Virtual experimentation in the service of theoretical and experimental science

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Abstract

In this paper a concept of virtual experimentation is introduced. The paper discusses in detail the role of virtual experimentation rigs in modern science. It then explains how virtual experimentation complements both theoretical and experimental science. Virtual experimentation concepts introduced in the paper are also demonstrated by virtual experiments based on discrete element simulations.

Keywords: Virtual experiment; Theoretical science; Discrete elements; Emergent properties

1. 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. A classical example is the story of a so-called Galileo's balls problem. Before Galileo it was widely considered that heavier objects fall faster than lighter objects. Galileo reasoned that two bricks glued together must fall at the same speed as two bricks that are not glued together. From this initial assumption he concluded that heavier objects must fall at the same speed as lighter objects. He tested his assumption using the famous Galileo's balls experiment.

The experiment Galileo did was relatively simple. Very often this is not the case. For instance, very often it is not possible to make observations using a naked eye. In such cases one would, possibly, use a microscope. In other cases 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 the rest of the paper the role of virtual experimentation in modern science and its link to theoretical and experimental science is discussed. Also the necessary conditions for feasibility of virtual experiments, the key benefits of virtual experimentation and key structural blocks for building virtual experimentation rigs are explained in some detail.

2. Experimentation in virtual worlds

In Fig. 1 the role of virtual experimentation 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 coupled with experimental observation. Virtual experimentation is based on building a parallel virtual world. Virtual experimentation rigs are used to perform virtual experiments in this virtual world. The results of virtual experiments complement both theory and experiment, and play an important role in gaining knowledge and understanding, obtaining predictive capability, developing new technology, improving productivity, environment, learning, life, etc.

Thus, virtual experiments complement both theory

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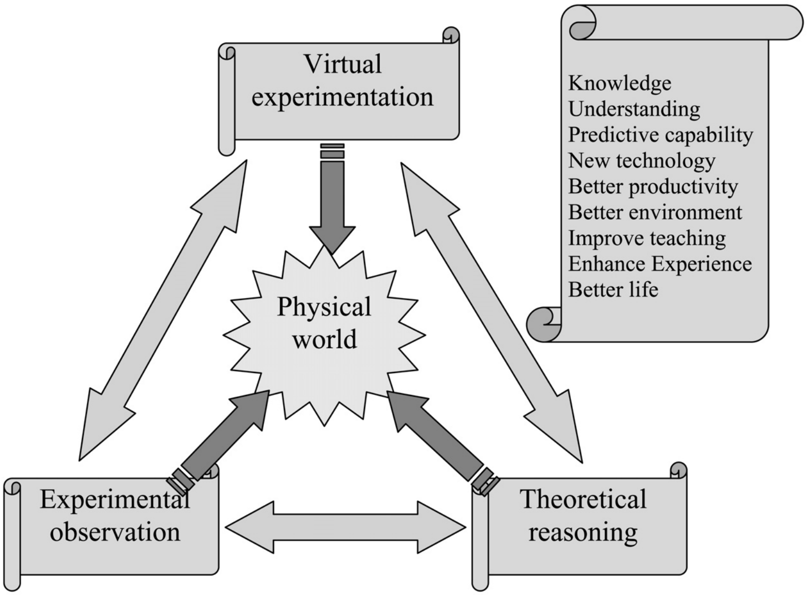

Fig. 1. The role of virtual experimentation in modern science.

and experimental observation. Virtual experiments are built from fundamental equations and what emerges is trustworthy. Virtual experiments serve science in a similar way that a microscope does. Using a microscope one can observe things that otherwise could not be observed. Using a virtual experiment one can observe things that are difficult or impossible to observe in the real world. For instance, one can go inside a long runout rockslide. One can follow trajectories of individual atoms with very short time-scales and very small-length scales. One can go inside the earth core with its massive confining pressures. One can almost ‘experience’ future, such as what it is going to be like if the climate changes.

In summary, virtual experiments complement both theoretical and experimental science and offer exciting opportunities in terms of:

(a) scale (nanoscale, atomic scale, very large scale)
(b) speed (very fast processes – pentosecond, very slow processes – cosmic timescale)
(c) size of data (It is software, i.e. the brain, that connects dots into lines and lines into shapes to enable us to recognize each other; Modern neuroscience has confirmed that the brain builds a parallel virtual world using the information supplied by the eye.)
(d) configuration, temperature, pressure, etc.

