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The Use of Lattice Discrete Particle Models in Selected Civil Engineering Problems

Využití částicových modelů ve vybraných úlohách stavebního inženýrství

SUMMARY

The Lattice Discrete Particle Model (LDPM) is an advanced numerical approach that effectively models the behaviour of various materials by representing them as a collection of discrete particles interacting over the facets. This method surpasses conventional finite element models by accurately capturing the heterogeneous nature of materials such as concrete, fibre-reinforced composites, and particulate polymers.

The thesis focuses on several civil engineering applications, highlighting the indispensable role of LDPM in simulating complex phenomena such as fracture mechanics, material failure, and multi-physics interactions. These applications include adhesive anchors, prestressed/post-tensioned concrete beams, the viscoelastic behaviour of macro-synthetic fibre-reinforced concrete, and fibre-reinforced polymer-concrete joints.

Key findings demonstrate the LDPM's ability to predict the mechanical behaviour of structural elements under various loading conditions. The particle-based nature of the model allows for precise simulation of crack patterns and stress distribution, offering valuable insights into the design and analysis of civil engineering structures. Moreover, the research underscores the necessity of multi-physics simulations in capturing the complex behaviour of materials. Therefore, the thesis emphasizes the LDPM's versatility and adaptability and stresses its potential for broader application in civil engineering.

SOUHRN

Tato práce se zabývá částicovým modelem LDPM (Lattice Discrete Particle Model) a ukazuje možnosti jeho využití při řešení úloh stavebního inženýrství. LDPM je pokročilý numerický model, který popisuje chování materiálů jako soubor diskrétních částic, které na sebe vzájemně působí přes plošky (facety) na rozhraní. Oproti běžně používané metodě konečných prvků umožňuje LDPM zachytit heterogenitu materiálů, jako je beton, vlákny vyztužené kompozity a reaktoplasty s plnivem.

Práce se zaměřuje na několik vybraných aplikací a zdůrazňuje klíčovou roli LDPM při simulaci složitých jevů, jako je lomová mechanika, poruchy materiálů a interakce více fyzikálních jevů. Tyto aplikace zahrnují chemické kotvení (vlepovanou výztuž), předpjaté betonové nosníky, viskoelastické chování betonu vyztuženého syntetickými vlákny a spoj mezi betonem a vlákny vyztuženým polymerem.

Předložené výsledky ukazují schopnost LDPM přesně zachytit chování konstrukčních prvků za různých zatěžovacích podmínek. Částicový model také umožňuje věrohodné zachycení vzorů trhlin a rozložení napětí, což poskytuje cenné poznatky pro návrh a analýzu stavebních konstrukcí. Výzkum navíc zdůrazňuje nezbytnost popisu všech fyzikálních jevů pro zachycení složitého chování materiálů. Předložená práce vyzdvihuje univerzálnost a přizpůsobivost LDPM a ukazuje jeho potenciál pro širší uplatnění ve stavebním inženýrství.

Keywords

lattice discrete particle models; multi-physics; fracture mechanics; failure; calibration; validation

Klíčová slova

částicový model; multi-fyzikální jevy; lomová mechanika; porušení; kalibrace; validace

CONTENTS

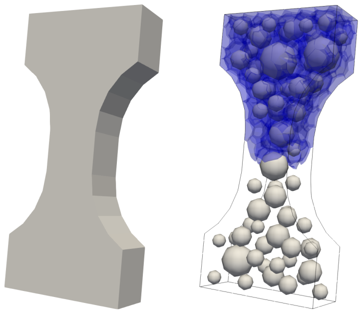
1 INTRODUCTION

Computer analysis of civil engineering structures requires general and robust material models to capture the behaviour of various materials, such as plasticity, strain hardening, distributed cracking and other types of strain-softening damage. The material models must perform realistically under a wide range of circumstances [4]. Two different groups of approaches have been formulated and developed throughout the years: (1) the continuum approach; (2) the discrete (or lattice) approach. In the former approach, the material is characterised by a general nonlinear triaxial stress-strain relation [6, 13, 22, to cite few], and the structure is usually solved by a finite element discretisation (although boundary elements and other methods are possible). The latter approach is a discrete element method or its variants (the random particle or lattice model). The material is represented by a lattice of particles and connecting bars for which simple rules of deformation and breakage must be defined [14, 16].

Conventional finite element software and associated numerical models are typically used to analyse the mechanical and non-mechanical behaviour of civil engineering structures or elements. However, these tools often fail to capture the inherent heterogeneity of materials such as concrete, particulate polymers, and fibre-reinforced cementitious materials. This limitation underscores the need for advanced numerical approaches. In response, the Lattice Discrete Particle Model (LDPM) is introduced to model the behaviour of selected civil engineering elements accurately. The standard LDPM, developed by Cusatis and colleagues ([15, 16]), is a discrete model for concrete that has demonstrated the capability to reproduce concrete behaviour under various loading conditions when properly calibrated and validated. Therefore, this thesis outlines selected civil engineering problems and the corresponding LDPM-based approaches to address them.

2 LATTICE DISCRETE PARTICLE MODEL

The lattice discrete particle model, a reliable and robust tool, is often employed to simulate the behaviour of quasi-brittle materials, such as rocks [2] and concrete [16], if the internal structure should be considered. The material is viewed as a group of stiff bodies (cells) interacting over the facets that are defined between them. These facets are considered between the neighbouring cells and can be thought of as possible crack surfaces. First, the studied volume is filled with spherical particles (Fig. 2.1). The lattice system that depicts the mesostructure topology is defined employing a Delaunay tetrahedralization of the particle centres and nodes used to characterize the external surface of the volume. Next, the system of polyhedral cells is designed according to the 3D tessellation. Note that many alternatives are used for the tessellation, as explained in [16] and [19], for example. Cells are formed by the aggregate and the matrix phase that surrounds the particles (Fig. 2.1).



