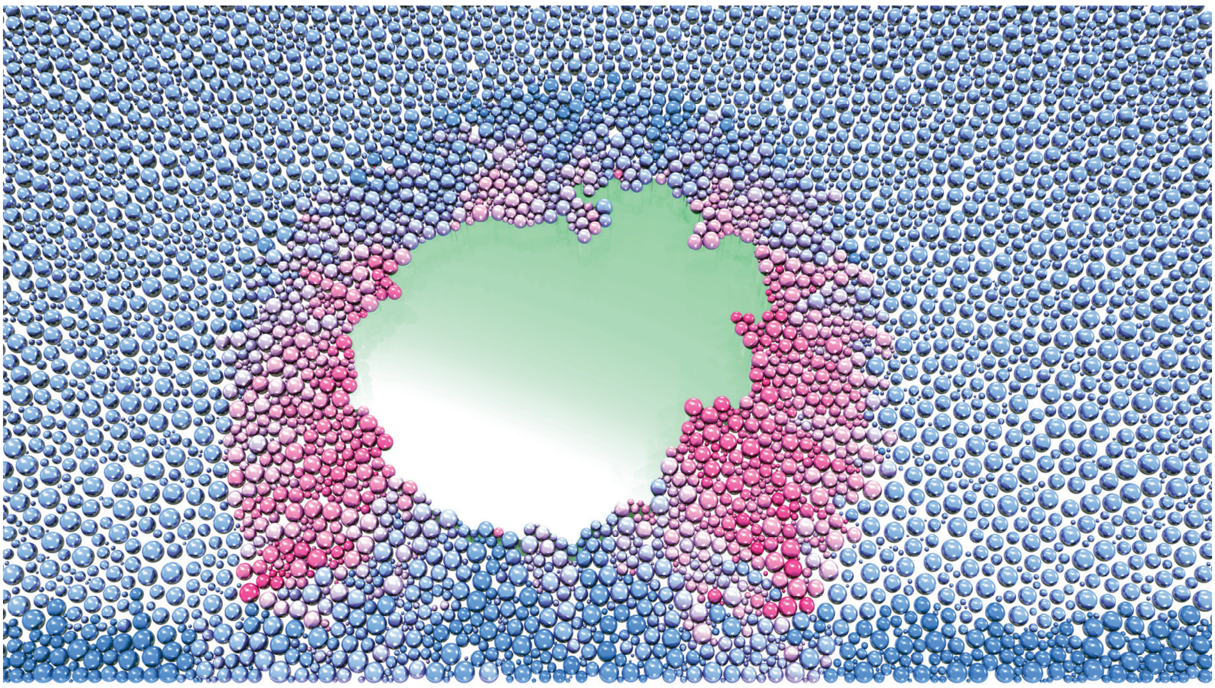

Figure 3: Interaction of a particle packing with an expanding gas bubble. Colours represent velocity magnitudes. (J.L. Vinningland, HJH)

Up to now, particle collisions had no consequences for the properties of particles. Imagine if each collision goes along with contact electrification, building up significant charges on the individual grains (see Fig. 4). In nature, this happens during desert sand storms that produce sparks and noticeable radio interference. The same is known for charged particle clouds that regularly lead to devastating dust explosions, e.g., in coal or grain plants.