3. Emergent properties

As previously mentioned, 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, particles or blocks, and simulate the interaction between these elements using fundamental equations [1]. The results of a set of such experiments are shown in Fig. 2. Different packs obtained using discrete element [1,2,3,4,5,6,7,8] simulation (it is worth noting that very often simulation is a major part of a virtual experiment) are shown. The packs range from monosized spheres to uniform size distribution and power-law size distribution. All packs comprise the same volume of solid material. By visual inspection, it is evident that monosized 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. Quantitative measurements of the actual packing density as function of the distance from the bottom of the pack is shown on the left graph. The graph shows that the power-law size distribution (curve $m = 2.25$) has produced the most dense pack, while monosized spheres (curve S1) have produced the lowest density pack. In addition, from the second graph, it is possible to observe that with increasing number of particles for monosized spheres, i.e. with decreasing size of spheres, the density of the pack increases. This density increase follows a smooth curve for spheres smaller than 0.15 (normalized diameter of the sphere relative to the length of the bottom edge of the box). In both graphs the normalized density relative to the theoretical density of closed packed monosized spheres (cubic closed packing) is given

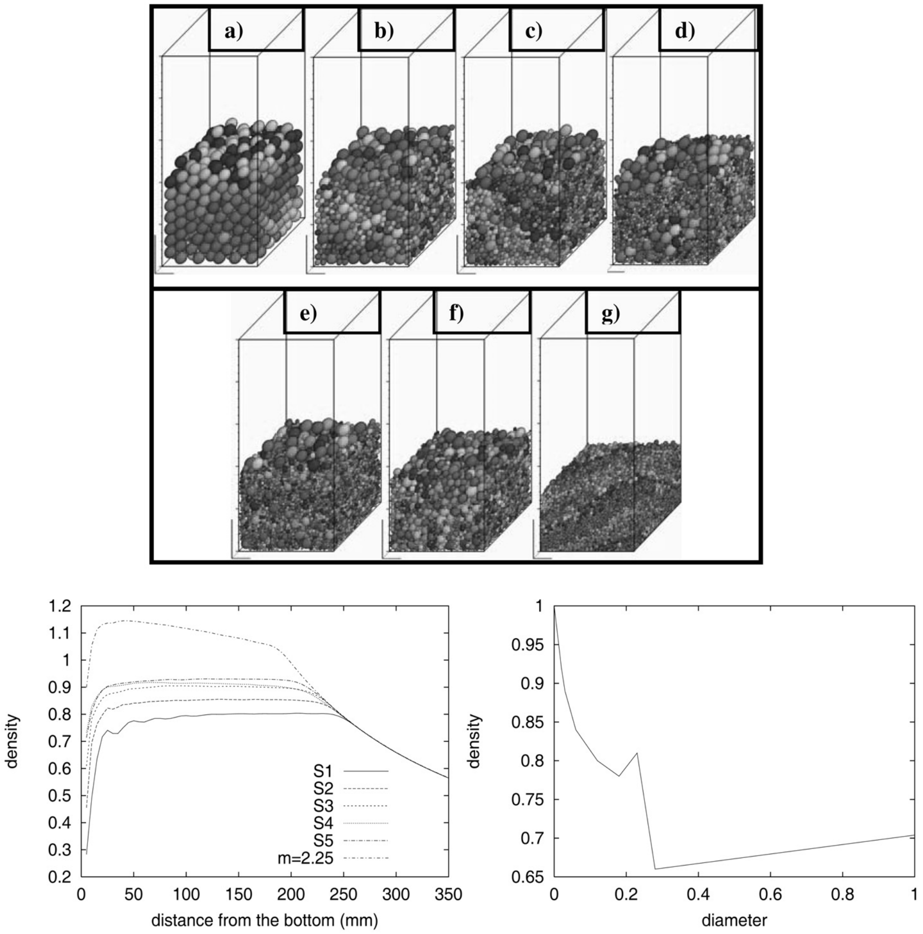

Fig. 2. Virtual experiments for packing problems.

$$\frac{V_{spheres}}{V_{space}} = \frac{\pi\sqrt{2}}{6} = 0.74048\ldots \qquad (1)$$

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 particles. 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'.

In Fig. 3, after considering the matter being made of individual atoms and employing virtual experiments incorporating discrete element simulation, the pressure of Argon gas has been obtained as emergent property. Also, by looking at trajectories of individual atoms, the liquid phase is distinct from the gas phase (diagrams right top and right bottom respectively). By visual inspection (animation), Fig. 4, liquid droplets of Argon are observed. Theoretically, due to surface tension these droplets should be spherical. In the animation itself, due to inertia forces, droplets are initially of irregular shape. As inertia forces decrease, droplets assume spherical shape due to the surface tension. However, it is worth noting that the simulation 'does not know' anything about surface tension, i.e. no surface tension is included in any models employed. The surface tension is, in fact, obtained from the experiment as an emergent property. It is simply the consequence of the way individual atoms interact.

