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FROM PARTICULATES TO SCIENCE OF DISCONTINUA: GENERALIZATION OF PARTICLE SIMULATION METHODS

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Abstract. In this work, we demonstrate that the rapid developments of methods of discontinua, when coupled with virtual experimentation and complementary discontinua based experimental and theoretical methods, are resulting in a significant paradigm shift from continuum-based analyses to either discontinuum and/or combined continuum discontinum-based approaches. Applications of these new approaches are so diverse (covering topics from traditional mineral processing to applications such as medical research, nano-science, social sciences, astrophysics, etc.) that what started as research on particulate media is rapidly transforming into the science of discontinua. In this paper, this trend is clearly demonstrated through a comparative study of both the fundamental developments in the core simulation technologies (together with synergies between different simulation tools) and their diverse fields of applications.

1 METHODS OF DISCONTINUA

It was during the mid-1980s that affordable computers started becoming widely available. Within a decade reasonably powerful workstations played a key role in the exponential development of continuum-based simulation tools, such as the finite element method (FEM) and the computational fluid dynamics methods (CFD). Computational technological advances, such as an increase in the CPU clock speed, carried on for another decade.

Now, the realization of affordable parallel computer architectures is available to the extent that an average researcher may already have one or more reasonably priced powerful parallel computers on their desk including a massively parallel graphics processing unit (GPU) device possibly comprising over three thousand float point processing units.

These advances have had a significant effect on the development of discontinua-based simulation tools, such as molecular dynamics (MD), discontinua deformation analysis (DDA), discrete element methods (DEM), combined finite discrete element methods (FDEM), smooth particle hydrodynamics methods (SPH), etc. The common thing to these methods is the fact that the continuum assumption has been replaced with discontinuum based model of matter characterized with discrete entities (elements) of predefined length scale – the length scale may be as small as individual atoms or as big as rock boulders or even planetary bodies.

In order to understand the concept of discontinua, it is worth to summarize some key historical stages of the modern scientific age. One could argue that the modern scientific age was a logical continuation of the work done by ancient civilization in the different fields of knowledge, such as geometry, algebra, logic, etc.

Researchers such as Galileo [1], Copernicus [2] and others were able to make significant discoveries by using both the algebra and geometry; for instance it was possible to formulate the concept of average velocity

$$v = \frac{\Delta s}{\Delta t} \tag{1}$$

where Δs is the distance travelled and Δt is the time interval. Without the convenience of the toolbox of algebra, this would not be possible. This is not to say that people would not understand the concept of velocity – they just would not be able to write it in such an elegant way that contains both the definition of the velocity and the quantitative measurement of it.

Early pioneers of the scientific age had reached an invisible barrier here and Newton was the first to discover that Δt can be infinitesimally small (smaller than any time interval, yet greater than zero). This was the eureka moment resulting in the discovery of the concept of instantaneous velocity, which Newton wrote as

$$\dot{s} = \frac{\mathrm{d}s}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{\Delta s}{\Delta t} \tag{2}$$

Leibnitz generalized the concept and differential calculus was born. For instance, the concept of point density simply becomes

$$\rho = \frac{\mathrm{d}m}{\mathrm{d}V} = \lim_{\Delta V \to 0} \frac{\Delta m}{\Delta V} \tag{2}$$

where ΔV is the volume and Δm is the corresponding mass. Thus, density becomes mass divided by volume provided that the volume is infinitesimally small. Of course, as the volume gets smaller and smaller the concept breaks down - because the material is not continuous. Nevertheless, one can assume that the material stays the same regardless of how small the volume is. This is the essence of the assumption of continuum, which is implicit in differential calculus. Differential calculus opened a whole range of possibilities for theoretical science starting with Newton's differential equation of motion (classical mechanics), through Navier stokes differential equations (Fluid Mechanics) to Maxwell's equations (electromagnetism), theory of relativity and numerous other applied scientific disciplines.