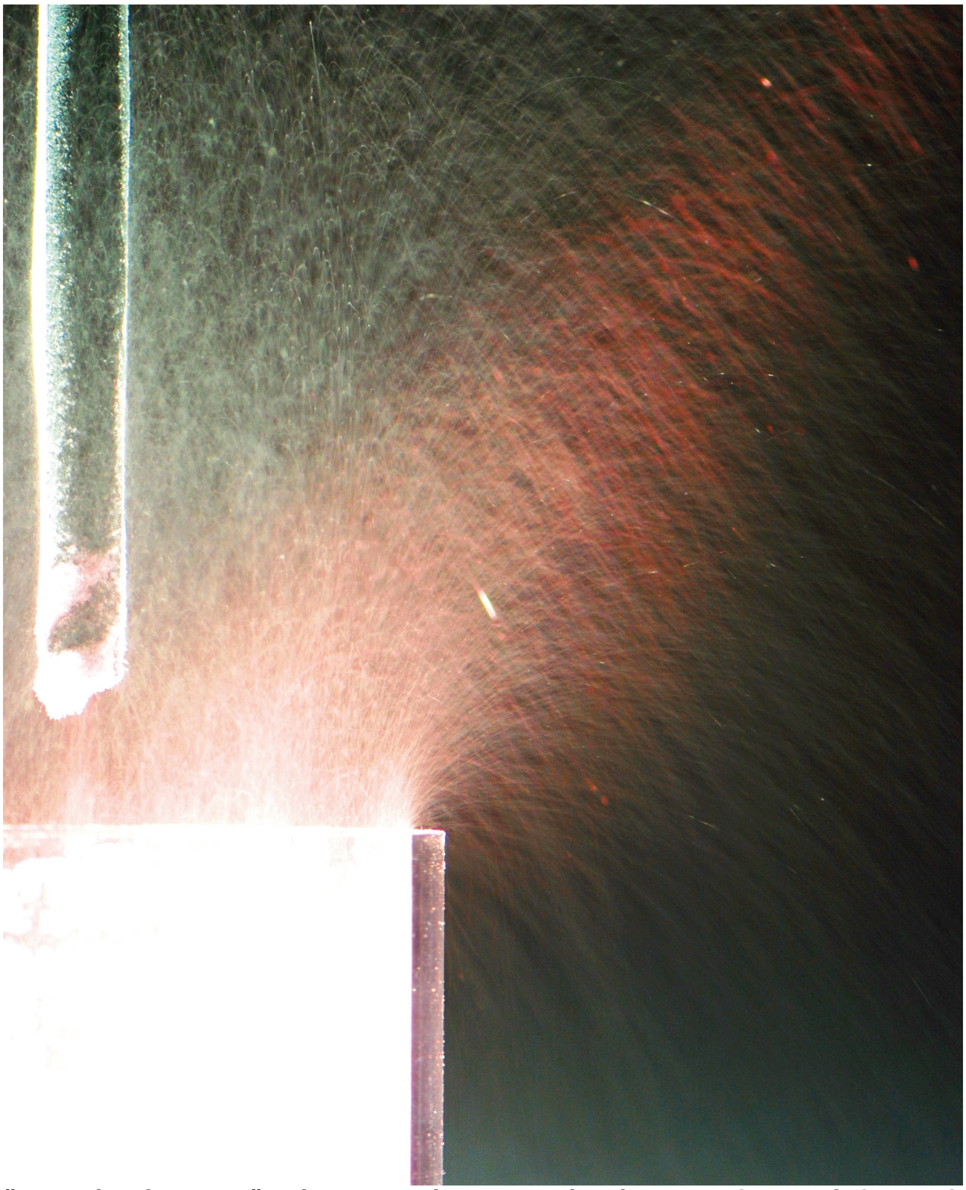

Figure 4: "Granular fountain". Glass particles are violently ejected out of the jar by electrostatic forces after they were charged only by pouring them through an acrylic tube. (FKW, HJH, T. Shinbrot)

Little is known about charged granular gas and even the nature of the electrostatic charging itself is still a puzzling phenomenon. However, particle models are top candidates to comprehend the dynamics of these complicated processes, including long-range interactions for attraction and repulsion of charges, and charge transfer when particles collide.

