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RANDOM AND GRADIENT BASED FIELDS IN DISCRETE PARTICLE MODELS OF HETEROGENEOUS MATERIALS

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Abstract. *The proper characterization of the microstructure and macroscopic properties of random heterogeneous materials may help to interpret the observed scatter in many engineering problems. In this contribution, a lattice discrete particle model is presented in a civil engineering framework with a special emphasis on concrete structures and infrastructure. The implications of spatial variability are investigated with regard to the observed scatter in standard concrete tests. In particular, classical experiments, such as three-point bending tests, may exhibit various levels of scatter which have to be accounted for if material characteristics are to be derived from such experiments and consequently used for the analysis and design of structural systems. Therefore, random and gradient based fields are combined in this paper in an attempt to realistically capture the material properties and associated variability stemming from the microstructure and macroscopic features such as the placement of coarse aggregates. Various mechanical and statistical aspects of simulated test series are investigated, such as macroscopic fracture energy or distribution of load bearing capacity. The presented application example of three-point bend specimens incorporates not only the inherent spatial variability owing to the placement of aggregates, modelled by random fields, but also various production artefacts, such as concrete compacting characterized here by gradient based fields.*

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1 INTRODUCTION

The estimation of uncertainties in probabilistic structural analysis may improve if the spatial variability concept is properly introduced. The presented paper addresses various discrete particle placement choices and schemes for discrete particle models such that the governing realization(s) of random or gradient-based fields is correlated to a particular structural discretization (i.e. radius and placement of particles) in a discrete framework.

This work is partially motivated by the increasing demand in developing procedures for statistical estimates of structural response, including deteriorating structures, many of which are still in use due to socio-economic constraints, and by the increasingly available computational resources [1], [2]. This has prompted research into Monte Carlo (MC) based small-sample simulation methods [3], [4], where, despite the capacity of current computers, and in particular in the context of spatial variability, practical utilization requires the availability of an effective sampling strategy that would dramatically reduce the number of required realizations while maintaining accurate estimates of the response characteristics (low-probability large-consequence events) [5]. Recent attempts addressing the sampling strategy for spatial variability in the MC simulation framework include [6], [7], which is based on the original work of [8], where critical samples of stochastic processes are identified.

In this paper the main focus diverts from the reliability aspects of spatial variability and aims to investigate how particle placement schemes may be used to characterize various microstructural and macroscopic properties of random heterogeneous materials [9], while maintaining the material property fields constant. Any observed scatter can therefore be directly attributed to the chosen particle placement scheme and its parameters. This implies a causal relationship between spatial variability, auto-correlation length of the random fields, type of spectral function and meso/micro-structure of the material which is an open research question.

2 LDPM

The so-called lattice discrete particle model (LDPM) naturally accounts for material heterogeneity by random particle placement and size, which is also constrained by a grading curve [10]. This approach captures most microstructural effects of concrete very well, when compared to the continuum framework, however introducing higher order spatial variability enables to control and interpret the response scatter [6], [9].

As a well-established member of the discrete framework, LDPM has been extensively calibrated and validated and has shown superior capabilities in reproducing and predicting concrete behavior [10]–[14]. It simulates the mesostructure of concrete by a three-dimensional (3D) assemblage of particles that are generated randomly according to a given grain size distribution. Delaunay tetrahedralization and 3D domain tessellation are used here to generate a system of cells interacting through triangular facets. Displacements and rotations of such adjacent particles form the discrete compatibility equations in terms of rigid body kinematics. At each cell facet the mesoscale constitutive law is formulated such that it simulates cohesive fracture, compaction due to pose collapse, frictional slip and rate effect. For each single particle, the equilibrium equations are finally evaluated. An extended version of LDPM is currently being developed and simulates various coupled deterioration mechanisms, such as Alkali-Silica reaction (ASR) [12], [15]. A further development is the age-dependent LDPM framework in which the local material properties are derived by chemo-mechanical coupling with a chemo-hygro-thermal model [16], [17] which also drives the creep and shrinkage analysis in a rate type form [18].

3 ABSTRACTION LEVELS FOR LDPM

The proposed particle placement schemes have become part of the spatial variability package for LDPM and, as will be shown in the next chapter, may influence not only the scattering and asymptotic properties of the spatially variable models but also shift the mean value of repeated identical experiments. By introducing the spatial variability package for LDPM a significant contribution to the general understanding of physics and reliability of spatial variability may be achieved.

