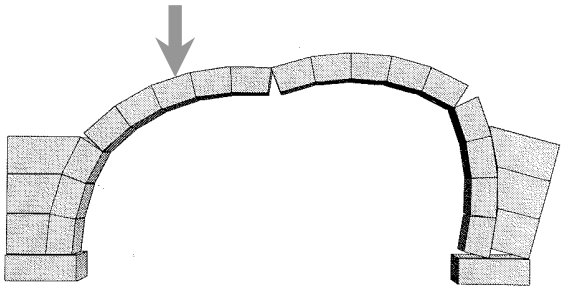
1. INTRODUCTION TO DEM

1.1 What is DEM?

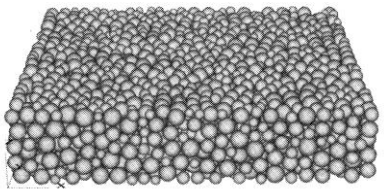
Engineers often have to face problems in which the mechanical behaviour of materials or structures consisting of separate components like grains, stone blocks, bricks etc. have to be predicted. Materials like corn stored in a silo, dry sand or rubble, ice blocks floating on the river; structures like masonry arches, domes, old stone bridges etc. are mechanical systems whose behaviour is fundamentally determined by the fact that they have a characteristic discrete internal structure which changes as a response to the external effects. In the failure of a masonry vault the separation or the sliding of neighbouring voussoirs usually plays a basic role. The deformation of a sandy soil originates basically from the sand particles rolling and sliding along each other which leads to the rearrangement of the microstructure. The wall pressure acting on a silo is caused by the internal "arches" and "chains", i.e. load-bearing arrangements of particles.

The usual, continuum-based calculation techniques like FEM or finite difference methods are unable to directly reflect these phenomena. This was the reason why engineers have been searching for alternative modelling methods, and already from the 1970ies started to develop different discrete element techniques.

DEM became an everyday tool for modern engineers in the 1990ies when the development of computer hardware reached the level where realistic problems could already be analysed on PC-s in reasonable computational time.



(a)
Discrete element model of a masonry arch: elements correspond to the voussoirs
Bicanic, 2003



(b)
3500 spherical discrete elements representing a sand layer which consists of millions of particles
Calvetti et al, 2004

Figure 1.

Any discrete element model consists of two basic components: the ***elements***, and the ***contacts*** between them. The elements may either directly correspond to those physical units which form the analysed system (e.g. stone voussoirs, sand grains, bricks), or, alternatively, the collection of elements as a whole represents a collection of a much larger number of real particles. Figure 1 illustrates these two possibilities: in 1(a) the discrete elements represent the stone voussoirs (one-to-one correspondence), while in 1(b) a few thousand discrete elements simulate the behaviour of a sand layer consisting of millions of particles.

Slightly modifying the original definition of Cundall and Hart (1992), a numerical technique is said to be a discrete element model if

→ it consists of separate, finite-sized bodies ("discrete elements") each of them being able to displace (and in many codes to deform) independently of each other;

→ the displacements of the elements can be large (i.e. not infinitesimally small);

→ the elements can come into contact with each other and loose contact, and these changes of the topology are automatically detected during the calculations.

The ability of the elements to move independently of each other is a basic difference from FEM where different continuity conditions have to be satisfied at the common nodes of neighbouring elements. In addition, while several FEM, frame or fracture mechanical software are able to simulate the separation of elements, a DEM code must possess the ability to handle contact creation too.

1.2 The elements

1.2.1. Geometrical shape

The elements in the different discrete element softwares have a wide variety of shapes: convex or concave, smooth or nonsmooth, polyhedral, spherical, elliptical or any composition of simple regular bodies. UDEC (Cundall, 1971) and DDA (Shi, 1988 or 2001), for instance, use polyhedra; PFC (Cundall and Strack, 1979), OVAL (Kuhn, 2003) or EDEM apply "clumps" prepared by rigidly gluing together intersecting spheres of different radii; the model of Ng (2001) contains ellipses etc. A few 2D illustrations are shown in Figure 2.