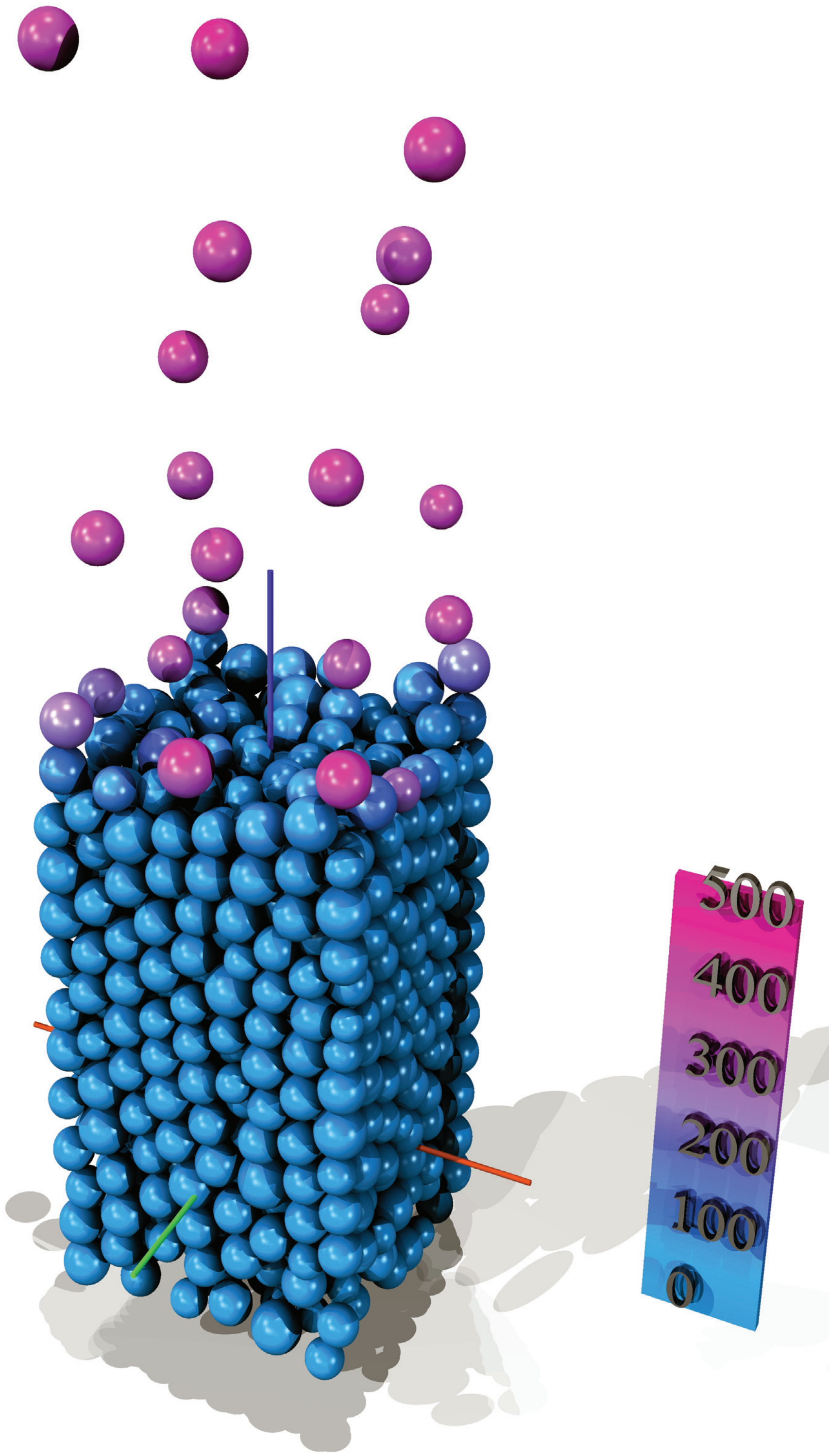

Figure 5: Snapshot of the simulation for electrostatic charged particles due to contact electrification when particles collide. Colours represent charge in meV. (T. Pähtz, HJH, T. Shinbrot)

We model this by a set of self-driven particles inside a box that produce a charge each time they collide. As time goes by, a charge profile builds up with particles on the top that are even levitated (see Fig. 5). Certainly particles with opposing charge attract each other. A small cohesive force is also used for contacting particles in the collapsing soil model. However, to create models for cohesive solids, additional cohesive elements need to be incorporated.