The independent and random particle placement (IRPP) scheme, as implemented in the original LDPM, may be considered as a first abstraction level. Here, the random diameters are generated according to the size distribution curve until the required volume fraction is reached (figure 1). No conflicting requirements are to be solved. Overlapping or less than minimum distance particles are resampled. Implications are scarcely populated boundary regions and an invariant coefficient of variation. The original procedure for generating particles is described in detail in [10].

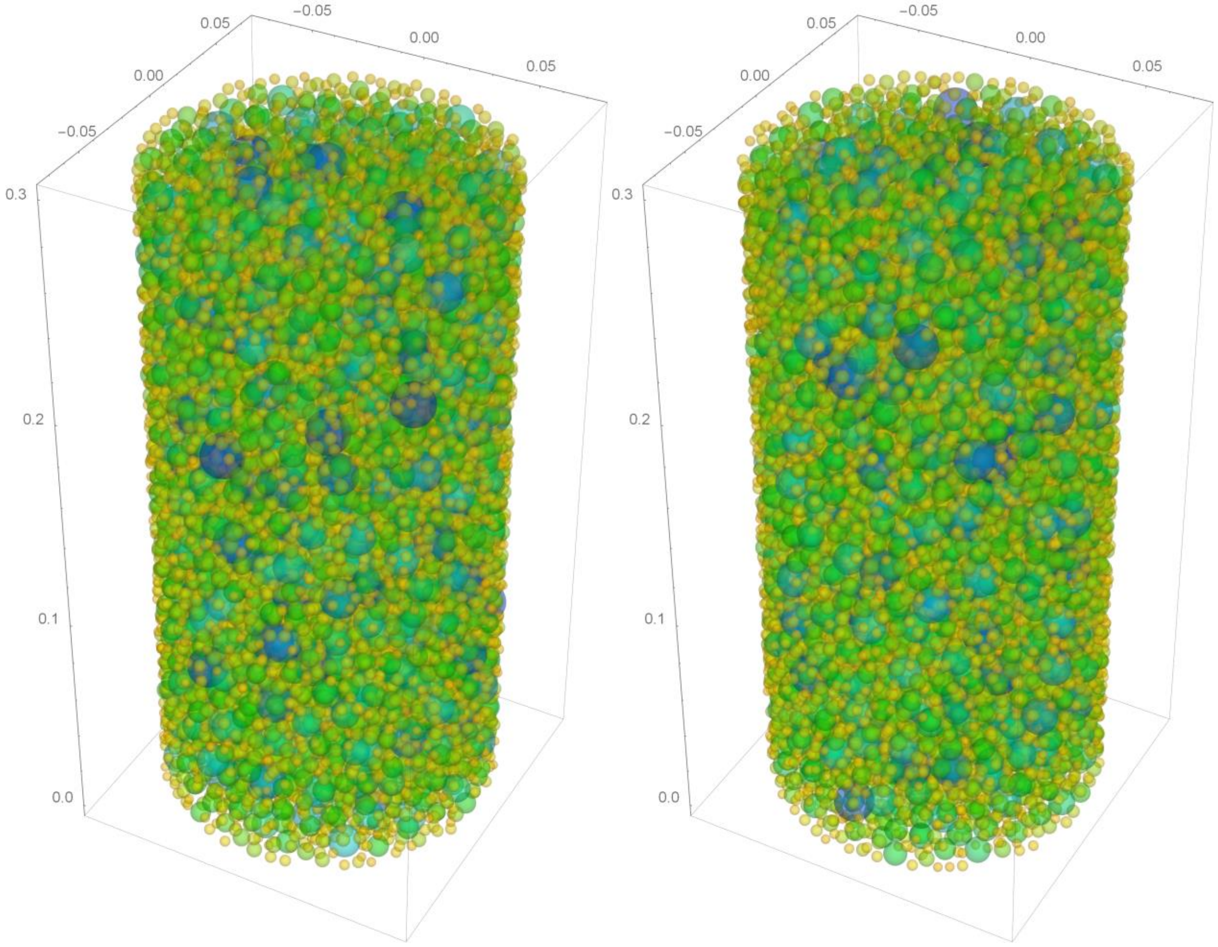

Figure 1: Maximum (left) and minimum (right) strength realizations of LDPM using the random and independent particle generation scheme.