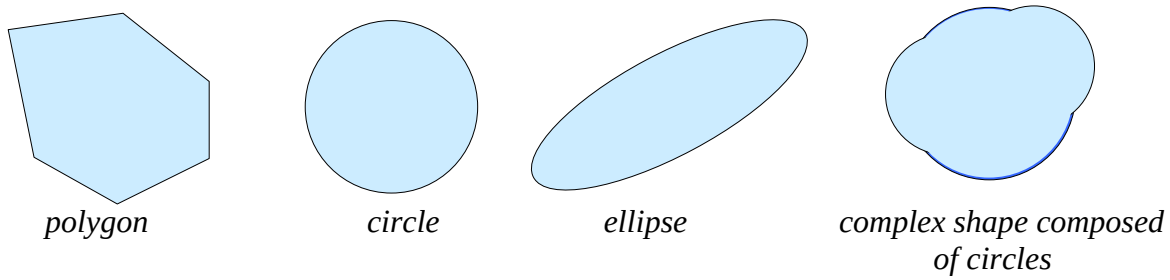


Figure 2.: 2D element shapes

Though perfectly circular or spherical elements are most easy to treat from computational point of view, it is a basic experience already from the 1980ies (e.g. Rothenburg and Bathurst, 1993) that the application of such elements may lead to very unrealistic behaviour of the model, particularly in the case of non-cemented assemblies of particles. (Spherical particles have an extreme rotating ability in comparison even to slightly elongated shapes.) Hence, irregular particles are often composed of simpler units (e.g. spheres or cylinders), whose treatment inherits the simplicity of the analysis of the original components. As illustrated in Figure 3, realistic particle shapes can easily be produced this way.

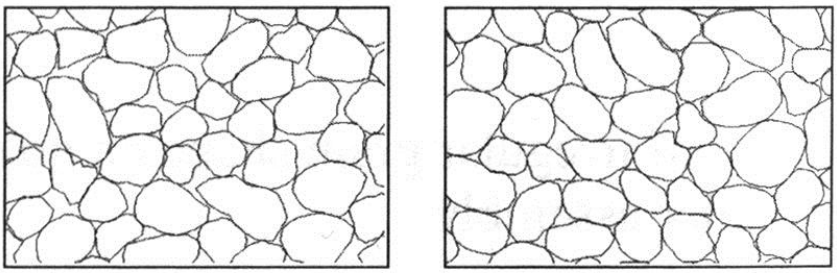


Figure 3.: Simulation of sand samples with the help of irregular elements composed of circles. (Matsushima, 2005)

In modern DEM investigations the individual particles may be made breakable (e.g. McDowell and Harireche, 2002; Cheng et al, 2003): they can fall into their components or groups of components under suitable mechanical conditions.

1.2.2. Mechanical properties of the elements

In mechanical sense the elements may either be perfectly rigid bodies, or deformable according to different (e.g. isotropic linearly elastic) constitutive relations; in some codes the user has the option to define the material behaviour. If applying a deformable element, the constitutive relations specify the relations between the stress and the strain over the characteristic domains of the element. (In UDEC, for instance, the polyhedral elements are subdivided into simplexes, i.e. triangles in 2D and tetrahedral in 3D, and the constitutive relations describe how to calculate the stress belonging to a simplex from the strain which is uniform inside the simplex. The different simplexes inside the same discrete element carry different strains, so complicated deformation and stress patterns can be simulated inside the individual elements. Another possibility is applied in DDA where the element carries a uniform strain and hence a uniform stress, in all its points, independently of its shape.) Failure conditions (e.g. plastic limits) can also be prescribed, and these conditions also belong to the constitutive relations of the element.

1.3 The contacts

1.3.1 Contact detection algorithms

The detection of contacting pairs of elements is a fundamental part of any discrete element model. Where two elements get in touch, forces (perhaps moments too) are transmitted, and these forces determine the static state of the whole system.

The identification of contacting pairs is a very time-consuming task. In principle, all pairs of elements should be considered one by one; and the shortest distance between the points of the two elements should be determined. If this shortest distance is greater than zero, then the two elements are not in contact; otherwise they touch or intersect with each other. The number of necessary calculations are proportional to the square of the number of elements.

There are several approaches to shorten this computationally very expensive process. The most common idea is to restrict the exact calculations only to a small set of pairs

("candidates"), and exclude those pairs from the exact analysis which are surely not in contact. According to "***body based search***" techniques, each element is considered separately: a window is assigned to the element under question, and only those other elements are checked for contact by calculations which are inside this window. In case of the "***space based search***" techniques several (strongly overlapping) windows are specified inside the complete domain of the analysis, and these windows are analysed one by one: only those pairs of elements are checked by exact calculations which are inside the same window.

