Conversion of Fractal Fields into Heterogeneities inside SPH Simulations

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Abstract. The inclusion of material heterogeneities in numerical simulations enables us to come close to the almost perfect description of the behaviour of structures. There are various ways and methods of introducing heterogeneity into a computational model. One of the methods is the creation of areas (fractal fields) in which material properties differ. The shape of such fractals is most frequently based on simple mathematical functions. However, this destroys the ability of the model to represent reality, as the structure of a real material is not based on any mathematical function. Fractals do not have to be based just on one simple mathematical function. On the contrary, they can be based on more complex inputs, such as real images of materials. In the case of images of concrete, fields can be generated which correspond to the presence of an aggregate, a cement binder or an air void. The contribution therefore describes fundamental steps in the creation of fractals, or the creation of fields based on real images of a material. The contribution also deals with the creation of material parameter oscillations and their subsequent inclusion in the numerical code of the Smoothed Particle Hydrodynamics (SPH) method. The conditions necessary for successful simulations if the SPH method is used are described. The whole process is clearly demonstrated using a pressure test conducted on a cylindrical concrete specimens. The presented results show the consequences of the inclusion of material heterogeneity in numerical simulations. These include randomness in the failure type or differences in the stress–strain diagrams of the monitored specimens. The functionality of the proposed process is supported by the results.

1. Introduction

The original idea in the very foundations of structure designing and related domains consisted in creating a simple and robust concept. With the progress of time, simple outlines gradually became more complicated, eventually reaching a stage where a mere pencil with a sheet of paper had ceased to suffice. Interestingly, at present we are often faced with efforts to design structures as simple as reasonably possible; after being completed, however, such structures may not necessarily be the simplest ones in terms of their behaviour and the presumptions of structural mechanics [1-3].

In concrete structures, the material heterogeneity offers a new dimension of complexity. Concrete, as the mixture of a concrete additive, a cement binder, and water, does not constitute a regular structure from any perspective or at any scale; with respect to this fact, not even the behaviour of the given structures can be assumed to remain identical in all cases. The introduced randomness is further multiplied by the type of load, which is invariably comprised in structural mechanic’s analyses [4-6].
In real-world conditions, countless loading tests can be carried out, and the rates of occurrence of an effect enable us to presume the most probable result of the series of tests to follow. However, numerical analyses and simulations, using common computational techniques such as the Finite Element Method (FEM), Finite Difference Method (FDM), or Smoothed Particle Hydrodynamics method (SPH), will not provide divergent results even with an infinite number of computations unless special add-ons are applied. In simulations where concrete-based materials are involved, we always encounter the problem of what material model is to be used [7, 8]. The results obtained from the varied models and their modified versions can differ fundamentally. Yet it is not advisable to introduce the heterogeneity directly into the description of the material model, mainly due to the increasing complexity of the operations and the lack of knowledge concerning the sensitivities of the model’s individual parameters before running the actual computation [9, 10].

A hitherto scarcely employed option consists in implementing the heterogeneity directly into the source code of the numerical method; however, there still remain the questions of whether this approach can be used to define the random behaviour of the monitored area, or the heterogeneity, and whether such numerical treatment can be further interconnected and explained using a real concrete structure. Numerical attenuation is utilized in fracture mechanics simulations, where the FEM often finds effective application. As the material model is the same in the entire monitored area, the finite element geometry can be modified such that any failure is immediately localizable at a pre-selected point (for example, via notching on a concrete beam). In high-speed loading, however, the FEM does not offer a suitable solution [11, 12]. Conversely, the attractivity of the SPH approach intensifies with the increasing loading speed, meaning that SPH method is more usable in diverse scenarios. Yet we also need to note that, in the case of the SPH, there is no physical mesh to interconnect the individual particles, and a mere change in the configuration of the particles may not provide the desired results (in fact, this type of action may even cause adverse effects, including the formation of numerical cracks) [13, 14].

