

# Virtual Nanotechnology Workbench for Engineering Education

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**Abstract** - During 1990s discrete element methods have been combined with finite element methods and a new simulation tool has been developed and named the combined finite element method. The first textbook on the combined finite-discrete element method has been published recently and key algorithms have been implemented in commercial codes. In recent years work is in progress to integrate these tools into the so called virtual experimentation framework covering different scales including atomic and molecular scales. The computational tools developed have a great potential in uncovering the mysteries of nano-scale world. This is done through advanced simulation and visualization techniques comprising millions and even billion of entities. In research terms these are able to put new light on the meaning of emergent properties. In the context of engineering education, these are very useful tools that can help students better understand the complex processes on atomic and nano-scale leading to both microscopic and macroscopic emergent properties. In this paper some key aspects of the new technology are presented together with simulation results covering some nano-scale applications. In the presentation itself, the potential for engineering education will be demonstrated through “movies from virtual world”. These are basically virtual animations covering nano-meter pento-second domains.

*Index Terms* – Engineering education, Nanotechnology, Virtual experiment, Workbench.

## INTRODUCTION

Traditionally, both theoretical and experimental approaches have been used to further human knowledge. Theoretical science is usually based on initial assumptions. From these initial assumptions conclusions are derived using logical reasoning. In experimental science, these conclusions are tested using experiments.

In real-world experimentation an experimental scientist may opt for extensive instrumentation in order to make necessary experimental observations and measurements. However, even these are very often not enough; confinement, temperature, distance, time-scale, etc. can make observation and measurements very difficult and very often impossible.

One solution for such experimental problems is to build a parallel virtual world. Experiments performed in such a world are called virtual experiments. The restrictions of real world very often do not apply to virtual worlds. For instance, in a virtual world one can easily consider very small or very large time-scales.

In this work virtual experimentation based on simulations using combination of discrete and finite element methods [1] is introduced and its possible role in engineering education is explained.

## VIRTUAL EXPERIMENTATION IN GENERAL

In figure 1 the general role that virtual experimentation can play in modern science is illustrated. In the centre of the diagram is the real world. To gain knowledge about this world traditionally theoretical reasoning has been employed resulting in theoretical scientific disciplines. These are then coupled with experimental observation.

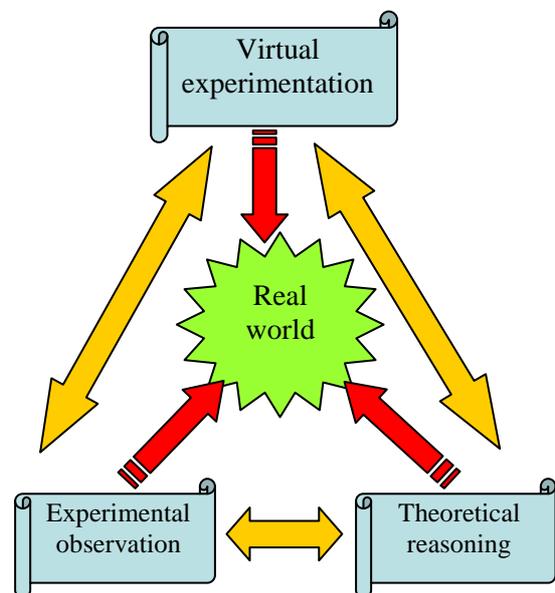


FIGURE 1  
THE CONCEPT OF VIRTUAL EXPERIMENTATION.

Virtual experimentation is based on building a parallel virtual world. Virtual experimentation rigs are used to perform virtual experiments in this virtual world. The core of these rigs is made of numerical simulation, key diagnostics and visualization tools.

The results of virtual experiments do not replace but complement both theory and real world experimentation. They play an important role in gaining knowledge and understanding and can enhance learning and teaching methods.

Virtual experiments are built from fundamental equations and what emerges is trustworthy. By using virtual experiment it is possible to observe things that are difficult or impossible to observe in the real world. For instance, trajectories of individual atoms can be followed despite very short time scales and very small length scales.

Virtual experiments offer exciting opportunities in terms of:

- scale (nanoscale, atomic scale, very large scale)
- speed (very fast processes – pentosecond, very slow processes – cosmic timescale)
- size of data
- configuration, temperature, pressure, etc.