When the elements have a complex shape whose distance from other elements is difficult to calculate precisely, the analysis of a pair can be done in two steps. First, a bounding domain of simple shape (sphere or brick) is defined around the first complex element so that all points of the element are inside the bounding domain. The same is done for the other element under consideration. If the two bounding domains have no common point, the two elements are surely not in contact, and further calculations are unnecessary. However, if the two domains overlap, a detailed analysis can follow.

1.2.2 Mechanical behaviour of the contacts

When two elements get in touch with each other, contact forces are transmitted between them. The constitutive relations of the contact describe how to determine these transmitted forces, usually from the overlaps and relative displacements of the two material regions forming the contact.

A few older DEM codes contained non-deformable contacts where the transmitted forces could be arbitrary while the contact was undeformed, and the contact forces were calculated from the equilibrium of the elements. However, these methods had several disadvantages and did not become widespread, their application remained restricted to special research softwares only. The contact models in the usual commercial codes work in such a way that after the contact is formed, its deformations (i.e. the relative displacements of those two material points forming the contact) during the analysed process are detected, and from them the contact forces are updated again and again. A very simple illustrative version is shown in Figure 4 where the elements are circular and perfectly rigid, and the two material points forming the contact are marked by black dots.

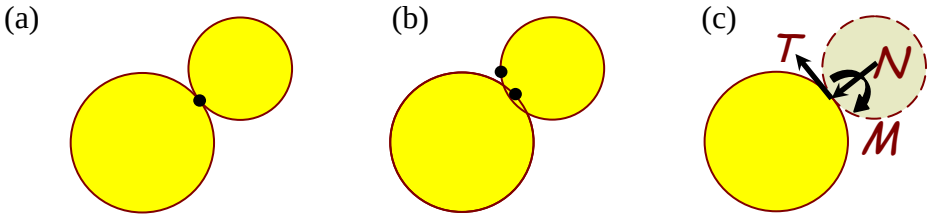


Figure 4.
Contact forces

Figure 4(a) shows the situation when the contact is just formed: two small material regions, just at coinciding position at this stage, are shown with the same dot. As the elements move, these material regions are displaced in a different way: consequently, a relative translation in the normal and in the tangential direction, and a relative rotation occurs (Figure 4(b)). A normal and a tangentional force, and a bending moment are consequently expressed by the two elements on each other (Figure 4(c)). The constitutive relations of the contact have to specify how the contact forces and moments depend on the relative displacements of the contact. Limits to the statically admissible forces and moments can also belong to the

constitutive relations, e.g. frictional limit for the tangential force, or a maximally possible tensile force etc. can be specified.

The system of contact forces may of course be much more complex in the case of complicated elements, particularly in 3D.

1.4 The initial geometrical arrangement

Similarly to the first step of FEM analysis, the discrete element modelling of a problem starts with the preparation of the ***geometrical*** model of the analysed system: the starting position and shape of the discrete elements have to be specified. This is rather straightforward if the discrete elements directly represent the units of the real structure whose geometrical data are known.

However, for the discrete element modelling of e.g. an assembly of corn stored in a silo, or a sand sample under a building, this is not the case: in several engineering problems a random ***dense initial arrangement*** of touching discrete elements has to be applied as the starting geometry. But to produce such an arrangement of thousands (perhaps millions) of densely packed particles can be a rather challenging task.