The second abstraction level assumes the original particle placement scheme, i.e. the IRPP, combined with one or more spatially variable fields, which are used to describe local fluctuations of material properties resulting from its inherent variability (random field, figure 2) and construction or transport processes (gradient-based fields). Similarly to the previous case, there are no geometry-related conflicting requirements and overlapping or less than minimum distance particles are resampled. Boundary regions may be normally populated by adopting a simple modification to the re-sampling algorithm. Please note that material characterizations derived from random fields must be verified for inadmissible values, such as negative strength, modulus, etc. This may lead to a conflict if the governing probability distribution, used for the random field generation, is to be maintained. Otherwise, truncated distributions may be used or the realization of random field can be rescaled to fit admissible range [6], [19], [20]. This is a quite popular abstraction level, especially for continuum models, but stipulates full independence between microstructure, i.e. particle placement and material properties. The later assumption is reasonable for continuum models but questionable for lower-scale models such as LDPM.

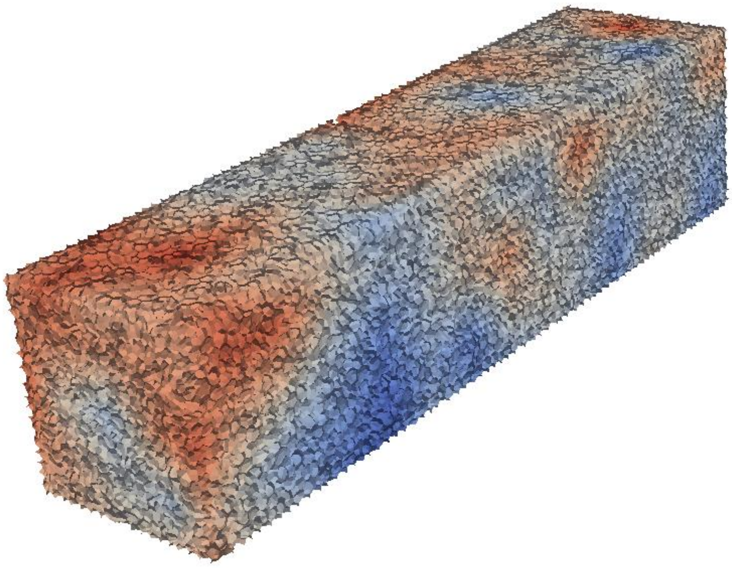

Figure 2: Sample realization of a Gaussian random field with a power spectral function $\#^{-2}$ as a material property field only.

The third abstraction level assumes that an initial random or gradient-based field of choice (or their arbitrary combination) governs the particle generation process (i.e. the position and size of each particle). If the particle generation is to be governed not only by granulometric distributions, but also by an initial random (figure 3) or gradient-based field (figure 4), the particle generation becomes a complex problem and has to be approached by balancing trade-offs between conflicting goals. Clearly, the global requirement on particular size distribution can lead to a local conflict with the initial random field, the role of which can be further ambiguous if we consider it to affect both the position and size of the particles (clustering of large particles). Details regarding the associated steps/choices for random fields were published in [9]. For higher volume fractions this becomes a computationally expensive procedure, however local conflicts can be resolved in parallel and terminate with the first valid particle.

Alternatively, the initial random or gradient based field may not only govern the particle generation process but also be used to modify the material property fields and thus maintain compatibility between the two domains.