### SOME EXAMPLES OF VIRTUAL EXPERIMENTATION

Virtual experimentation serves both theoretical and experimental science. The key idea behind virtual experimentation is to take small individual elements of the real world say atoms and simulate the interaction between these elements using fundamental equations.

An example of the results of a set of such experiments involving a simple packing problem is shown in figure 2. Different packs (obtained using discrete element simulation [1-3]) are shown next to each other. The packs range from mono-sized spheres (a) to uniform size distribution (b-e) and power-law size distribution (f). All packs comprise the same volume of solid material.

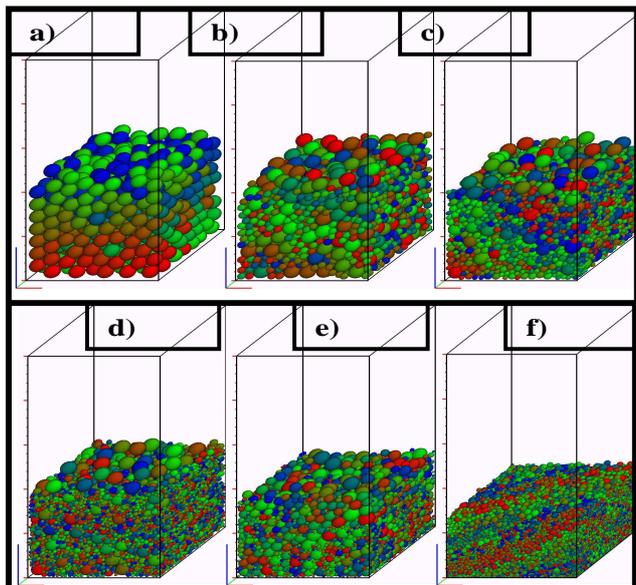


FIGURE 2  
VIRTUAL EXPERIMENTS FOR PACKING PROBLEMS.

By visual inspection, it is evident that mono-sized spheres occupy the largest space, i.e. have the lowest packing density. Power law size distribution has produced the pack

occupying the smallest space, i.e. having the largest packing density.

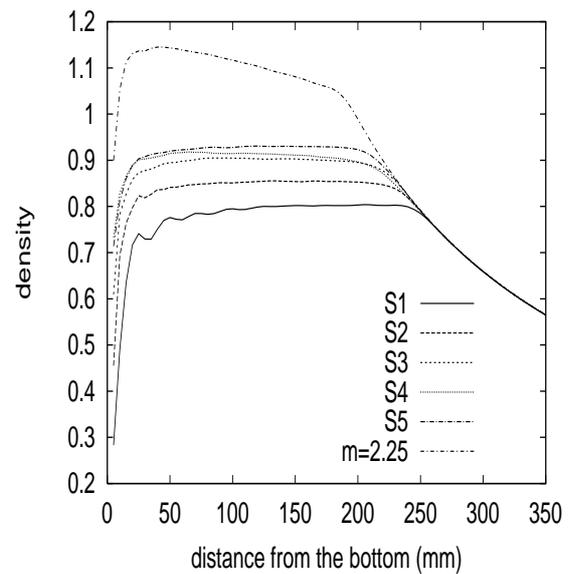


FIGURE 3  
VIRTUAL EXPERIMENTS FOR PACKING PROBLEMS.

The actual packing density as function of the distance from the bottom of the pack is shown in figure 3. The graph shows that the power-law size distribution (curve  $m=2.25$ ) has produced the most dense pack, while mono-sized spheres (curve S1) have produced the lowest density pack.

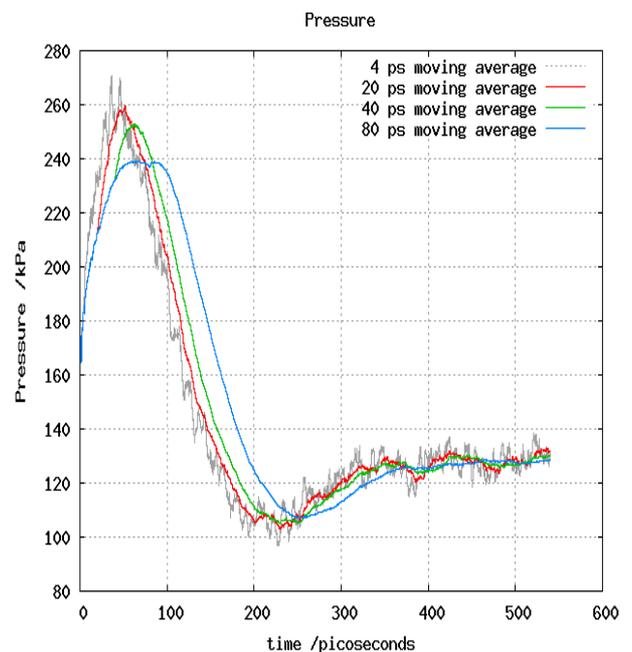


FIGURE 4  
PRESSURE AS EMERGENT PROPERTY .