2 DEFINITION OF DISCONTINUUM

Engineers have encountered discontinua in their practice for long time. A classic example is discontinuities in rock masses, dam foundations, discontinuum nature of coastal protection units, wave breakers, powders, blood fluid with all its red blood cells, etc. In the example of historical structures subject to earthquake, it is the interaction between individual stone blocks that is respectable for the bulk of energy dissipated. In the example of red blood cells, it is tempting to write a non-Newtonian fluid based differential equation based on the assumption of continuum and model blood flow using continuum based computational tools. However, when one tries to design, for instance, an artificial heart, the mechanical concepts employed break due to the accumulated damage to the red blood cells – in other words, what the continuum assumption has rejected has become the key stone. In all problems of discontinua starting with nanotechnology a great scientific revolution is happening to the extent that one can now talk about the science of discontinua, i.e., mechanics of discontinua.

Discontinuum can be defined as a frictional material similar to continuum with the key difference that at a certain length scale the assumption of continuum is explicitly broken, and the material is assumed to be made of discrete entities, such as atoms, molecules, crystals, nano-particles, pebble size particles, house size blocks (of rock), and terrestrial size bodies; with carefully defined interaction between these entities.

Methods of discontinua range from DDA, DEM, FDEM, SPH to MD and even meshless methods and may also involve both solids and fluids. One could say that the serious work on discontinua started with the developments of the simulation tools. These included the pioneering work of Shi on DDA [2]-[5], Cundall on DEM [6]-[10], Mustoe [11]-[17], Williams, Preece [18], [30]-[36] on applications and advanced solvers, Munjiza on FDEM [18]-[29].

The power and versatility of modern computational science of discontinua and especially computational mechanics of discontinua can be demonstrated using a number of software packages, both research and commercial being developed all over the world such as Y-code (open source), ELFEN (Rockfield Software), ITASCA packages, Lawrence Livermore FDEM package, in-house packages at MIT, CSIRO (Australia), Toronto, specialized MD, DDA and other packages.

3 FROM SIMULATION TO VIRTUAL EXPERIMENTATION

The continuum based problem involves solving differential equations in such a way that one looks for a specific continuum function (field) such as the density of the material at each point. With discontinuum based problems, one has the system of interacting entities such as atoms, red blood cells, particles, rock blocks, etc. With such a system, one performs a virtual experiment. As a result, one gets the so called emergent properties such as a droplet of liquid emerging from a cooling gas cloud. This droplet is in a sense a “surprise” from the virtual experiment (usually computer simulation) - it is not just another quantity, but is fully a new quality.

For instance, should one try to apply the second law of thermodynamics to solar cells, it would produce a completely misleading result in terms of the possible efficiency of the solar cells. Should one try to apply the continuum formulation to flow through a cracking solid, similar misleading results will be produced. The reason is quite simple, what the continuum assumption has smeared out from its formulation plays the key-stone role in the behaviour of the system.

As such the science of discontinuua stretching from nanotechnology to material science, rock mechanics, medicine and even economics, has become a logical extension of continuum based scientific reasoning; and it is responsible for many modern scientific discoveries..

4 INTEGRATED APPROACH TO DISCONTINUA

At Los Alamos National Laboratory different discontinua simulation tools have been, for the first time, integrated under a single umbrella that includes fluid as well. The end objective is to provide a comprehensive environment for virtual experimentation using state of the art software design concepts. The new platform called the Hydrofrac Optimization Software Suite (HOSS) bridges the gap between different solvers, different applications and between solvers and applications. The current capabilities are demonstrated through some sample simulations that are listed below.

Dry real shaped particle systems. A cubical, hollow raster of particles of general shapes placed inside a rigid spherical container is shown in Figure 1. The raster is centered with respect to the spherical container. There is no initial overlap between the particles. Each particle is given an initial velocity pointing towards the center of the spherical container. The obtained motion sequence is shown in Figure 2.

