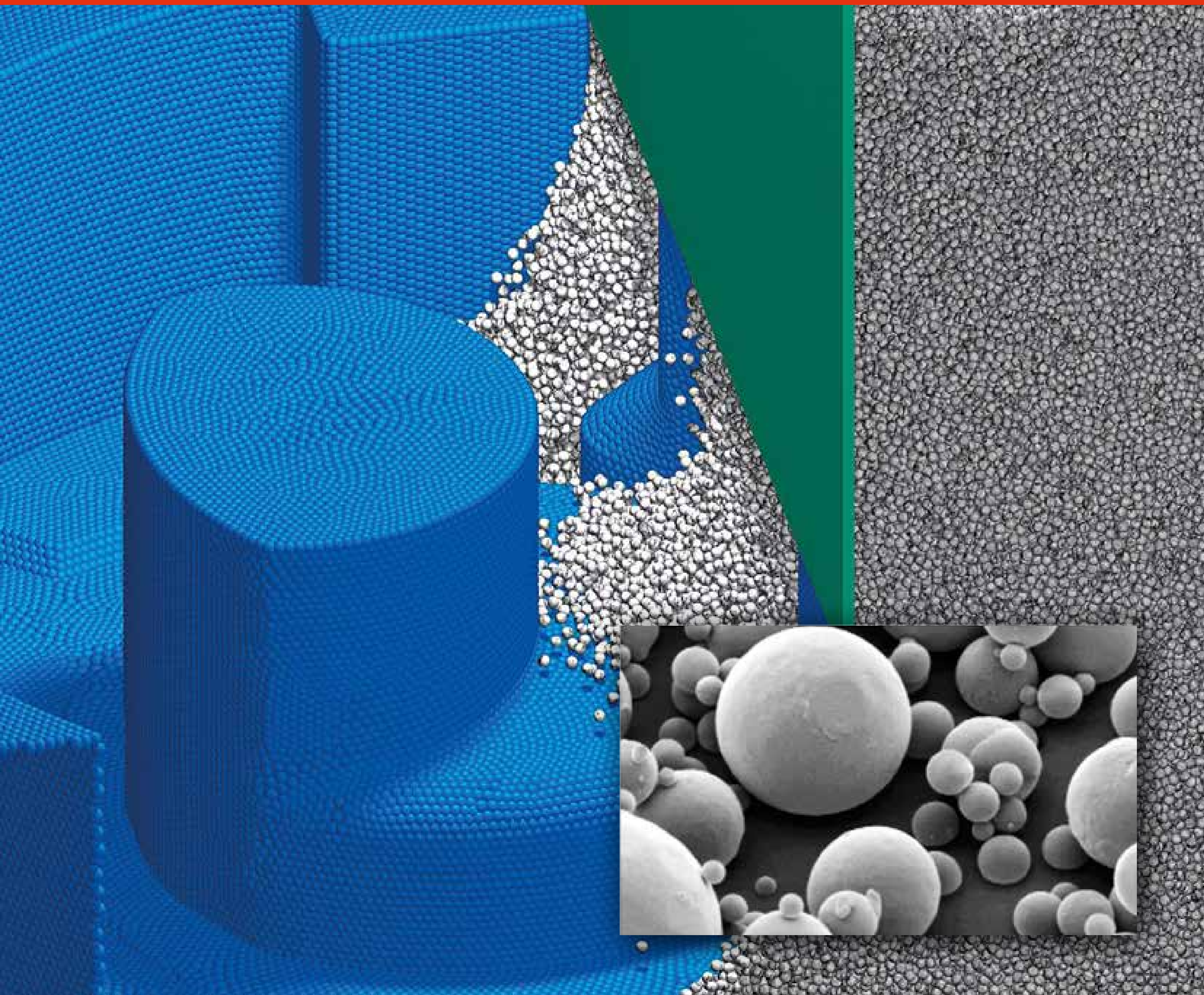
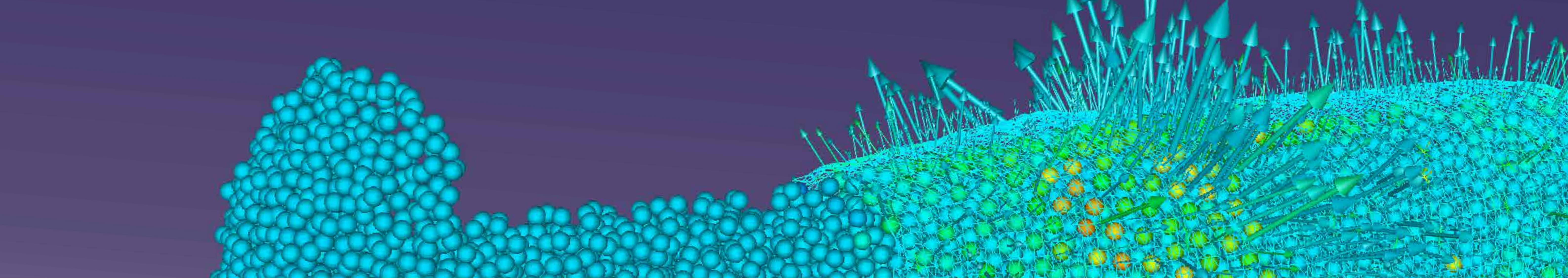
PARTICLE-BASED SIMULATION AND CO-SIMULATION FOR GRANULAR MATERIALS AND COMPLEX APPLICATIONS