It is evident from the above set of virtual experiments that the packing density has been obtained as an emergent property of what can be termed as agent based simulation. The agents here are individual spheres. The interaction between these agents has been simulated using a discrete

element method. Never in the course of the simulation has the pack as such been considered, neither have any pack properties been assumed.

This is in sharp contrast to traditional numerical simulations such as say linear elasticity using finite elements. In finite element simulations constitutive law and material properties such as density are supplied as input parameters to the simulation. In the above virtual experiment the material has been built particle by particle and density has emerged as the result of the experiment. It has emerged as an “emergent property”.

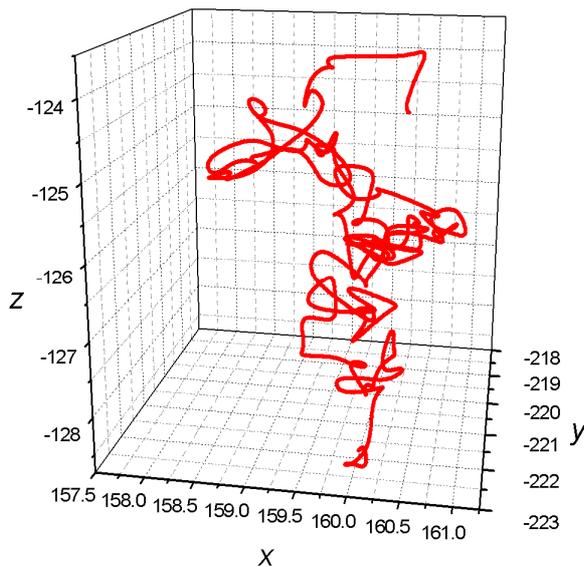


FIGURE 5

A TYPICAL TRAJECTORY OF ATOM INSIDE A LIQUID DROPLET.

By considering matter to be made of individual atoms and employing virtual experiments incorporating discrete element simulation (with interaction forces between atoms implemented in a similar way to molecular dynamics simulation [4]), the pressure of argon gas has been obtained as emergent property as shown in figure 4.

Using virtual experimentation it is also possible to look at trajectories of individual atoms. One such trajectory for the liquid phase is shown in figure 5. It is evident that the trajectory implies constant interaction with neighbouring atoms, i.e. close proximity of individual atoms.

#### VIRTUAL EXPERIMENTATION AND ENGINEERING EDUCATION

The results of virtual experimentation are very often best presented using so called movies from virtual world. These enable students to observe on their screens processes at nano-meter and pento-second spatial and temporal scales respectively. Students can therefore “experience” how the emergent macroscopic properties (usually described by differential equations) are formed. In this context, virtual experimentation has a potential of playing an important role in engineering education.