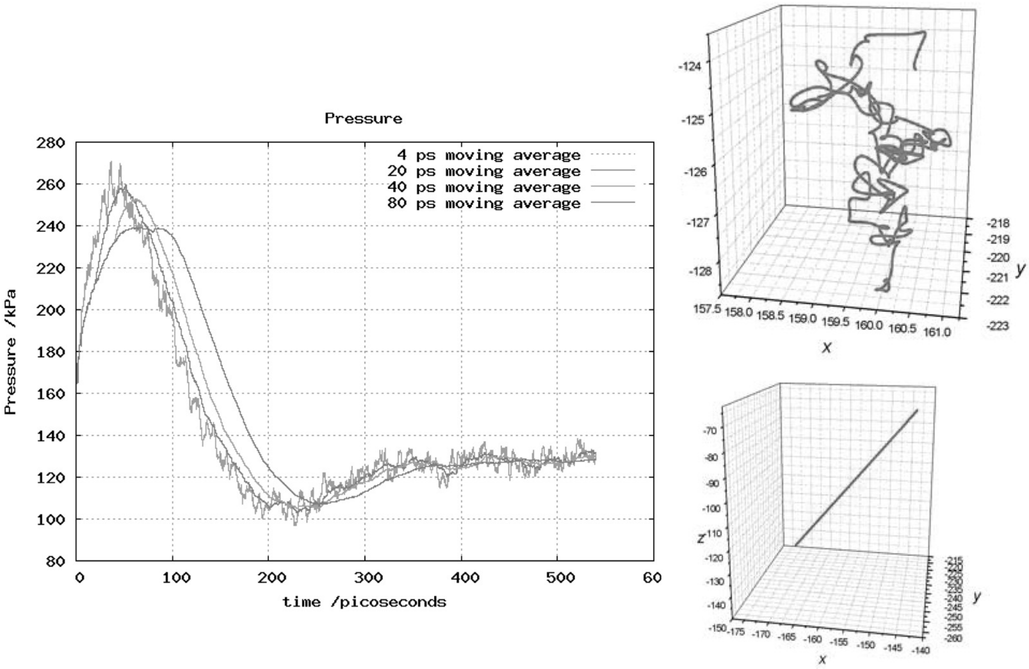

Fig. 3. Using virtual experiments in which individual atoms are agents, pressure is obtained as emergent property (left) and so is the state of matter: liquid (top right) or gas (bottom left).

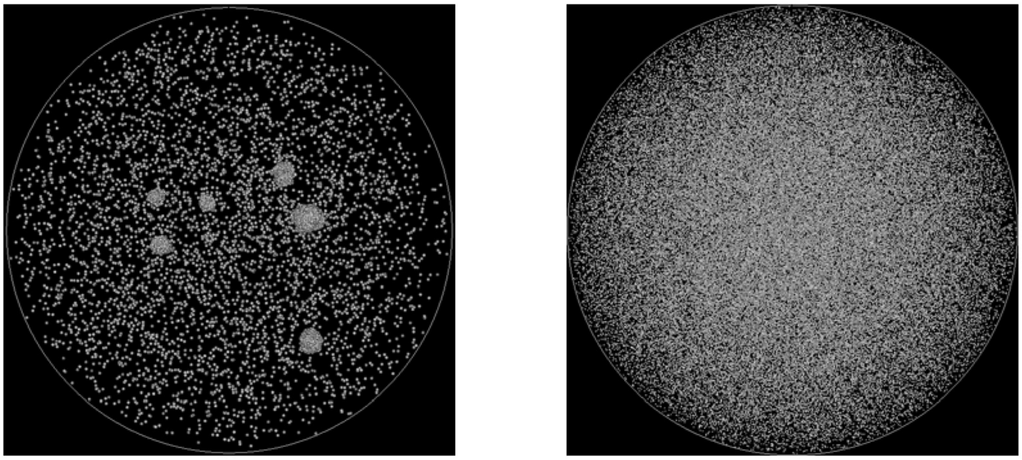

Fig. 4. Using virtual experiments in which individual atoms are agents, surface tension is obtained as emergent property – observe spherical shape of liquid droplets (left) as opposed to gas atoms (right).

In Fig. 5 sensitivity to initial conditions is obtained as an emergent property. The figure shows the results of two successive experiments shown side by side. In both experiments a pill-shaped particle moves inside a rigid box. Initial setup of both experiments is identical, except that in the second experiment the particle is inclined by 10^{-11} rad. Initial motion sequence in both experiments is similar. However, the final motion sequences are completely different from each other, thus demonstrating the well-known sensitivity of multibody systems to initial conditions. It would be interesting to observe such sensitivity and possible chaotic behaviour of virtual systems comprising trillions of particles.