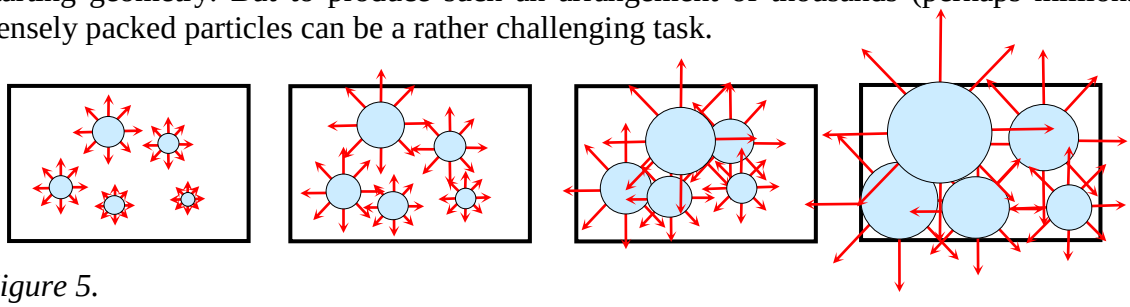


Figure 5.
Gradual increase of the elements

1.4.1 Dynamic methods

Most engineers use their DEM code itself for the preparation of the initial arrangements, and generate the geometry of their assemblies with the help of different ***dynamic methods***. A typical approach is to place the required number of elements (with diameters much smaller than their final size) into the domain of interest; then the particle diameters are gradually increased, and they push each other until a dense arrangement with the desired porosity is reached (Figure 5). Alternatively, having assigned the final size to the particles, they can be placed into a large domain whose walls are slowly moved inwards until the required density is reached (Figure 6). Both methods involve multiple collisions during the densification process, until the particles push each other into an evenly dense arrangement.

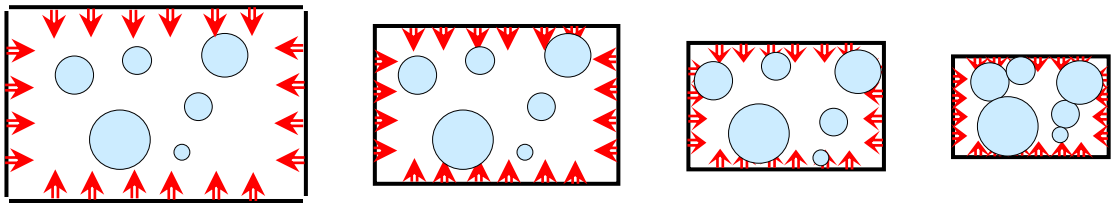


Figure 6.
Isotropic compression

Another possibility is to simulate some kind of a gravitational deposition: the particles (having assigned their final size) fall down into the domain as if into a container, and find their equilibrium position under the effect of gravity (Figure 7).

These dynamic techniques can be applied for any element shapes.

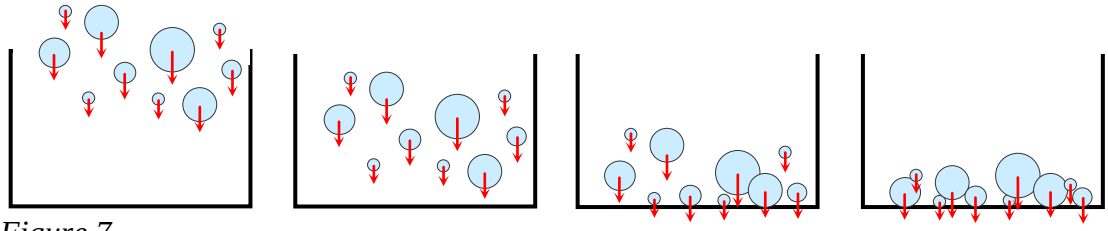


Figure 7.
Gravitational deposition

1.4.2 Constructive algorithms

Since the motion of each particle has to be simulated with the DEM code during the whole process, these preparation methods require a huge amount of calculations hence they are rather time-consuming. Another set of approaches, called ***constructive algorithms***, may provide advantageous alternatives to the dynamical methods. The basic feature of these algorithms is that the assemblies are prepared with the help of purely geometrical calculations, without simulating the dynamics of particle motions. They are, on the other hand, mostly restricted to circular/spherical elements („particles" or „grains").

Sedimentation techniques, e.g. Jodrey and Tory (1979; 1985), can indeed quickly produce dense arrangements. The typical implementation can be introduced as follows. In order to fill up a parallelepipedal domain (as if a container), the first step is to produce an initial collection of pheres, usually a layer at the bottom of the container. Every subsequent step places a new sphere into the container, and translates it downwards, until the sphere hits an already existing sphere in the system. Then the new sphere is further moved just as if rolling down along the contacting sphere, until it finds a stable position by being supported by three previous spheres. It is important to emphasize that the new sphere is 'translated' and 'rolled' (i.e. the coordinates of its centre are modified) with purely geometrical calculations, without analyzing the dynamics of the system. The „dropping method" proposed by Bagi (1993) and the „open front technique" of Feng et al (2003) work basically in a similar manner.