The contribution describes a procedure which can be utilized to make use of images of real material structures for the generation of fractal fields (areas where heterogeneity will occur). At the same time, it shows how these heterogeneities can be amplified using the source code of the SPH method in such a way that the individual particles behave like a cement paste or aggregate and in this way create random material structure. As a result, the failures occurring in loaded specimens involve a variety of crack shapes. The whole process of heterogeneity generation is described by a simple experiment from the area of fracture mechanics in which a concrete cylinder is exposed to pressure load. The deformation results are compared with stress–strain curves.

2. Essential formulation of the SPH
The formulation of the SPH method is often divided into two key steps. The first step is the integral representation of field functions, and the second one is particle approximation. Assuming that the finite volume $\Delta V_j$ is assigned to the SPH particle $j$, the following relationship applies

$$ m_j = \Delta V_j \rho_j $$

(1)

where $m_j$ and $\rho_j$ are the mass and density of the particle $j$. The value of the monitored quantity $f(x_i)$, which is the product of integral representation and particle approximation operations, can thus be written as:

$$ f(x_i) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(x_j) W(x_i - x_j, h) $$

(2)

where $W$ is the so-called smoothing function and $h$ denotes the smoothing length defining the influence area of the smoothing function $W$. Equation (2) states that the value of a function at particle $i$ is
approximated using the average of those values of the function at all the particles in the support domain of the particle $i$ weighted by the smoothing function shown in figure 1, [13].

Figure 1. The particle approximations using particles within the support domain of the smoothing function $W$ for particle $i$

3. Fractal fields and material heterogeneity

The shapes of the fractal fields in which oscillations of material parameters occur can be based on various mathematical functions or distribution theories. However, such assumptions are not based on the real structure of the material. They are only some kind of effort to introduce randomness to a numerical model. A far more accurate approach would be to generate a fractal field directly from images of the structure of the material. In the case of an image of concrete, it would be possible to distinguish aggregate and cement paste from one another. Colours could subsequently be assigned to these particles, thus simplifying the image of the structure into an image of some coloured areas. The colour scale can be very simple, based only on shades of grey. These areas can be projected very easily into a space in such a way that every colour has a spatial depth allocated which is, e.g. dependent on any distribution function of random distribution. An algorithm is thus created which is able to generate spatial fractal fields from real images. Examples of real images of concrete transformed into simplified areas in various ways are shown in figure 2. These structures will subsequently be used in simulations. They will be compared with homogeneous material.

Figure 2. Examples of real images of concrete transformed into simplified areas in various ways.

Black – cement paste; white – aggregate
4. Numerical heterogeneity

If a numerical model is interleaved with generated fields, various material parameters can subsequently be assigned to these fields. For example, a generated field representing a cement paste will be given the material properties of the cement paste, a generated field which represents an aggregate will take on the material properties of that aggregate, and so on. However, this process can of course be amplified further in such a way that the heterogeneity is increased even more. For example, the oscillation of material properties can be modelled at the cement paste-aggregate interface, or directly inside the generated field. If the simulation is executed using the SPH method, its numerical code can be modified advantageously in order to achieve the aforementioned result. This can then be referred to as the introduction of “numerical heterogeneity”.

The implementation of the numerical (material) heterogeneity into the tested models was performed via modifying the weight value function of the individual SPH particles; in other words, the particle mass $m_j$ included in (2) was modified. Further, the same density value was preserved in all the particles, meaning that – with respect to the validity of (1) – the volume assigned to the individual particles was virtually modified (enlarged/reduced). However, due to the necessity to maintain the best possible particle distribution regularity in the tested models (an identical smoothing length for all the particles), the initial particle distributions were generated for the state where all the particles are assigned the same volume $\Delta V_j$. This operation is graphically represented in figure 3.

5. Mass distribution and experiment set up

As the individual SPH particles had to be assigned various masses, it was necessary to build the entire distribution algorithm upon the precondition of a constant weight of the resulting body – concrete cylinder in the tested scenario. The algorithm can nevertheless satisfy the conditions of any distribution function (including, for example, the normal, uniform, or Poisson distribution variants). For the actual testing, the uniform distribution of the occurrence of masses was selected. The reason for choosing uniform distribution consisted in testing the computational stability. The properties of the smoothing function enable the SPH method to suppress or highlight the heterogeneities contained in a computational procedure [13]. By another definition, the sensitivity of the computational stability in the presence of particles with significantly different masses was tested.