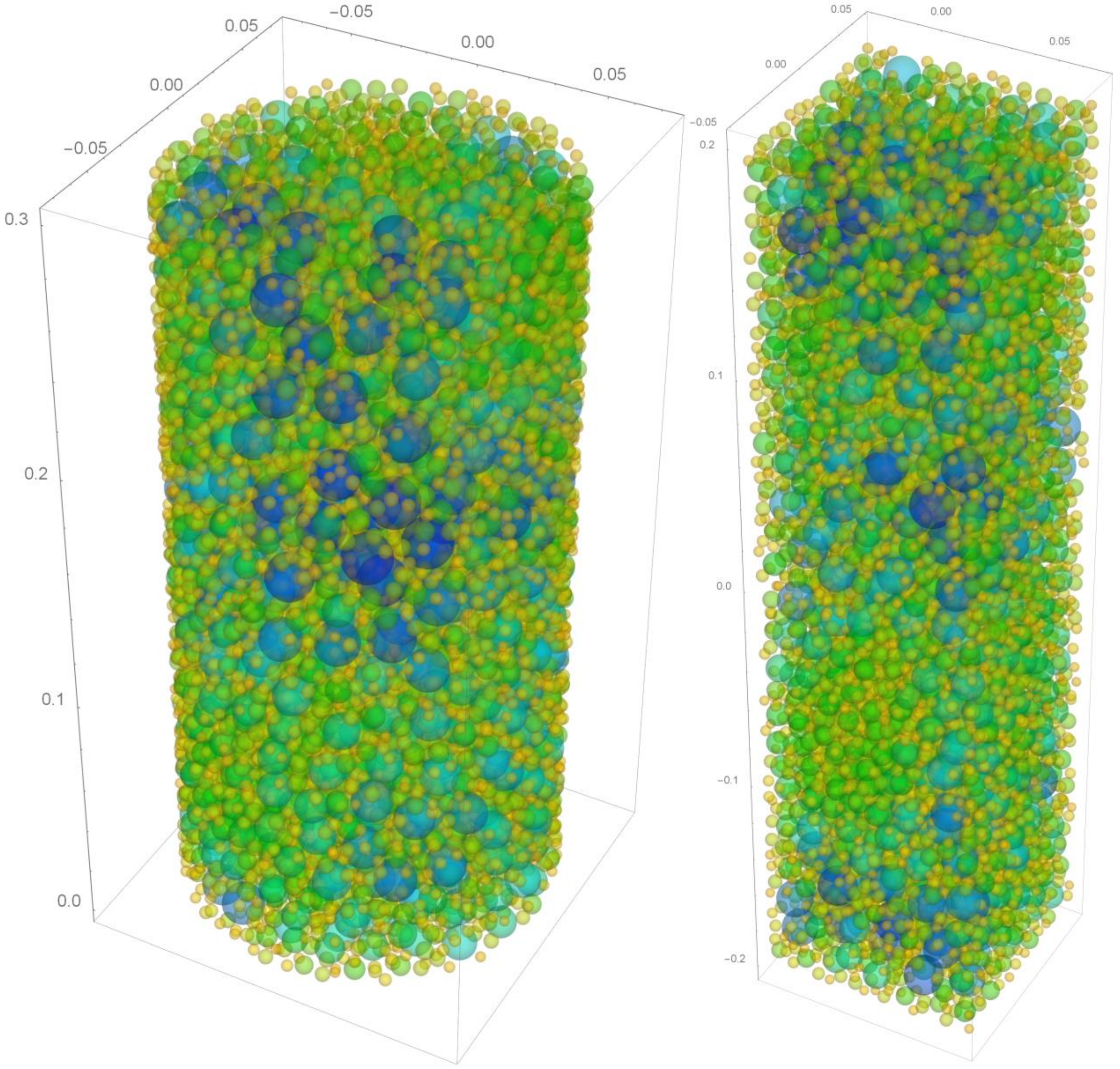

Figure 3: Maximum strength realizations of LDPM experiments based on a governing Gaussian random field with a power spectral parameter ($\#^{-2.00}$) maximizing the COV of load capacity.