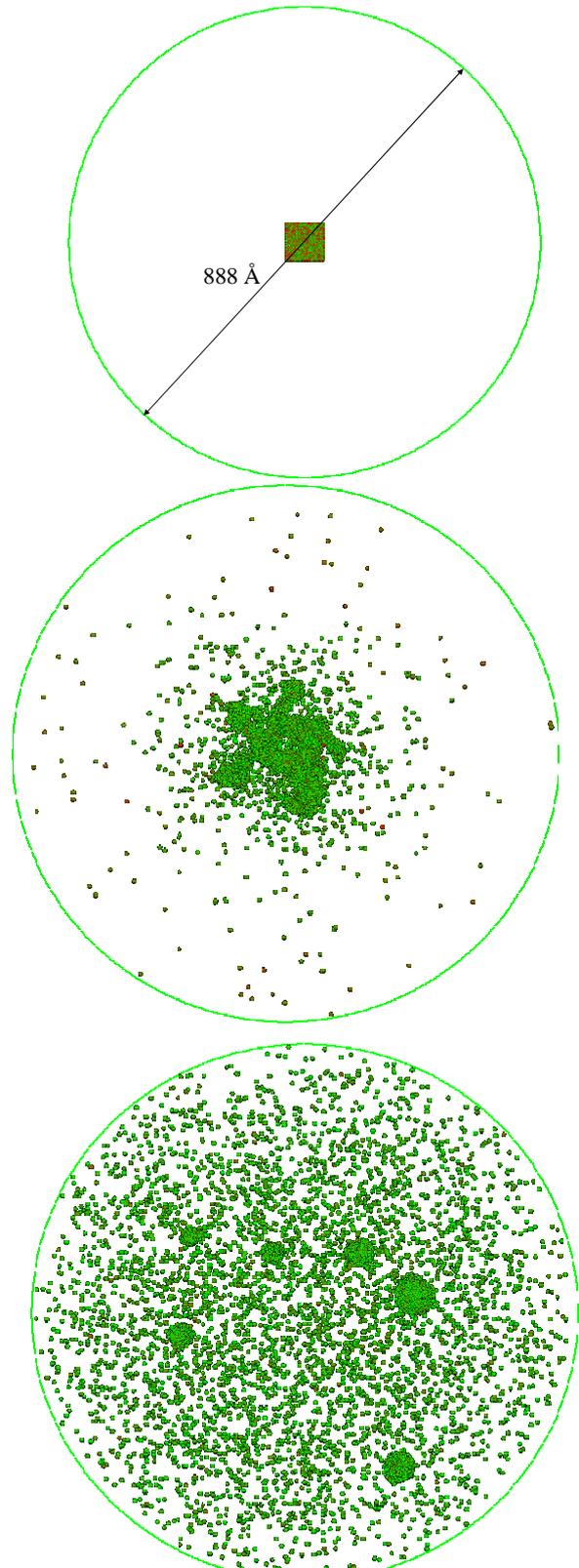


FIGURE 6

ARGON CRYSTAL MELTING INSIDE A RIGID SPHERICAL CONTAINER.

This is best demonstrated by the example shown in figure 6, where a crystal of Argon comprising 9842 atoms ordered in a face centred lattice is placed inside a spherical rigid container. The initial temperature of the solid Argon is 83.8 K. The crystal is heated instantaneously to 350.0 K at

time  $t=0$ . After that no energy is either added or taken from the system.

The crystal starts melting and evaporating as shown in figure 6 and eventually some droplets of liquid Argon are formed. After the transient stage is over, the system comprises of gas phase of Argon in equilibrium with suspended liquid droplets. The droplets have spherical shape, which is due to surface tension. Surface tension is therefore an emergent property.

The still images shown are not enough to visualize the complexity of the problem, thus in the presentation movies from virtual world will be shown, which will immerse the viewer into the complex phenomena occurring at nano-scale, pico-second level.

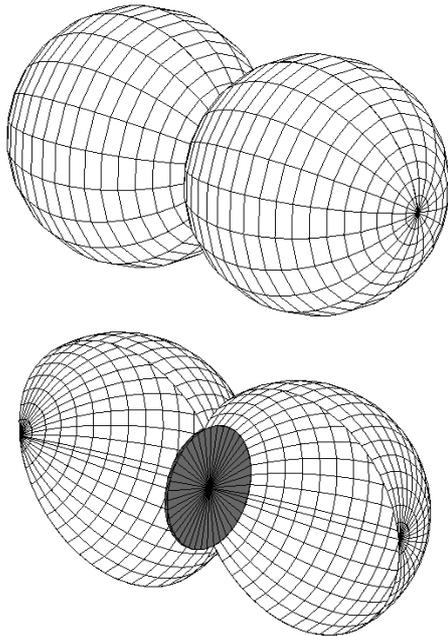


FIGURE 7

MAXWELL DEMON: (TOP) THE CONTAINER; (BOTTOM) THE GATE.

Very often in teaching and learning demonstration examples are designed to illustrate extreme and limit cases and also “what if” scenarios. This is relatively easily done in theoretical works. In real life experiments these may be more difficult to obtain. In virtual experimentation it is in general possible to create processes that do not normally occur in the natural world. For instance in figure 7 a virtual experiment showing the so called Maxwell’s demon problem is shown. Maxwell presented the demon in his book called “Theory of Heat” in 1871 [5]. Since then, a lot of effort has been done in order to “exorcise” the demon.