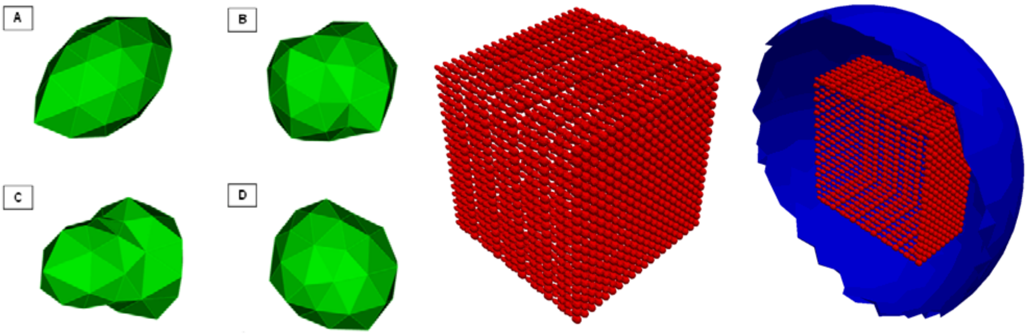

Figure 1: An example of real shaped dry particle system.

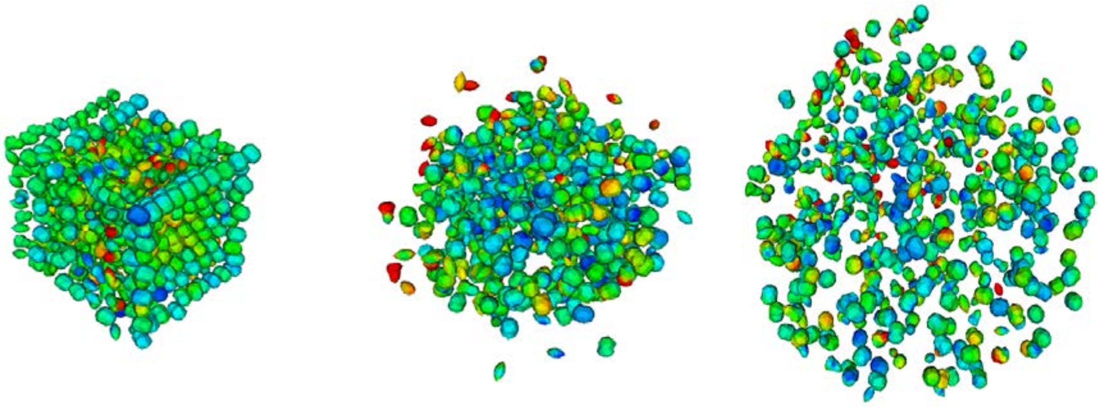

Figure 2: Obtained motion sequence of the dry particle system.

Combined continuum-discontinuum simulation. In Figure 3 a typical example of the combined continuum-discontinuum problem is shown. It resembles a bench blasting simulation that starts as a continuum and finishes as discontinuum through complex dynamic fracture and fragmentation processes.