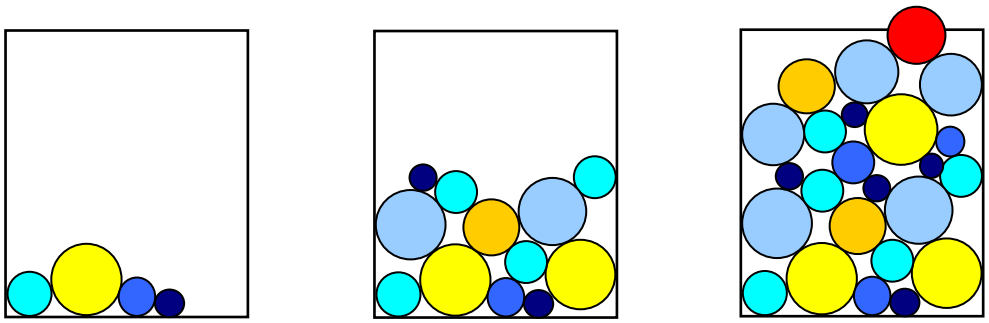


Figure 8.
Sedimentation techniques

In the sedimentation techniques the particle diameters may either be equal, or they can follow any user-defined size distribution. Rather high coordination numbers (i.e. average number of contacts per particle) can be reached: in 2D it is nearly 4, and in 3D this number approaches 6.

A common disadvantage of the sedimentation techniques is that a slight anisotropy is introduced into the microstructure: the produced assemblies are slightly stiffer in vertical compression than in horizontal compression. Another and more serious disadvantage is that (in general case) small ***gaps*** remain under the 'top'wall that cannot perfectly be filled up.

The ***closed front method***, also suggested by Feng et al (2003), fills up the desired 2D domain along an outwards spiral. At the beginning a triangle of three touching particles (circles) are placed into the middle of the domain. Then the additional particles are added one by one, by exactly attaching each new particle to two pre-existing grains (see Figure 2): While the method produces an isotropic geometrical arrangement, in the case of a general grain size distribution large gaps may remain at the edges of the domain. These gaps may turn out to be impossible to fill up, and it is possible for the walls to have no contacts at all with the assembly.

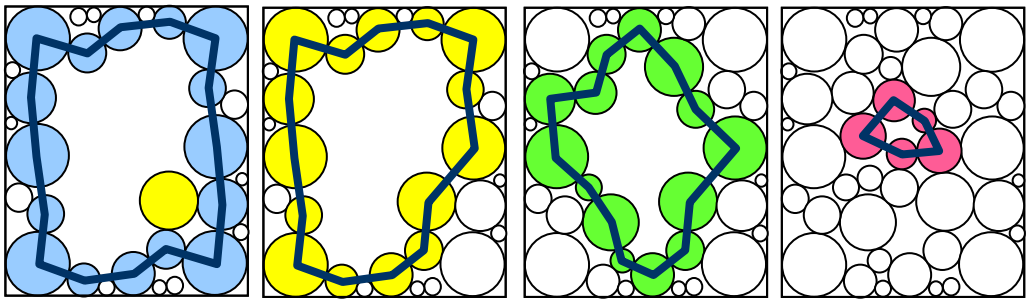


Figure 9.
The Inwards Packing Method

The ***inwards packing method*** proposed by Bagi (2005) proceeds in an opposite way: a chain of particles (either touching, or being close to each other) is formed first along the edges of the desired 2D domain, and then new elements are attached to its interior. The front proceeds inwards, until there is no more space for a next element. The 3D version of this technique was developed by Benabbou et al (2009). The great advantage of the method is that there are no gaps remaining along the edges.