From Fracture to Fragmentation

Strong cohesive forces are responsible to maintain the integrity of engineering materials. In particle models, this is achieved by connecting the particles by combinations of elements of arbitrary rheological behaviour like linear or non-linear springs, beams, or dashpots, just to name but a few. The simulations basically all follow the scheme that first a material section is assembled by particles and cohesive elements. When the system is loaded, consecutively cohesive elements are weakened or removed as a reaction to a mechanical or thermal load that exceeds the element's failure criteria. The secret of the success of this model approach lies in the local dynamic interaction of particles that can reproduce the complex behaviour that emanates from failure processes on small length scales inside the material. This is exemplified by studies on three different types of fracture, namely creep fracture of asphalt, dynamic crack propagation inside a brittle, disordered material, and a full three dimensional simulation of impact comminution.

Asphalt fails in a very peculiar way, especially in fatigue damage. This is due to microcracks that not only form, but also completely heal when crack surfaces contact again during mechanical or thermal load cycles. The competition between microscopic damage accumulation and the healing of defects basically determines the lifetime of a costly highway construction. In our simulations, we allow cohesive elements to accumulate damage and, if compressed again, to heal completely. If an element is damaged, part of its load is dynamically redistributed to its neighbours. If they cannot bear the additional load, damage grows (see Fig. 6). By this approach, the detailed process of damage, fracture and failure of the solid is revealed, providing excellent agreement with experiments and, more importantly, open access for material design of specific asphalt mixtures.

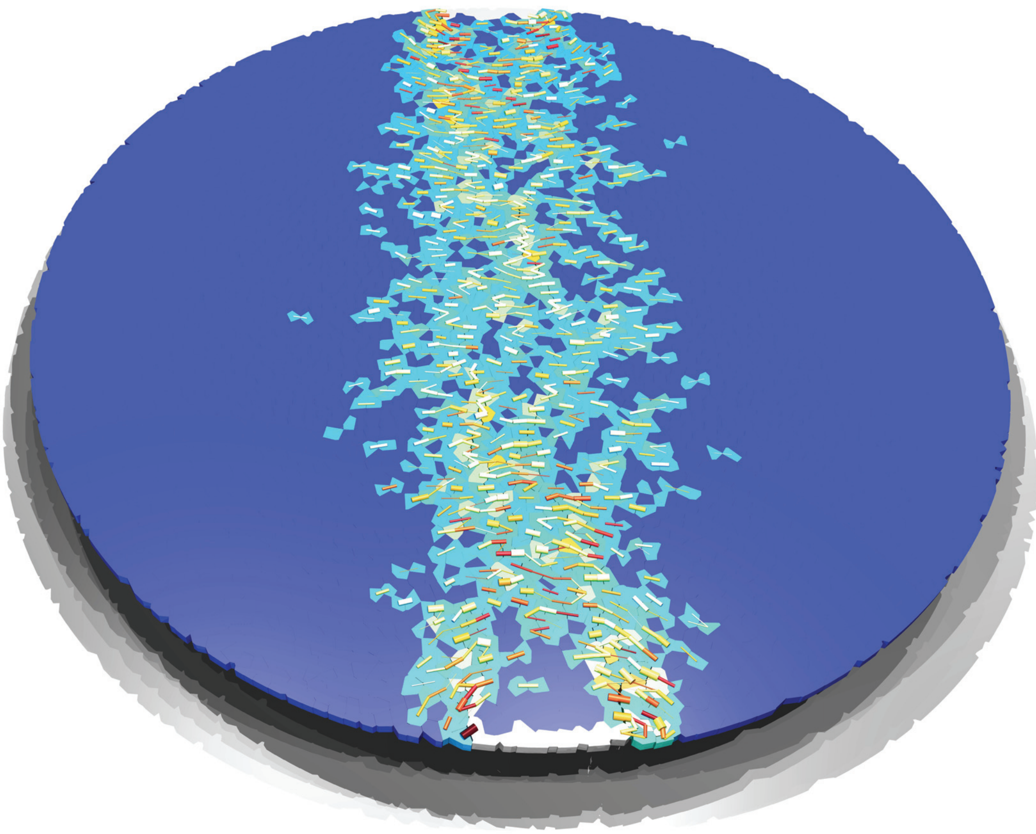

Figure 6: Snapshot of a Brazilian test. Polygon colours represent the spatial damage level, while beam colours represent the breaking times. (H. Carmona, F. Kun, HJH)

Due to the dynamic nature of the particle interactions, such models are powerful tools in the study of dynamic fracture processes. These incorporate the interaction of the stress release wave due to post-critical crack growth with the stress field in front of the crack leading to crack tip instabilities. The resulting crack branching has strong influence on the further crack propagation speed, crack roughness and the energy release rate. We apply simulations to study the interplay of the material heterogeneity with the branching instability and resulting crack surfaces (see Fig. 7). For computational reasons, particle contacts are neglected and only the part of the system is solved that contains the crack tip with a sufficiently large environment.