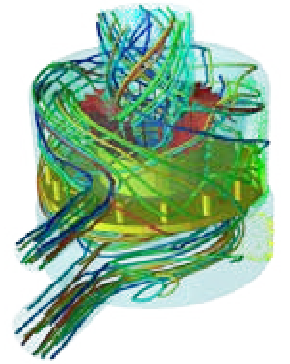
GRANULAR MATERIALS, COMPLEX FLUIDS AND PROCESS SIMULATION

The transport and processing of solid particles is fundamental to process engineering. Sample applications include grinding, classification, filtration, and the deposition of granular products.

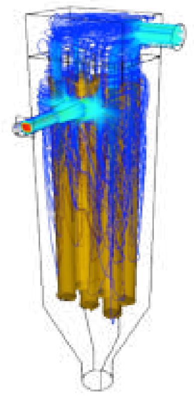
In the case of multi-phase flows with low concentrations of solids, granular matter is carried by a surrounding fluid. The interactions within the individual phases are often negligible. At higher particle concentrations, e.g. in the case of sedimentation in fluidized beds or in the transportation of slurry, inter-particle collisions exert increasing influence on the behavior of individual phases.

At very high concentrations of solids, the numerous interactions between the individual particles dominate the entire motion. This is the case with compaction of powders, moving soil and bulk material or contact between tires and soil. The fluid is then driven by the motion of particles rather than by any pressure drop. The presence of a fluid is virtually negligible.

The modeling and numerical solution of problems dominated by particle-particle interaction is a specialty of Fraunhofer IWM and Fraunhofer SCAI. The SimPARTIX® software, developed by Fraunhofer IWM, performs discrete element method (DEM)-based simulations of the motion of individual grains and their interaction due to impacts, friction, or cohesion. The basic discrete elements used in SimPARTIX® are spheres; more complex particle shapes can be approximated by rigid or elastic clusters thereof. SimPARTIX® can also simulate fluid motion through application of the smoothed particle hydrodynamics (SPH) method.



1 *Multiphase flow inside an air classifier mill.*



2 *Multiphase flow inside a baghouse.*

3 *Cast slurry with non-spherical solid particles.*

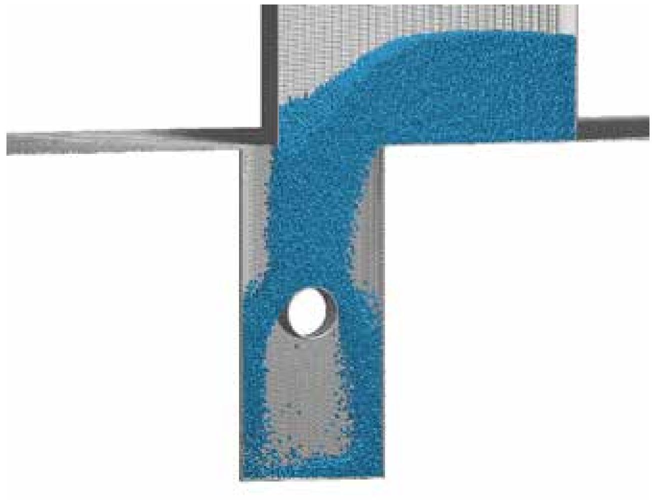
A FRAMEWORK FOR CO-SIMULATION

The combination of SimPARTIX® and a structural-mechanics simulation, typically a finite element method (FEM) solver, is a powerful tool for the analysis of particle/structure interactions. The co-simulation framework developed by Fraunhofer SCAI allows such codes to inter-operate seamlessly and efficiently.