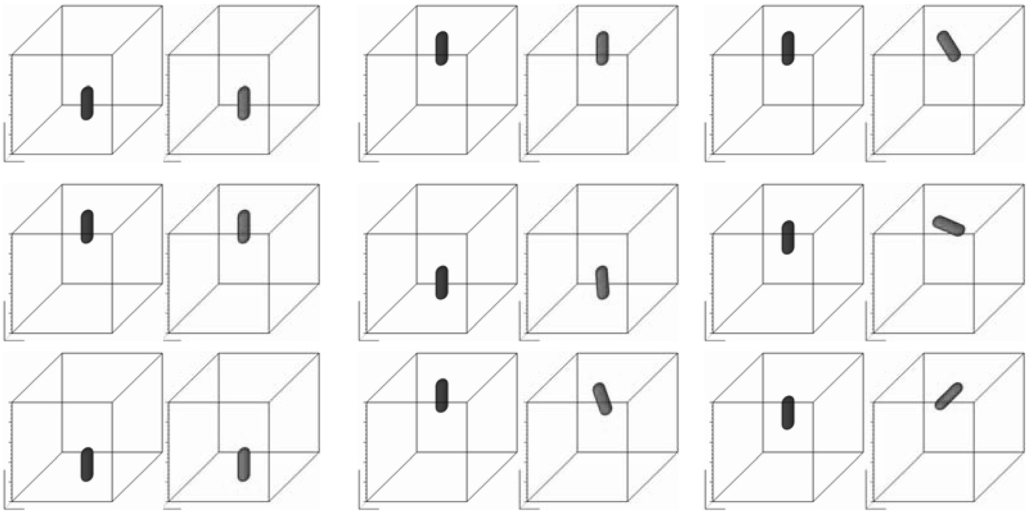

Fig. 5. Sensitivity to initial conditions as an emergent property.

4. Conclusion

The concept of virtual experimentation has been introduced in this paper. Virtual experimentation is, in essence, based on building virtual worlds and performing experiments in, most often 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. Such building blocks can be particles, atoms, concrete blocks, etc. However, there is no reason for such building blocks not to be humans, plants, bees, etc. Interaction between these individual building blocks requires description of individual blocks, while description of the system is not needed. The system can be granular material, human society, etc. Virtual experiment knows nothing about such a system. In fact, the purpose of the virtual experiment is to produce ‘emergent properties of such a system’.

Virtual experiments are built using ‘first principles’ and the results are trustworthy. In addition, in virtual worlds one can observe what in real worlds is impossible. With virtual experiments large data sets come naturally, which is not always the case with real experiments, where extensive instrumentation may be required. Integration of experimental and theoretical science with virtual experimentation has the potential for yielding fundamental leaps forward in research endeavours ranging from traditional disciplines to complex systems such as financial markets or the global economy (where real experiments on a large scale can have disastrous consequences).

In this work discrete element [1,2,3,4,5,6,7,8] 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 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 pentosecond to geological time-scale and from nanoscales 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.

5. Acknowlegements

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References

[1] Munjiza A. The Combined Finite-discrete Element Method, Wiley, 2004.

[2] Perkins E, Williams JR. Generalized spatial binning of bodies of different sizes. Proc 3rd International Conf on Discrete Element Methods, Santa Fé, NM, USA, 2002.

[3] Chung SH, Mustoe GGW. Effects of particle shape and size distribution on stemming performance in blasting.

Proc 3rd International Conf on Discrete Element Methods, Santa Fé, NM, USA, 2002.

[4] Preece DS, Chung SH. An algorithm for improving 2-D and 3-D spherical element behavior during formation of muck piles resulting from rock blasting. Proc 3rd International Conf on Discrete Element Methods, Santa Fé, NM, USA, 2002.

[5] Munjiza A, Andrews KRF. NBS contact detection algorithm for bodies of similar size. Int J Num Methods Eng 1998;43.

[6] Owen DRJ, Feng YT, Cottrel MG, Yu J. Discrete/finite element modelling of industrial applications with multifracturing and particulate phenomena. Proc 3rd International Conf on Discrete Element Methods, Santa Fé, NM, USA, 2002.

[7] Williams JR, Mustoe GGW. Proc 2nd US Conf on Discrete Element Methods, MIT, MA, 1993.

[8] O'Connor R, Gill J, Williams JR. A linear complexity contact detection algorithm for multy-body simulation. Proc 2nd US Conf on Discrete Element Methods, MIT, MA, 1993.