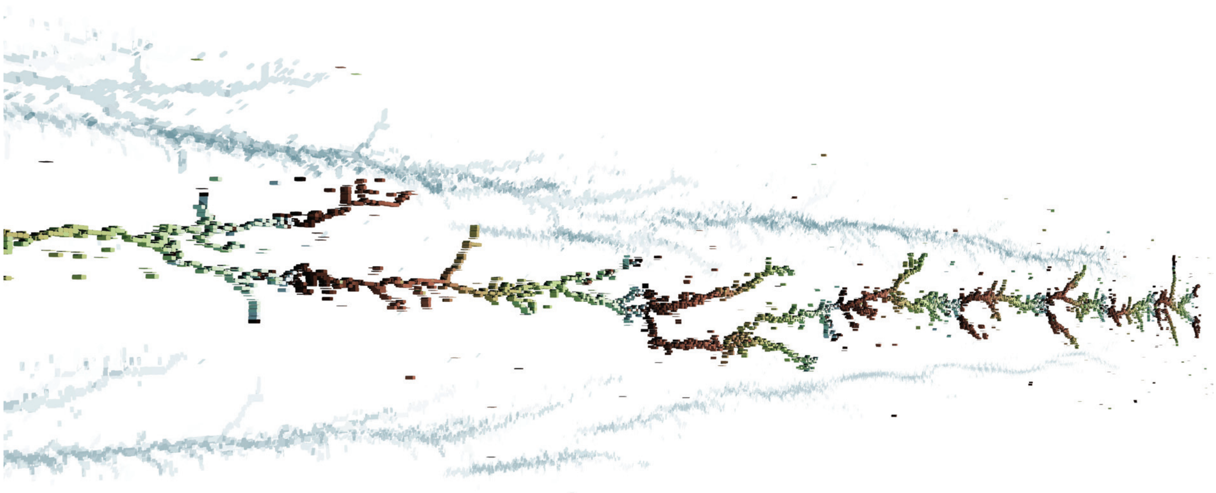

Figure 7: Dynamic mode I fracture with severe crack branching simulated via a moving lattice method. Colours represent breaking time intervals. (FKW, HJH)

Engineering materials are often particle compound materials or agglomerates of finer aggregates. To break up the agglomerates for re-use or to produce finer powders, they are, for example, impacted on a target.