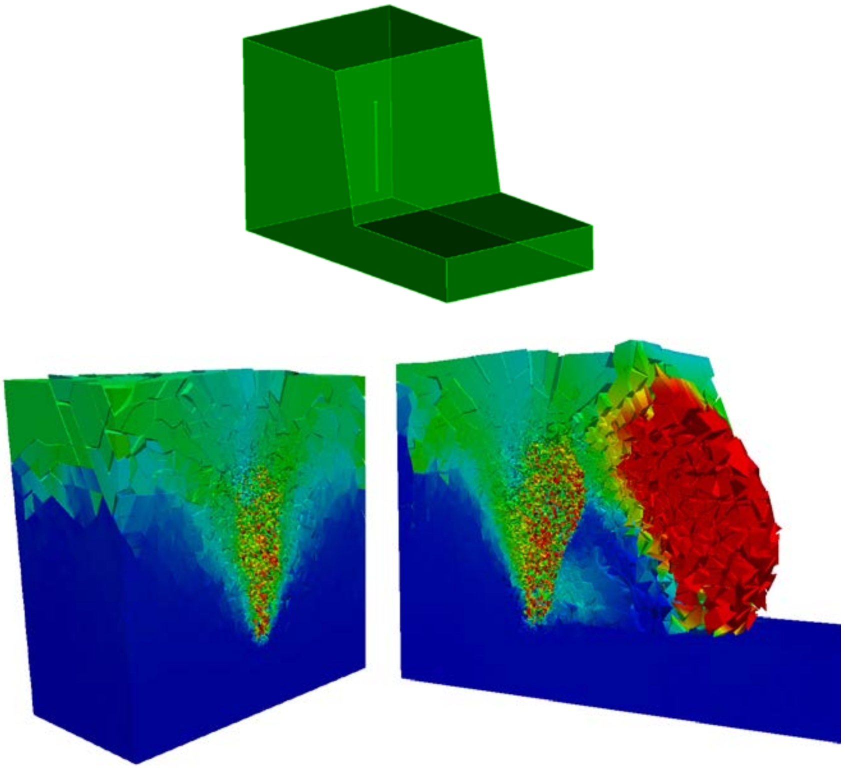

Figure 3: A 3D bench model with a borehole (top) and simulation results showing the fragmented solid (bottom).

Grand scale parallelization. Modern computers are by default parallel. HOSS has been designed to naturally take advantage of different parallel hardware platforms. In Figure 4 a parallelization example based on domain decomposition is shown. The little square shown in the figure represents particles assigned to a single processor. Despite a large number of processors employed, speedups of up to 90% of the total CPU power employed are possible – say 900 times for a 1000 processors problem.

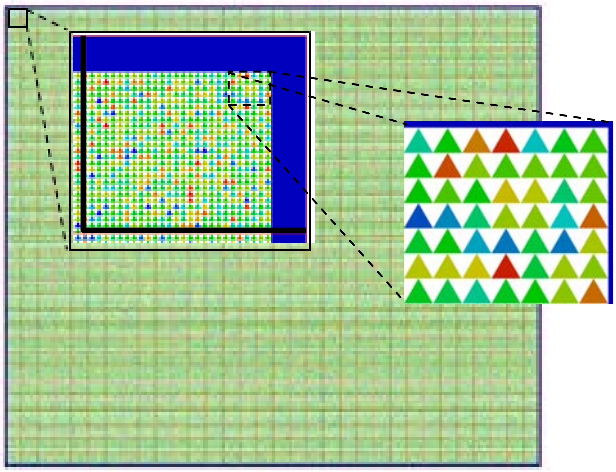

Figure 4: An example of domain decomposition using over thousand processors.

Industrial Scale Mining Applications. The application resonance of the above examples can be best demonstrated by a 3D simulation of a block caving mining operation. In Figure 5 an example of this simulation is shown. The model's external height is 31m with thickness and depth of 30m. The drawbell itself is 16m x 12.8m with a height of approximately 11m. The 3D mesh has an element size that ranges from between 10 cm near the 4 charge boreholes out to 1m at the extreme edges. As such, the total number of elements employed was 450,000. The four boreholes have charges that are ignited simultaneously at the beginning of the simulation. The obtained fracture, fragmentation and rock flow clearly demonstrate how the combined continua-discontinua model naturally captures different aspects of the problem.