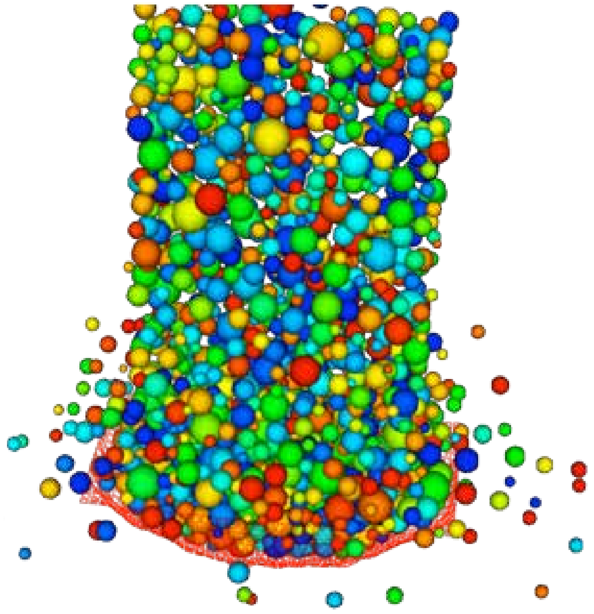
One compelling application for co-simulation is found in the modeling of contact between a granular material and a soft body. Here, the two simulations are coupled at the interface separating the granular material and the solid body. The structural mechanics simulation determines the displacements and velocities at the nodes of the finite elements; these are influenced by contact forces exerted on the surface. The calculated values are fed back into the simulation of the granular material, which drives further changes in the FEM model in turn.

In the co-simulation model developed by Fraunhofer SCAI, the simulation codes do not communicate directly. Instead, they pass messages through an intermediate service process, which is responsible for both the coordination of the simulations and the efficient distribution of data over the available computing resources.

A notable advantage of this architecture is the ability to execute both simulation codes concurrently, at scales ranging from a single multi-core workstation, up to a highly-parallel compute cluster.



4 *Bulk flow example.*

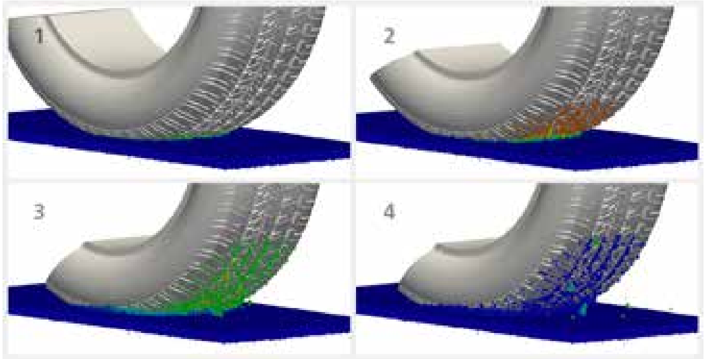


5 *Particles falling under gravity.*

DEM WITH STRUCTURES

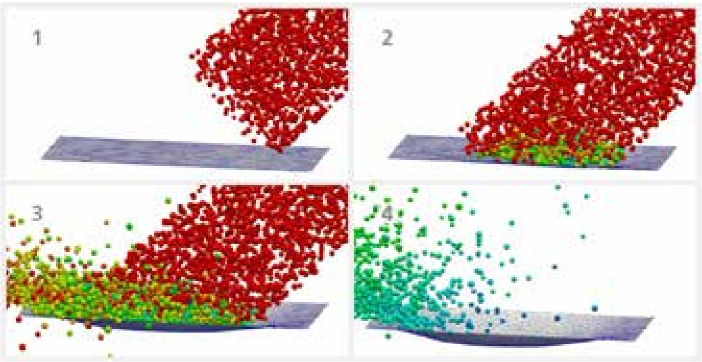
Tire traction

SimPARTIX® can be parametrized to represent various types of ground, ranging from sand through snow to mud. The diagram to the right displays a simulation of a spinning tire running over a strongly cohesive soil. The soil is represented in SimPARTIX® as a collection of approximately 300,000 distinct particles. Some of the soil can be seen to remain embedded in the treads of the tire, due to the effect of cohesion.