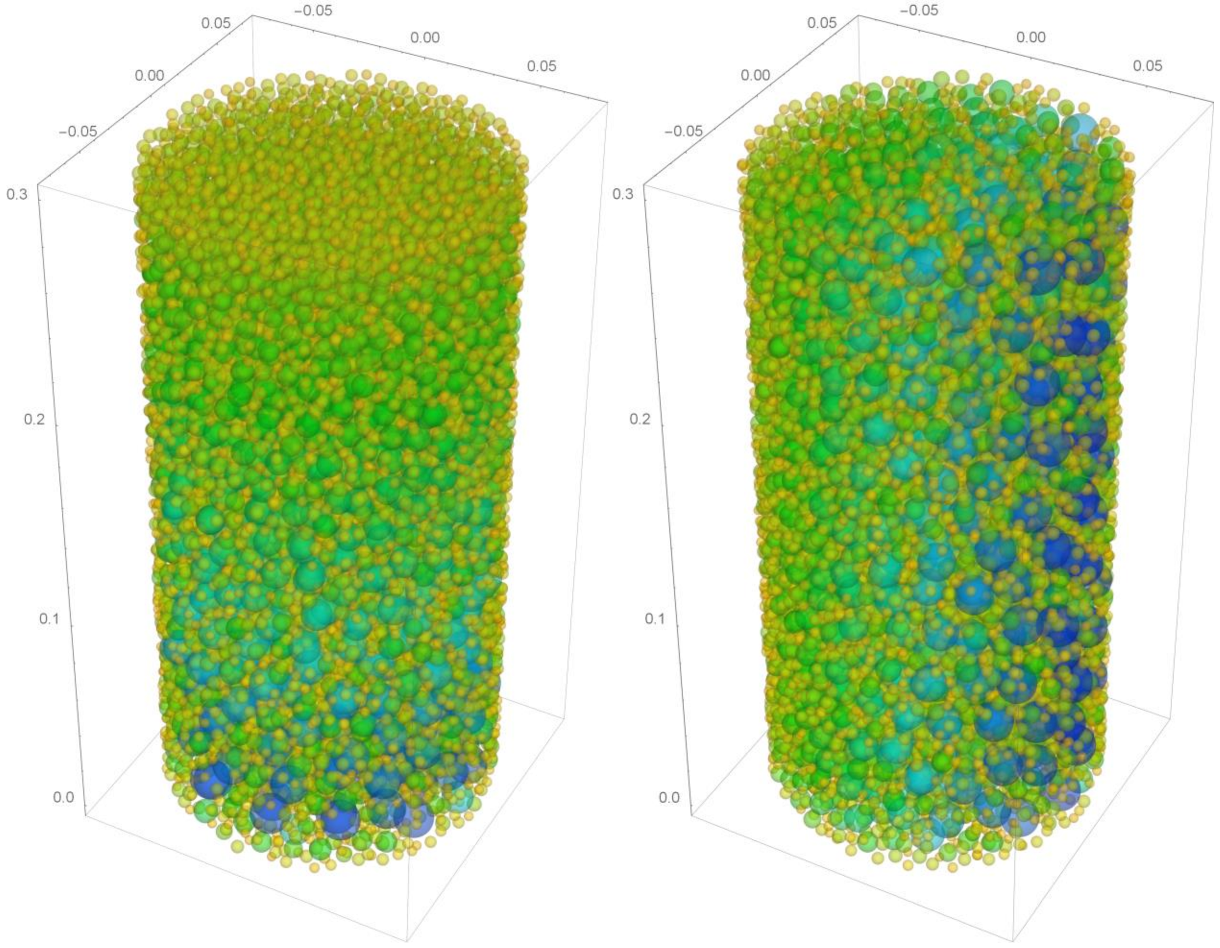

Figure 4: Maximum strength realizations of cylindrical compression tests with gravity-based gradient field (left) and normal-to-gravity-based gradient field (right).

4 RESULTS

Selected observation regarding the statistical characterization of parallel identical LDPM experiments and various particle placement schemes are discussed in this chapter. Two classical experiments for concrete, the cylinder compression test (D150x300 mm) and notched three point bending test (400x400x100 mm), have been statistically reproduced by LDPM and the spatial variability package. Each of the presented numerical experiments is characterized by 20 realizations. The same sequence of seeds for the random number generation is maintained throughout the experiment. Figure 1 shows the ensemble of particles for the abstraction level 1, i.e. the independent and random particle placement scheme for the maximum and minimum strength realizations. Figure 2 conceptually depicts the abstraction level 2, i.e. particular realization of a random material property field which is combined with independently and randomly generated ensemble of particles. Figure 3 shows the maximum strength realizations of a gradient and a Gaussian random field with a power spectral function $f(x) = \#^{-2.00}$ for the cylindrical compression test and three point bending test (notched). Figure 4 shows the maximum strength realizations of cylindrical compression tests with gravity-based gradient field (the failure is depicted in figure 5) and normal-to-gravity-based gradient field. The consequence of rotating the gravity-based gradient field is evident from figure 6 where the scattered load-displacement (LD) diagrams are shifted upwards for the rotated version (figure 4 right), i.e. the mean capacity is increased by ~2%.