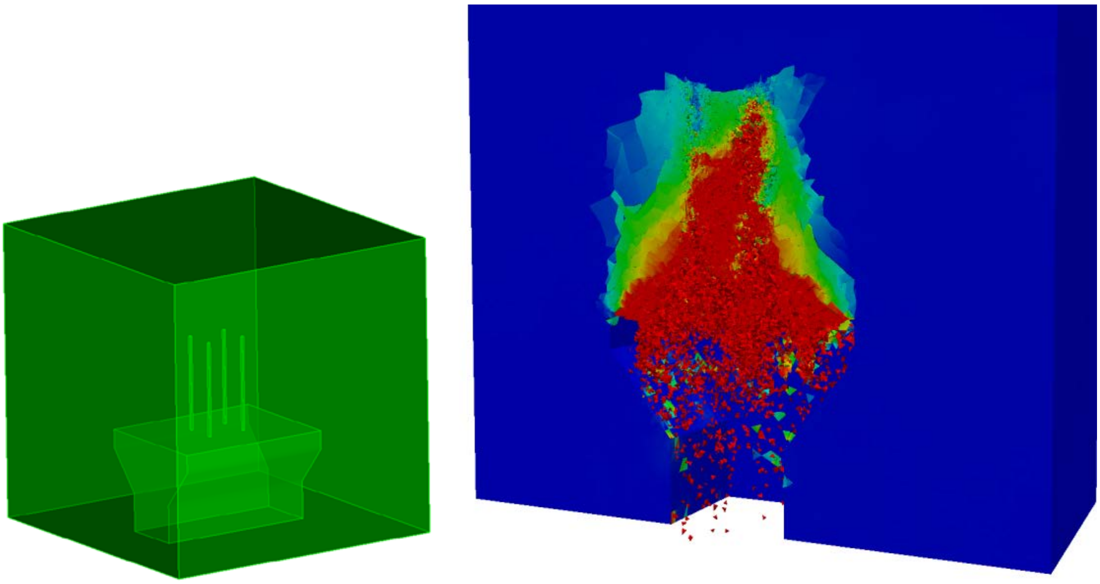

Figure 5: MUNROU drawbell simulation sequence: longitudinal cut clearly showing the cave formed by the flow of fragmented rock.

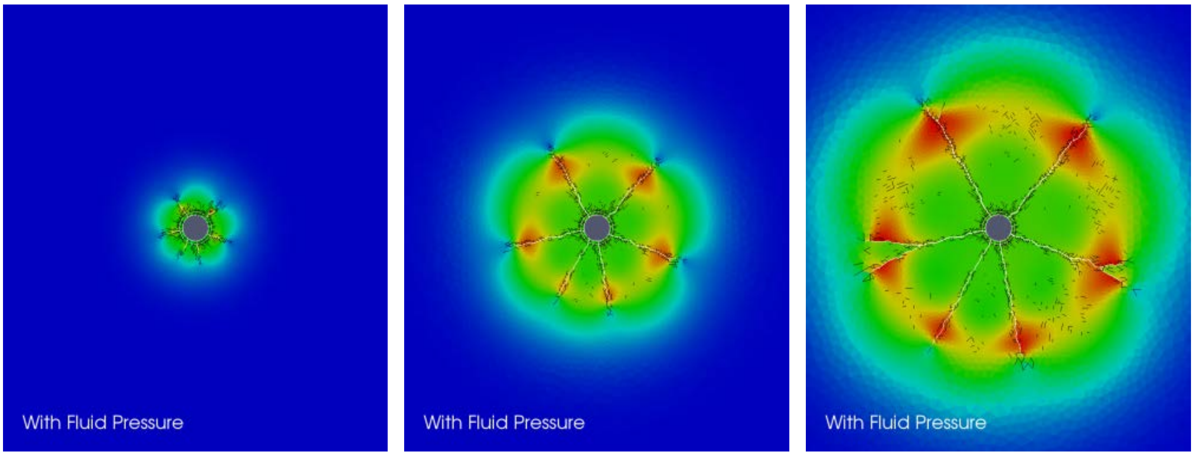

Figure 6: Fluid driven fracture simulation.

Fluid Driven Fracture. A constant pressure is applied to the inside of a borehole 0.4m in diameter. There is an annulus of concrete around the borehole. The rest of the material is shale. The simulation results obtained for borehole pressures of 40 MPa are shown in Figure 6 together with clearly visible individual cracks filled with fluid that has penetrated them.

Structures in Distress. In Figure 7 an example of a dome shaped structure under seismic load is shown together with the obtained damage (fracture) pattern. The seismic load is applied through actual motion sequence of the base obtained from a real earthquake.