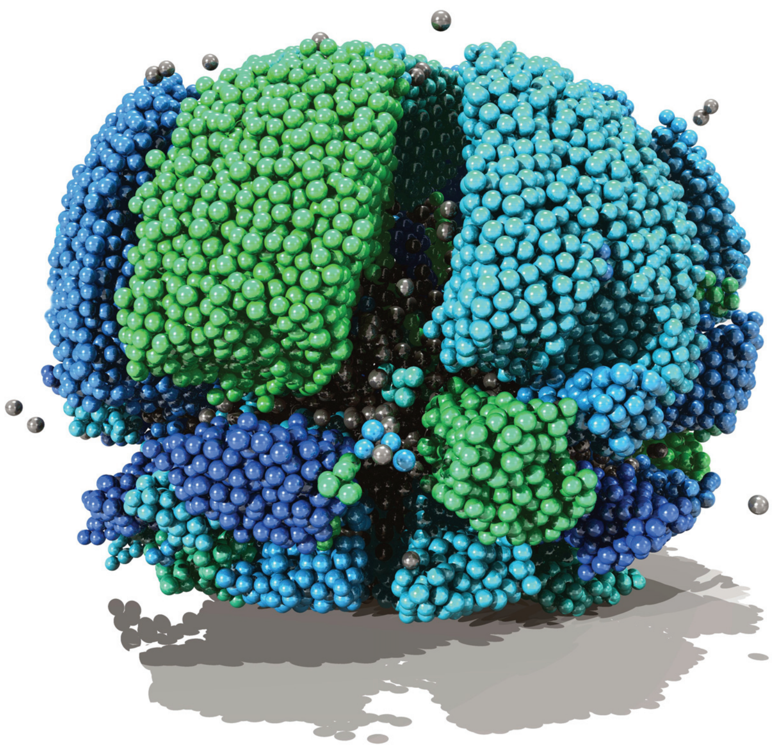

Figure 8: Impact fragmentation of a bulk sphere vertically impacting a hard ground. Particles are coloured according to the fragment they belong to. (H. Carmona, FKW, HJH)

Particle models with cohesive beam-truss elements are ideal for studying the impact fragmentation. With such models the simulation of the fracture and fragmentation processes that take place simultaneously during a very small time interval can be captured. Various fragmentation mechanisms, their origin, evolution and interaction during the process can be studied in detail. It was found that damage initiates and grows from the inside to the outside with a quasi-periodic angular distribution. The final shape of the experimentally observed large wedge-shaped fragments could be reproduced and explained. If more energy is accessible, these pieces further fragment (see Fig. 8). Simulation models for fragmentation are the future means for optimizing milling processes with respect to certain size distributions, minimal powder production and minimal energy input for various material systems.

From Stability to Collapse

The formation or demolition of structures can be the result of series of global and local instabilities due to multiple buckling and body contacts. When structures are formed, we talk about their morphogenesis, while their demolition is a progressive collapse. Both processes are of a dynamic nature and need to incorporate simultaneous multi-body contacts, both of which are essential parts of particle model simulations. We give two examples, one for the morphogenesis of a growing chain of particles in a constrained 2D space and one for a progressive collapse of a slab floor construction.