Figure 4 shows the tested specimens with a depiction of the distribution of the mass of the individual particles. These are cylindrical specimens with a height of 300 mm and a diameter of 150 mm. As one of the conditions for the functionality of the introduced algorithm is regular initial particle distribution, the cylinders were discretized by 50 particles along their height and 25 particles along their width or depth. The particles were arranged into a regular grid field, not a radial one.
A total of four specimens were tested. The first of them was a homogeneous specimen, a “reference sample” without any implementation of fractal fields or heterogeneity. The remaining three specimens already contained generated fractal fields as well as the heterogeneities described in Chapter 4. The fractal fields were based on figure 2. A distinction was made between the specimens marked fractal field 1 – 3. The cylindrical specimens were statically loaded with controlled displacement until failure occurred. Stress–strain curves were recorded. The simulations involved 24,050 SPH particles in total and were performed via the LS-DYNA program [15]. The Continuous Surface Cap Model (CSCM) was chosen as the material model of concrete to be used [16, 17], meaning that all fields had assigned the same material model. Table 1 shows the parameters employed in the simulations.

Table 1. The material parameters for CSCM concrete model.

| Parameter                        | Value  |
|----------------------------------|--------|
| Mass density, $\rho_c$ (kgm$^{-3}$) | 2207   |
| Compressive strength, $f_c$ (MPa) | 47     |
| Initial shear modulus, $G$ (GPa)  | 12.92  |
| Initial bulk modulus, $K$ (GPa)  | 14.15  |
| Poisson’s ratio, $v_c$            | 0.18   |
| Fracture energy, $G_F$ (Jm$^{-2}$) | 83.25  |
| Maximum aggregate size, $a_g$ (mm) | 8      |

Figure 4. Mass distribution of the tested specimens (units in kg)

6. Results and discussions

This section discusses the algorithm functionality and compares also the generated specimens’ behaviour where the heterogeneity was introduced. The gray-marked portions of the images invariably represent a crackless material, whereas the red sectors stand for complete failures (main cracks mostly). All the results were captured at the same moment.

In the case of the homogeneous variant of the tested specimen, it was expected that one of the basic types of failure would occur – a main slanting crack, or several vertical cracks. It is clear from figure 5 that a main slanting crack was created. The resultant failures of the tested specimens with introduced heterogeneities took a very different form, yet follow the trend of the generated fractal fields. In the case of tested specimen fractal field 1, there is an obvious kinked crack that almost goes around the aggregate (propagating at the interface between the aggregate and the cement paste). As regards tested specimen fractal field 2, which features a minimum amount of cement paste in the model, an extensive part of the specimen collapses (compressive failure of the aggregate occurs). With tested specimen fractal field 3,
in which the fractal fields actually become smooth, the failure starts to resemble that of a homogeneous specimen. Only one main crack is thus created. The results of the deformations also correspond to the stress–strain curves in figure 6.

![Figure 5. Deformation of the tested specimens](image)

From the practical point of view the presented algorithm is numerically stable, mathematically transparent and is able to simply produce various results. More about the topic can be found in [18, 19].

![Figure 6. Stress–strain curves of the tested specimens](image)

7. Conclusions
The contribution describes a simple method of generating fractal fields in which numerical heterogeneity is also introduced based on the adaptation of the numerical code of the SPH method. The principle of fractal fields is that they are based on real images of material structure. The numerical heterogeneity which fractal fields provide thus corresponds to the real properties of concrete-based materials. The fundamental ideas behind algorithms and conditions are described; these need to be fulfilled so that
numerical (false) cracks which are not related to numerical heterogeneity are avoided. The whole principle is presented via a simple loading test in which a concrete cylinder is statically loaded until it fails. The functionality of the algorithm is clear from the results.

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