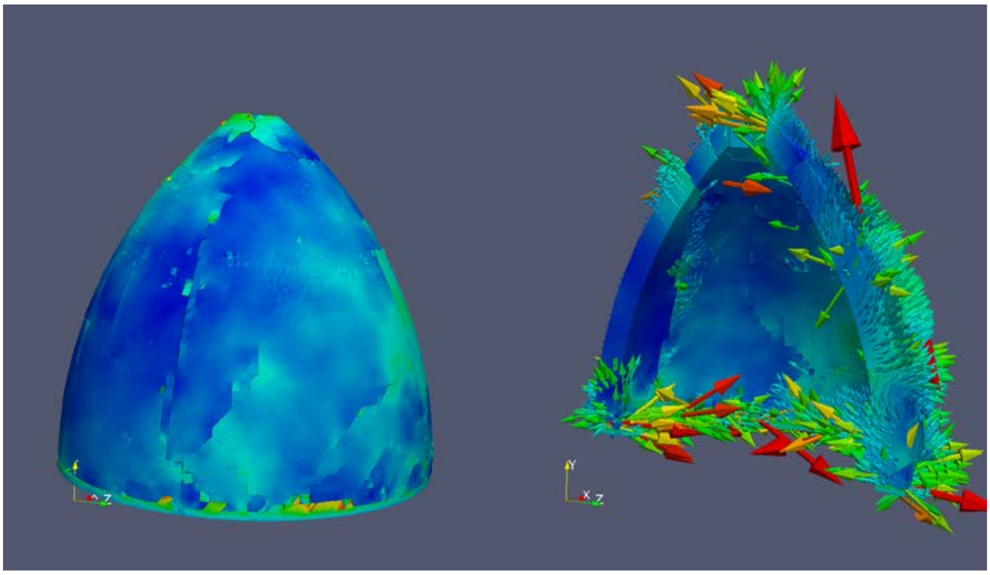

Figure 7: A dome fractured by earthquake load.

Safety and Security. In Figure 8 an example of laminated glass breaking under impact is shown, while in Figure 9 an example of laminated glass under a blast load is shown.

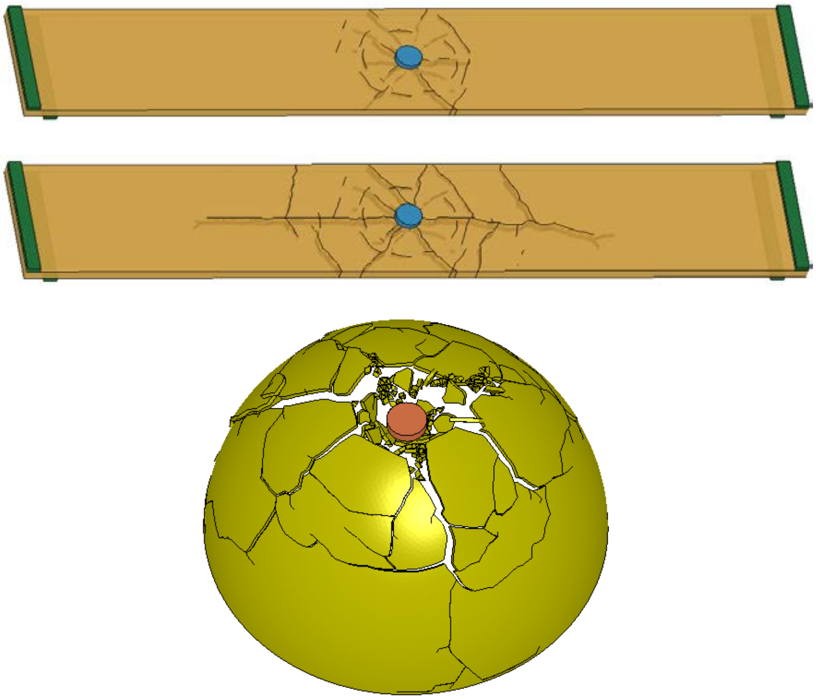

Figure 8: Examples of: fracture sequence for laminated glass under impact (top) and fracture pattern for spherical shell under impact (bootom)

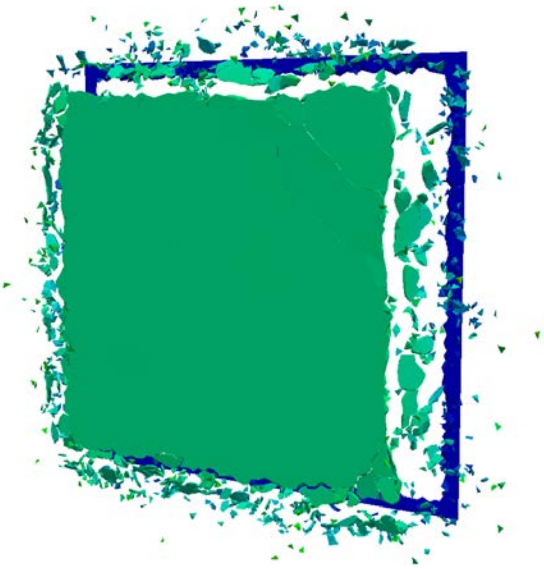

Figure 9: An example of laminated glass under blast.