Finally, the normalized statistical characteristics are plotted in figure 7 against various power spectral parameter values. Here, the 20 cylindrical compression tests share the same material property fields (constant) and differ only by the particular realizations of the particle generation, in this case based on the abstraction level 3 using a Gaussian random field with power spectral function $\#^{-n}$. For the reference, the dashed line is added into the plot to mark the zero correlation length, which corresponds to the level 1 IRPP scheme. Please note that the range of COVs for the cylindrical compression test series is 0.42 to 0.66 % and for the notched three point bending test series 2.11 to 3.71 %, considering the various particle placement schemes only.

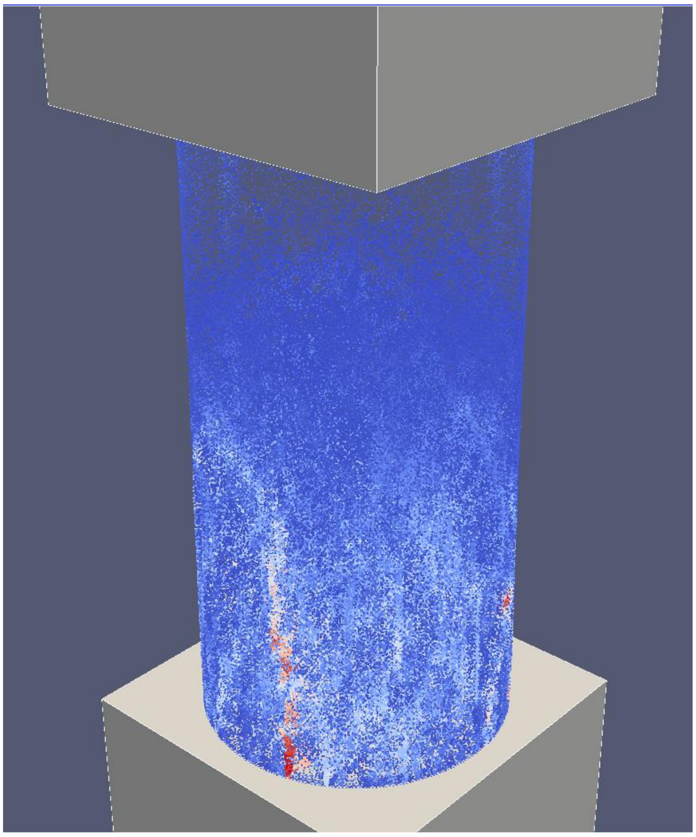

Figure 5: Visualization of a crack opening displacement (red color ~ 0.7 mm) at peak load at maximum strength realization of cylindrical compression tests with gravity-based gradient field (fig. 2 left).