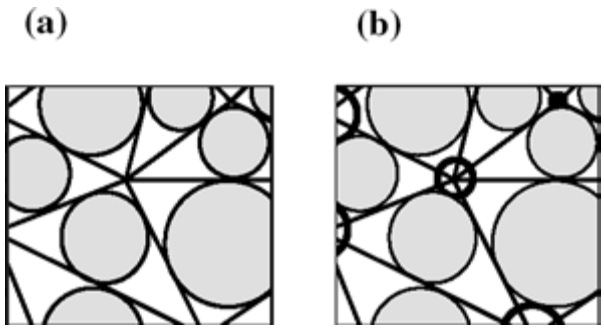


Figure 10.
The method of Cui and O'Sullivan:
(a): incircles of the triangular cells; (b): additional circles defined around the nodes

A completely different constructive algorithm was suggested by Cui and O'Sullivan (2003) for 2D and 3D assemblies of circular/spherical grains (see Figure 10). This method is based on creating a random mesh of triangles/tetrahedra in the domain of interest. The incircles/inspheres of the triangles/tetrahedra will be the grains of the assembly. The arrangements can further be densified by placing additional particles on the nodes of the mesh (not overlapping the previous grains, but touching the nearest one). The grain diameters cannot directly be prescribed in this model, the resulting systems are less dense, and the average coordination number is significantly lower than in case of any previous constructive technique. Significant advantages of this algorithm are, however, its simplicity, its easy generalization for 3D, and the very small computational cost associated with the preparation of an arrangement.

1.4.3 Collective rearrangement techniques

Finally the different ***collective rearrangement techniques*** have to be mentioned (Stillinger et al, 1964; Moscinski et al, 1989, Lubachevsky and Stillinger, 1990 etc; a novel version was published by Labra and Onate, 2009). In these methods the number of particles is defined by the user, and this number is fixed during the sample preparation process. Initially the particles are placed randomly into the desired domain. Overlaps are permitted, and their size is attempted to be reduced during the process by moving and sometimes by shrinking the grains in a stepwise relaxation manner. In every step the displacements of each grain is calculated from the overlaps of the grain with its neighbors, similarly to the dynamical sample preparation techniques (see Figure 11). Consequently, these algorithms are rather time-consuming, not much better than the dynamic methods.

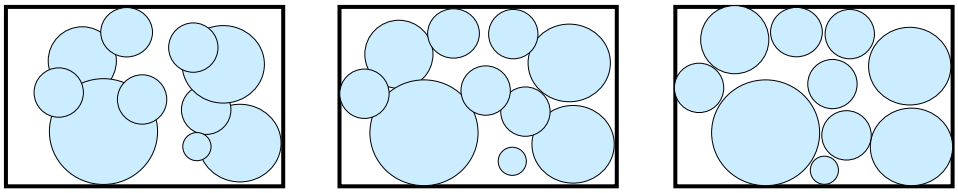


Figure 11.
Collective rearrangement techniques

1.5 The main steps of discrete element modelling

It was already explained that the first step of the simulation of an engineering problem is to prepare a ***geometrical model*** (Section 1.4). Then the ***mechanical characteristics*** of the elements and of the contacts have to be specified. After this, the ***loads*** acting on the system have to be given, the loads can vary in time.

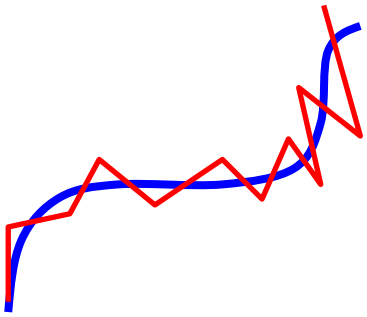


Figure 12.
The real motion of an element (blue) approximated by DEM (red)

The state changing process of the analysed system is approximated as a series of small but finite displacement increments (Figure 12). The calculation cycle for the determination of such an increment can be summarized in the following way:

– At the beginning of the cycle the geometry and the position of the elements, the contact topology, the forces acting directly on the elements and those transmitted in the contacts, the mechanical state (i.e. the deformations and the constitutive relations) of the contacts are known.
– Based on these data, the displacement increments are determined. There are several numerical calculation methods for this; the next lectures will focus on these details.
– The geometrical, topological, static and material data are updated, and a new calculation cycle can be started.

The forthcoming lectures will introduce the details of the most important DEM softwares.

Questions

1.1. What are the conditions to consider a numerical technique a discrete element model?
1.2. What is the task of the constitutive relations of the elements and of the contacts? From the point of view of mechanical behaviour, what basic types of elements and contacts are used in the different DEM models?
1.3. How can we prepare an initial arrangement of touching elements? What is the difference between dynamic, constructive and collective rearrangement techniques?
1.4. Introduce the main types of contact detection algorithms!
1.5. What are the three basic steps of discrete element modelling?