In both cases multiplicative decomposition based finite strain-finite displacement shell formulation is employed.

Nanoscale simulations. In Figure 10 a nano-scale MD simulation demonstrating the concept of emergent properties is shown. The droplets of liquid Argon appear “out of the blue” clearly demonstrating the ability of virtual experiment to not only measure quantity, but also to come with new quality.

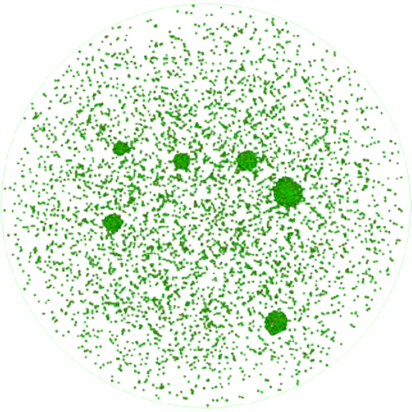

Figure 10: MD simulation of a mixture of different phases of Argon inside a container.

Medical Engineering. In Figure 11 an example of a micro-scale simulation of blood plasma with deformable blood cells is shown.

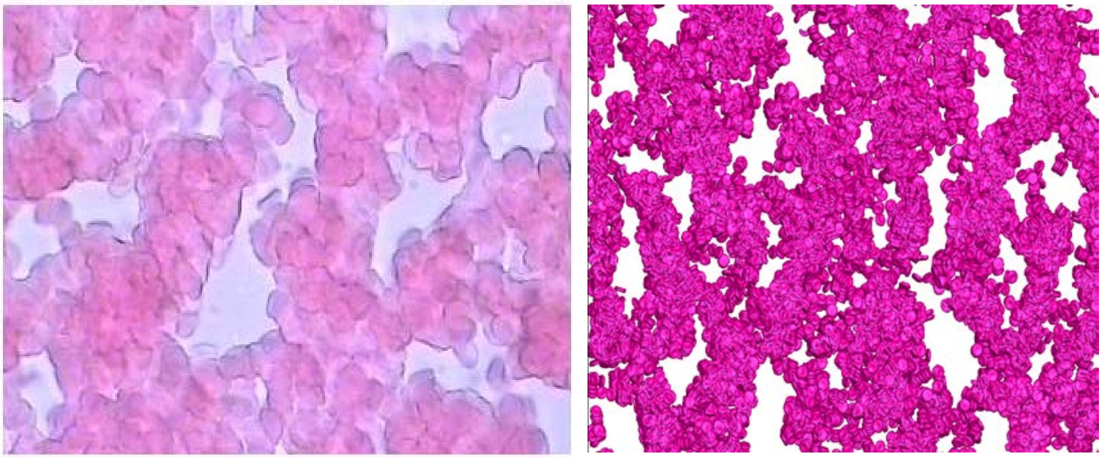

Figure 11: Side by side: experimental and simulation results for blood plasma containing red blood cells.

12 CONCLUSIONS

It has been clearly demonstrated that discontinua represents a paradigm shift occurring in many scientific, engineering and industrial disciplines spreading from nano-science, material sciences, medical engineering to mining, mineral processing, powders, etc.

Exponential research developments coupled by industrial applications are driving both experimental and theoretical approaches, which are now greatly helped by credible virtual experimentation tools based on grand-scale parallel or GPU based discontinua simulations that are able to discover emergent properties, in much the same way a real experiment would. The added benefit of these approaches is convenience, flexibility and a low cost for simulations when compared with real experimental rigs, for example, inserting sensors into a model is not troubled by physical constraints such as very high temperatures. In short, discontinua is here to stay, and it is likely to help in major discoveries of the 21st century.

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