The idea behind this thought experiment is quite simple: consider gas inside two containers connected by a gate. The gate is operated by an intelligent demon. Initially, the gas in both containers is at the same temperature and pressure, and ideally contains the same number of molecules. Each time a molecule approaches the gate, the intelligent demon decides whether to close or open the gate based on a velocity threshold appropriately selected.



FIGURE 8

MAXWELL’S DEMON EXPERIMENT COMPRISING 80,000 ATOMS.

Clearly, this thought experiment goes against the second law of thermodynamics, because in this system the heat is flowing spontaneously from a colder side to a hotter side without expensing any work. In the real world this experiment is therefore impossible to perform. In the virtual world the virtual demons are simply placed on the plane of the interface between the spheres, as shown in figure 7.

When considering the atoms that are allowed to pass from one to the other container, the demon works in the same way as a high pass filter, i.e. it lets through only those atoms that have a speed greater than the threshold. When considering the atoms that are allowed to pass from the right side to the left side, the demon works as a low pass filter.

The transient sequence produced by simulation is shown in figure 8. The colour indicates velocity of individual atoms and therefore temperature. The image sequence shown indicates the right hand side container increasing in temperature, while the gas inside the left hand side container is cooling.

In the simulation two types of demons were used: a) global demon that knows the position of all atoms at every time instance; b) sleeping demon that knows only the position of the atoms that hit it. Energy balance shows that sleeping demons are more efficient in energy terms. However, the net energy available per event is only about 100keV, which is approximately  $1.60e-17J$ . It is worth mentioning that this energy is not enough to remember even a single bit on present day computers. The conclusion is that even in virtual world Maxwell's demons do not produce a net gain of energy.

It is obvious that an experiment such as the one described above is not possible in real world. Performing an experiment in virtual world and observing the results can give students both qualitative and quantitative information about the processes involved and can also act as a motivator to study the related theory.

It is worth noting that simulations similar to those shown above have also been obtained on much larger systems comprising up to one million atoms. The largest simulation attempted comprises 0.6 billion atoms.

The paper has demonstrated that virtual experiments are useful as tools for explaining to students the processes involved on spatial and temporal scales where experimental techniques are either not available or may even be impossible. However, it is difficult to demonstrate the full potential of these tools using still black and white images. Thus, in the presentation itself more advanced techniques are used including the movies from the virtual world. These enable students to be immersed into nano-scale, pento-second worlds and fully experience them. Some of these movies will be shown during the presentation.

## CONCLUSIONS

The concept of virtual experimentation has been introduced in this paper and its potential role in engineering education has been explained. Virtual experimentation is in essence based on building virtual worlds and performing experiments using numerical simulation. In contrast to traditional numerical simulations such as finite element simulations,

virtual experiments consider the individual building blocks making the virtual world.

Simulations shown in the paper enable students to visually observe processes occurring at very small length scales and at very high or very slow speeds. Some of these processes are well understood on macroscopic level. Even in these cases actual development of macroscopic emergent properties can be observed, thus helping students to better understand the mechanisms and processes leading to differential equations that quantify the results of such processes. Problems such as evaporation and combustion, of a single droplet of fuel or flow in nano-tubes are currently beyond the capabilities of the virtual tools developed. However, the work is in progress to include these into the existing codes. It is hoped that these and other enhancements will enable observation of more complex phenomena on a nano- and micro-scale.

The paper has been limited to nano-scale mostly inter-atomic interactions. In other words the building blocks have been atoms and interactions between atoms. However, there is no reason for the building blocks not to be humans, plants, bees, etc. Interaction between these individual building blocks requires description of individual blocks. The system itself can be granular material, human society, biological population, etc. Virtual experiment knows nothing about such a system. In fact, the purpose of the virtual experiment is to produce "emergent properties" of the system.

In this work discrete element based virtual experiments have been shown. This is because the author is familiar with discrete element systems. However, there is no reason not to employ similar agent based simulation techniques, depending on the experiment itself.

It is not hard to visualize how virtual experimentation can change the way teaching is done and how it can give students the opportunity to experience processes on all scales from pento-second to geological time scale and from nano-scales to terrestrial bodies. Virtual experimentation can help students gain experience fast and can therefore play an important role in industry where the world changes fast and experience soon becomes out of date.

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