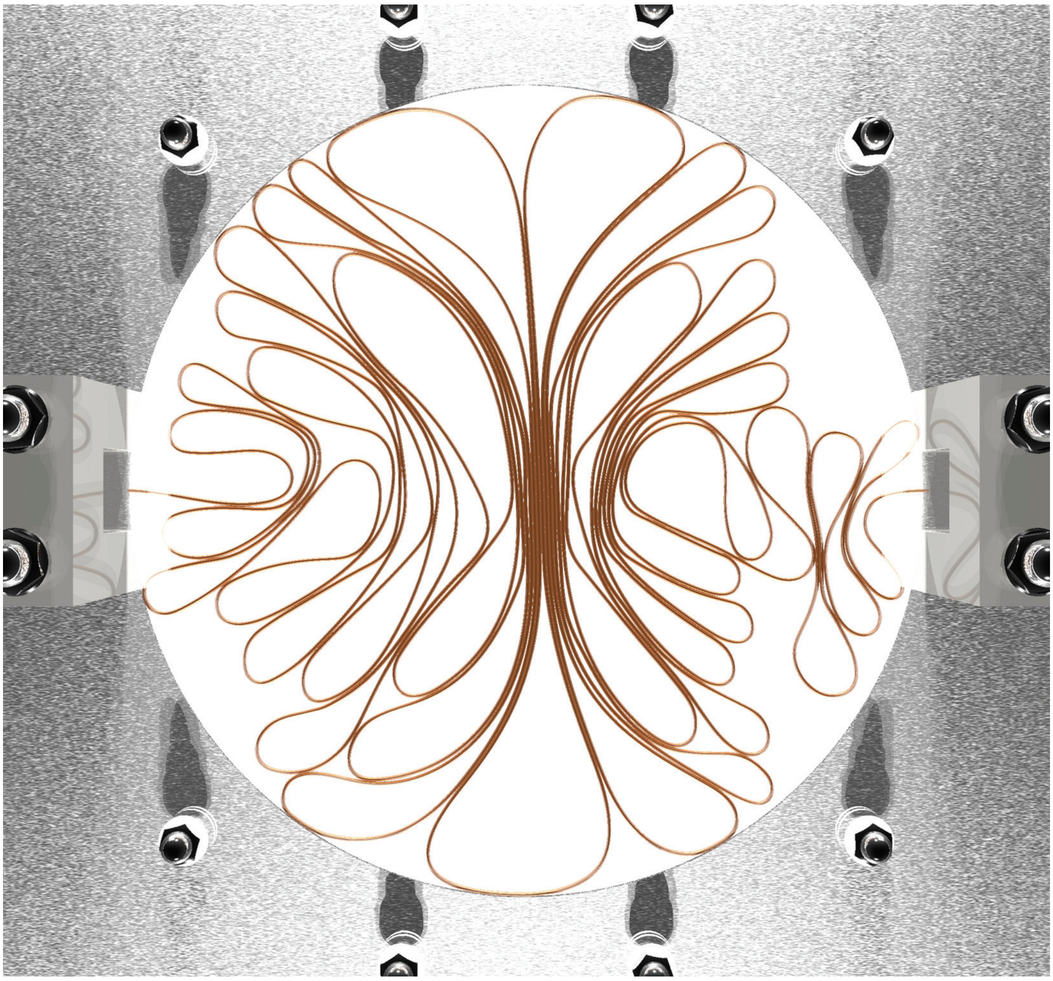

Figure 9: Simulation of the final morphology of an elastic-plastic particle chain pushed into a circular cavity. (N. Stoop, FKW, HJH)

We simulate the pushing of a chain of particles connected by elastic-plastic beams into a circular cavity from opposing sides. The particle chain is set to behave like a metal wire of certain thickness. When we push, the wire buckles and forms loop until the cavity is filled with stabilizing loops, making it almost impossible to inject more wire (see Fig. 9). Therefore, the system is self-stabilizing. By studying this simple system, we were able to construct a phase diagram for characteristic morphologies in the plasticity-wire-friction space. We found excellent agreement with experiments on various metal wires ranging from scaling relations for packing densities and loop formation to the structural stiffness.

In a further example, we allow elements to fail again. Starting from the regular geometry of a simplified slab floor construction, we add gravity and remove parts of a column. Element properties are chosen to represent concrete with steel reinforcement.