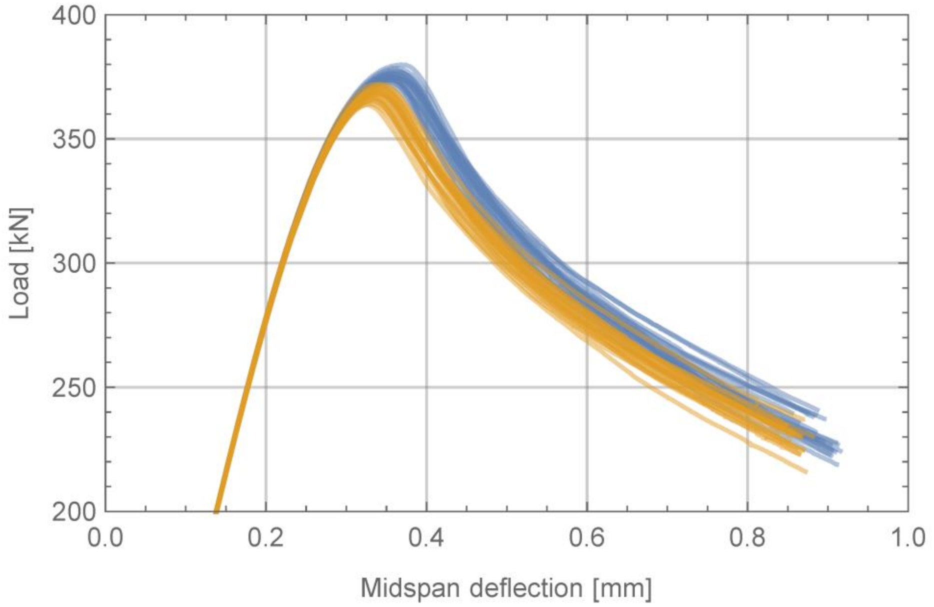

Figure 6: Scattering and shifted L-D diagrams (zoomed-in detail) of LDPM realizations of compression cylinder tests with two gradient-based fields (gravity angle is orange and normal to gravity angle is blue).

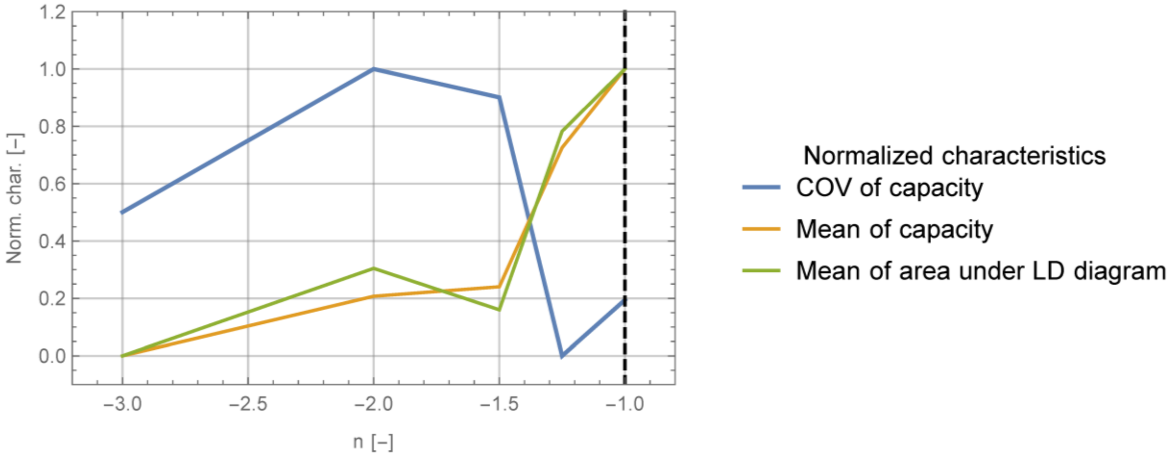

Figure 7: Normalized statistical characteristics vs. power spectral parameter *n*; response of cylindrical compression test series (20 realizations) and Gaussian random field with power spectral function $\#^{-n}$. The dashed line represents the zero correlation reference, i.e. the IRPP scheme.

5 CONCLUSIONS

- The inverse U-shaped curve for the coefficient of variation (figure 7) and various power spectral parameters clearly supports the hypotheses on a causal relationship between spatial variability, auto-correlation length of the random fields, type of spectral function and meso/micro-structure of the material. Please note that the material property fields are constant for all presented results.
- Although the relative differences resulting from the presented abstraction level 3 (i.e. correlated particle placement scheme and constant material property fields) may not always be significant, the ability to obtain the functional form for mean values and COV of response series represents a fundamental concept for spatial variability based structural reliability.
- The relative differences in terms of COV for parallel identical test series may increase dramatically if (a) the material property fields are randomized, (b) engineering failure probabilities ($\sim < 10^{-4}$) are introduced (by effective sampling strategy) rather than a first passage probability based on 20 realizations, and (c) structural components or structures are analyzed that are sensitive to damage localization leading to, e.g., the statistical size-effect.
- Even if the material property field remains constant, the various particle placement schemes derived from initial random or gradient based field may be used to control not only the scattering of simulated experiments, but also to shift the mean values of the response.
- Several abstraction levels for the lattice discrete particle models of concrete have been presented, together with a particle placement schemes derived from initial random or gradient based fields.
- The proposed spatial variability package for LDPM may dramatically increase the consistency and realism of the LPDM paradigm if a physical reference for the governing spatially variable field is established.
- Reliability of spatially variable LDPM models will require an objective statistical characterization in a small sample Monte Carlo simulation framework.

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