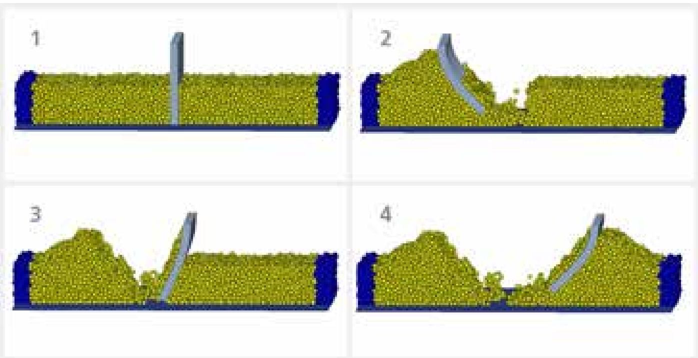
Shot peening

The simulation at right depicts a jet of DEM particles hitting a metal sheet. The sheet is modeled as a membrane using an elastic, perfect plastic material formulation. The particles are colored according to their velocity, from red (high velocity) to blue (low velocity). The deceleration of the particles can be observed upon their contact with the sheet, as can the deformation of the sheet itself.



Elastic wiper blade

The figures at right display a back-and-forth motion of an elastic wiper blade through a granular material. The top surface of the blade is path-controlled. The blue DEM particles surrounding the simulation are fixed, and define the boundaries of a box. Note the cohesive particles adhering to the blade.

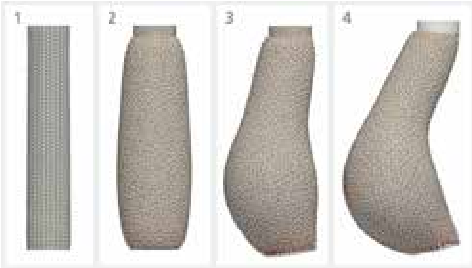


SPH WITH STRUCTURES

Classical mesh-based computational fluid dynamics (CFD) methods exhibit computational issues when large deformations of the flow domain are required, or when a topological change is required to the underlying grid. One such classical example is found when simulating the opening and closing of valves. The sudden change from an open gap to a closed one results not only in a topological change to the grid, but also in a sudden stop to any flow. The use of the SPH method instead of a mesh-based CFD approach avoids many of the restrictions seen in typical finite-volume CFD solvers.

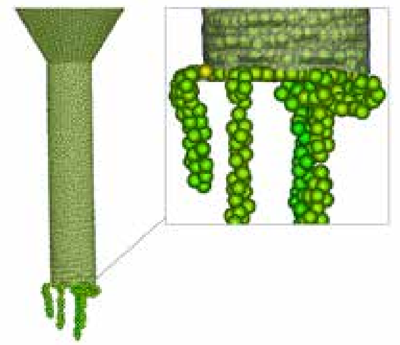
Nonlinearities and geometric changes

A fluid is forced into an impermeable hose made of a hyper-elastic material, with its lower end closed by a rigid lid. The hose first bulges and expands symmetrically due to increasing pressure, before buckling into a state of lower elastic energy.



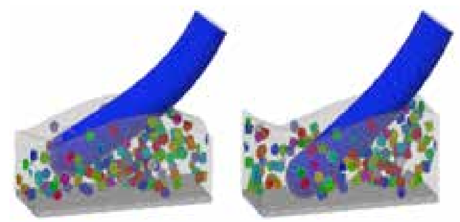
Topological changes

A fluid flows into a tubular membrane made of an impermeable elastic material. The lower end of the tube is initially closed by a rigid lid fixed in space, but unconnected to the tube. As it fills, the tube expands radially and contracts axially, opening a small gap at the lower end through which the fluid drains slowly away.



SPH, DEM, and elastic structures

The figures on the right show two elastic toothbrush bristles (blue), interacting with a toothpaste composed of abrasive particles (DEM) suspended in a fluid (SPH). The bristle on the far right is stiffer than that on the left, leading to less bending and direct contact with tooth enamel.

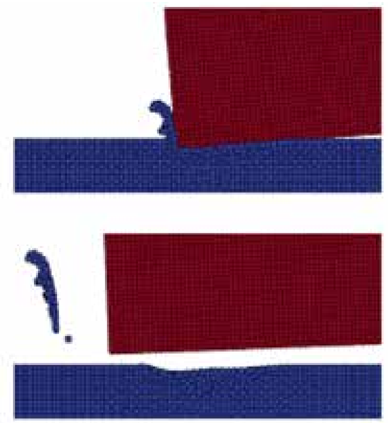


PLASTICITY AND DUCTILE MATERIAL FAILURE

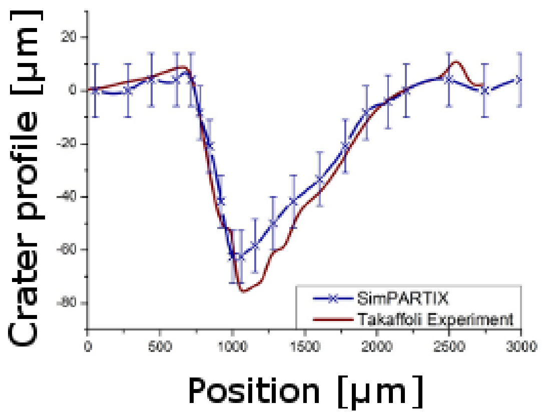
The simulation of processes involving both large deformations and high rates of strain imposes high demands on modeling tools. Reliable numerical simulations contribute significantly to a deeper understanding of material mechanics, and enable process optimization. By modeling plastic deformation and ductile fracture behavior, for example, removal rates in material processing may be predicted.