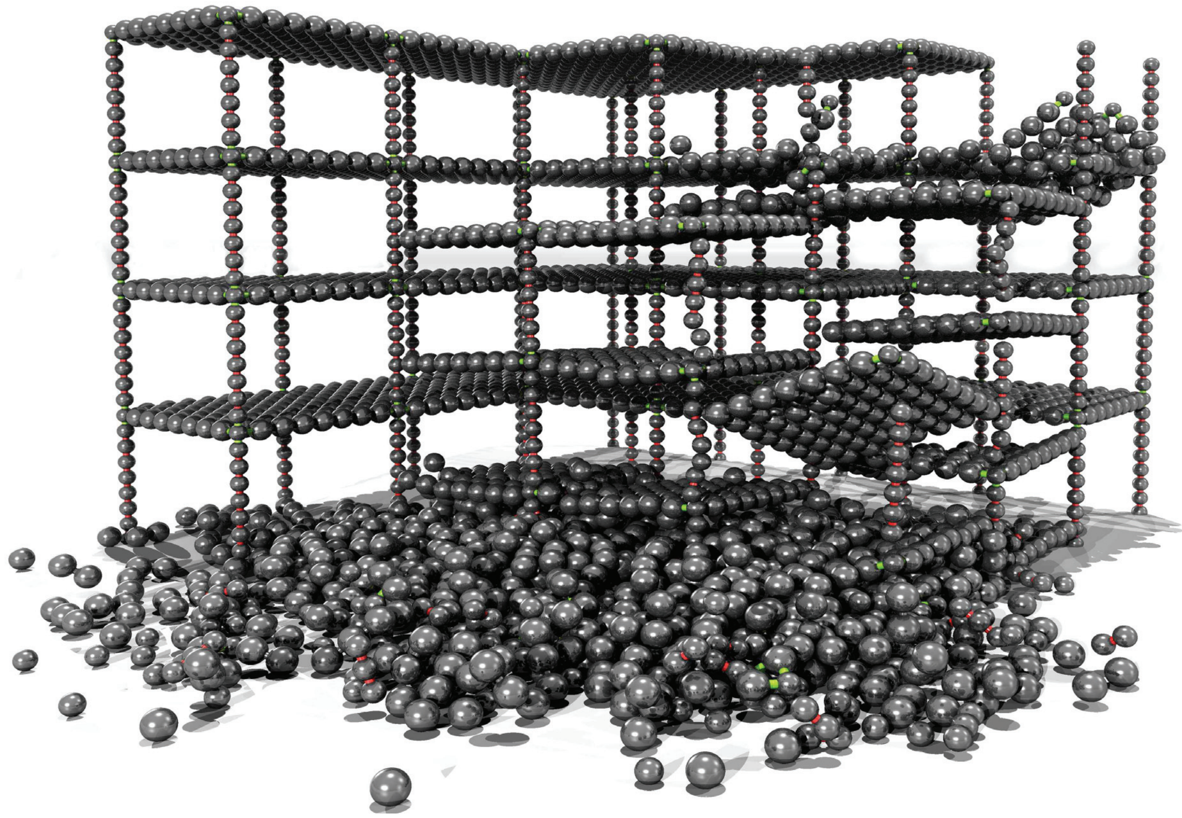

Figure 10: Snapshot of the progressive collapse of a simplified slab floor construction. (E. Masoero, FKW, HJH)

Large displacements, local ruptures and momentum transmissions due to contacts between structural elements are naturally considered by the simulation procedure. Depending on a morphology parameter for possible geometrical variations, non-robust structures can collapse partially or even entirely (see Fig. 10). Progressive collapse goes along with a multitude of sequential failure mechanisms due to the impact of rubble with intact portions of the structure. Interestingly, lateral bending failure of columns due to piling rubble in the basement is observed, a mechanism that can only be captured by such a model approach.

Future Trends

Today particle models are capable of accurately describing local processes like those shown. However, the number of particles is limited by available computational resources. Fortunately, in many cases, only a small portion of particles is really needed in active zones, while the rest, for instance, are only used to represent the elastic foundation.

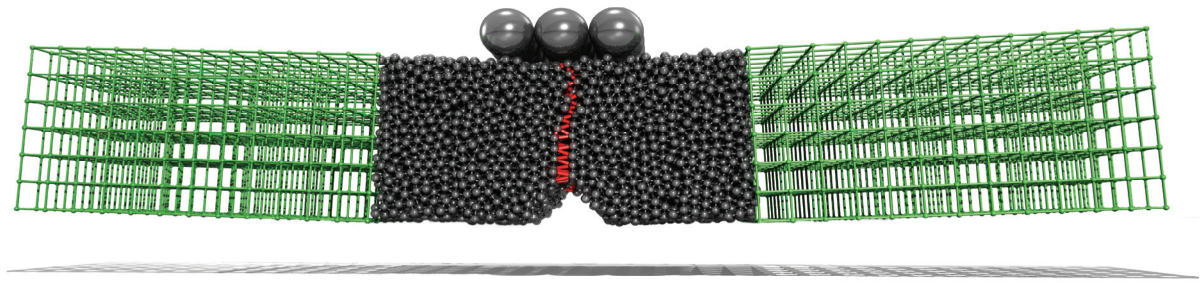

Figure 1: Hybrid FE-DE Simulation of the Charpy Test with edge-to-edge coupling. (M. Fuhr, FKW, HJH)

Hybrid methods are increasingly used to take advantage of this fact. For example, particle models can be used for the discretisation of the damage zone, while the Finite Element Method (FEM) is utilized to model the surrounding domain. Figure 11 demonstrates this technique called bridging scale or handshake method on a 3D simulation of a notched bar impact test with edge-to-edge coupling. It is our belief that hybrid methods together with advanced homogenization schemes will be the right track for particle models on the way from research-driven studies to become a valuable numerical technique of broad applicability in engineering.