The primary advantage of a particle-based methodology is its mesh-free approach. Thus, large plastic deformations and fragmentation can be simulated in a natural way. The deformation of the whole body or a crack formation within are not influenced by the deforming of a computational mesh.

For the simulation of ductile damage processes, the generated plastic deformations as well as the failure of the material have to be reproduced in detail by the numerical model. SimPARTIX® takes plastic deformations into account by using a plasticity model for the flow limit. To model failure of the material, a criterion is used which predicts the fracture of the material during critical plastic strain under dynamic load.



1 *Simulation of a solid grain (red color), which impacts an aluminum workpiece (blue color). In this case, the workpiece is plastically deformed and a chip is separated due to ductile material failure.*



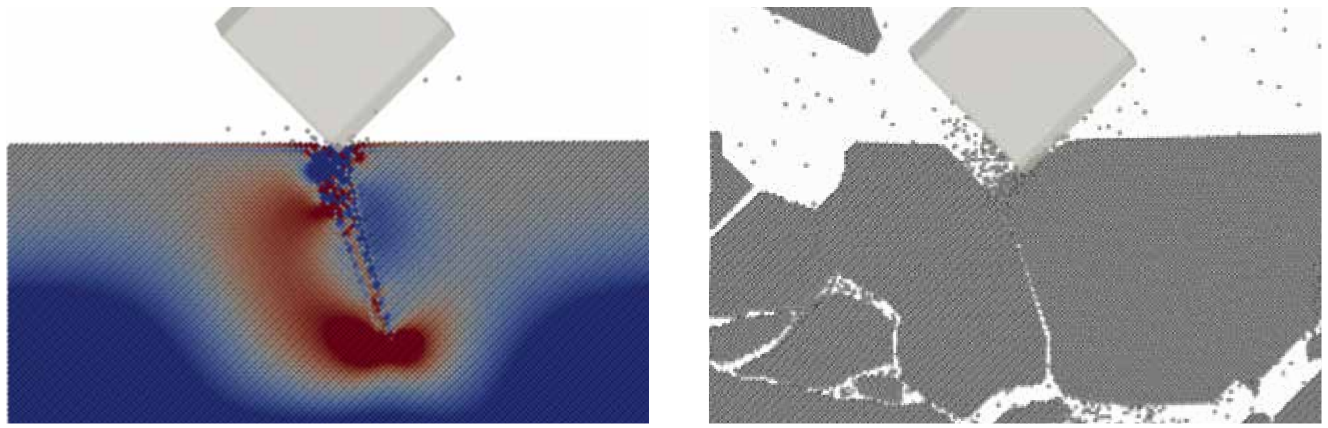
2 *The comparison of simulation and experiment (Takaffoli et al., Wear, 274–275:50–59, 2012) underlines the quality of the numerical modeling.*

BRITTLE MATERIALS

Ceramic materials and glasses generally exhibit brittle fracture behavior. Under tensile load, such a material initially behaves elastically, until a sudden break occurs, causing an instantaneous fall in tension. In the case of crystalline materials, the fracture surface is often oriented along a crystal plane, and is therefore smooth on the atomic length scale.

Quantitatively, the fracture toughness of a material can be described by the critical stress intensity factor. This quantity sets an upper barrier for the intensity of the stress field near the tip of the crack. When this barrier is exceeded, brittle fracture occurs in the material.

In SimPARTIX®, brittle fracture is described in the framework of peridynamics theory, a non-local expansion of classical continuum mechanics. Particle-based simulations are well suited to represent the mathematical models underlying peridynamics theory. The individual particles represent finite volumes of the material. The particles are connected by "force bridges" whose stiffness reflects the compressibility of the material. The fracture toughness is implemented as a critical strain on the force bridges; when this strain is exceeded, the force bridges are released.



The image shows the simulation of an indentation test of a silicon crystal. On the left, the tensile stresses (red color) and compressive stresses (blue color) inside the crystal are shown. On the right, the resulting fracture pattern after failure of the crystal under the load of the indenter is shown.

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