(a) (b)

Figure 2.1: LDPM representation of dog-bone specimen: (a) real geometry; (b) particles and corresponding cells (coarse).

2.1 Particle placement [1]

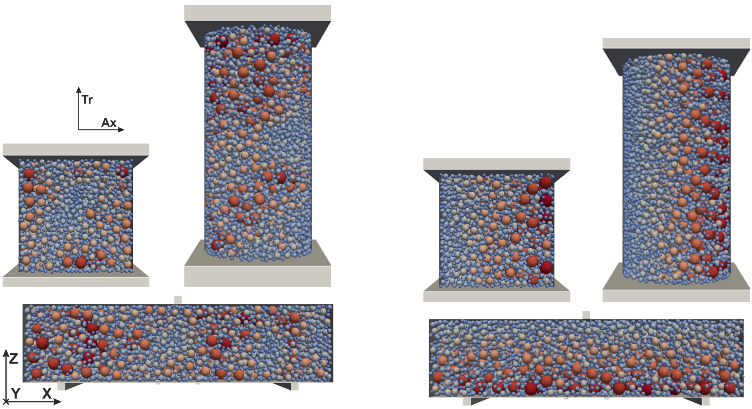
The LDPM material model's response depends highly on particle distribution, necessitating multiple simulations to achieve credible results [27]. This variability is often likened to experimental scatter. However, the numerical model scatter is usually much smaller than observed experimentally. Consequently, particle placement and its effect on response scatter are also investigated.

Numerical models of classical concrete experiments are presented, including cubes and cylinders loaded in compression and unnotched beams subjected to three-point bending, see [32] for more details. The material's internal structure is modelled using discrete elements to capture the fundamental aspects of heterogeneity. Essential inputs for these models include the maximum and minimum aggregate sizes, which drive a generation of particle sizes based on the classical Fuller curve. The upper bound of the sieve curve is defined by the maximum aggregate size, d_a, while the minimum aggregate size, d_0, defines the lower cut-off, under which no particles are generated and placed. The minimum aggregate size thus affects the refinement of the discrete mesh and, consequently, the computational cost.

A statistically isotropic random mesostructure is used to create the numerical models in its original formulation. Vorel et al. [32] introduced a new

[1] The section is based on the data presented in [32].

placement procedure to mimic the segregation or clustering of large particles in specimens caused by the casting process. Specifically, gradient-based generation is utilized. The response scatter of these approaches is compared, and conclusions are drawn. Both random and gradient field-based generations are studied, see Fig. 2.2.



(a) random field

(b) gradient field

Figure 2.2: Visual representation of particle placement for compression and three-point bending tests. [32]

Particle generation governed by a field is a modified approach to the standard geometrical characterization of concrete mesostructure presented in [16]. The generated mesostructure complies with the particle distribution curve and the distribution of a specified field, such as random or directional. The initial step involves generating particles, represented by spheres, according to the defined granulometric distribution. The primary difference between the standard and new methods lies in the particle placement strategy.

The process begins by generating N_0 random particle positions, with the intensity of each position evaluated based on the prescribed field. These positions are then ordered by intensity, from highest to lowest. The position with the highest intensity is assigned to the largest particle, which is placed there, provided it does not cross the domain's border. Both the particle and the position are then removed from their respective lists. Next, the second largest particle is placed at the position with the highest remaining intensity, ensuring no conflict with previously placed particles or the domain boundary. If a conflict exists, the position is discarded, a new random position is generated, its intensity is evaluated, and the positions are reordered by intensity. This particle placement process continues, with particles placed in descending order of size. A minimum distance between adjacent particles is defined as $\delta_s(r_1 + r_2)$, where r_1 and r_2 are the radii of the particles and $\delta_s \geq 0$ is the non-dimensional scaling parameter. This rule permits a smaller distance between small and large particles than between two large particles.

Based on the presented results, the following conclusions can be drawn:

- Directional effects, describing production processes (concrete casting) and represented by gradient-based fields, may slightly affect both the mean values of force at peak, displacement at peak, and their respective coefficients of variation of the response.
- Correlated spatial variability models (random fields) governing the particle generation process moderately influence the covariance of the response compared to the independent and random generation of particles.
- The investigated particle placement schemes with constant material and composition properties enhance the realism of the simulations but are insufficient to reproduce the experimental scatter.

2.2 *Particle facets* [2]

While LDPM has been shown to provide accurate predictions of the mechanical behaviour of concrete, its particle-based nature presents challenges in terms of computational costs. This primarily originates from the need to determine mesoscale parameters and the actual model processing. To tackle this, some researchers proposed an adaptive multiscale homogenization scheme to simulate damage and fracture in concrete structures [25]. Other researchers suggested implementing the proper orthogonal decomposition method to reduce the computational cost of model processing [12]. Pathirage et al. [28] compared the computational cost between dynamic implicit and explicit methods for the LDPM. Also, the use of machine learning techniques to rapidly determine model parameters has been investigated [26]. Nevertheless, keeping the LDPM computational costs at an acceptable level remains challenging.

A method is proposed in [36] to reduce computational costs by reducing the number of interaction surfaces between particles. For the original LDPM, each basic four-particle tetrahedron has twelve triangular facets. Two additional simplified interaction schemes are introduced in [36], one based on 6-facet interactions and one based on edge-based interactions. The model based on 6-facet interactions simplifies the tessellation of a basic four-particle tetrahedron, resulting in 6 quadrangular facets by combining the original two triangular facets corresponding to a point on the tetrahedron edge. The model based

[2] The section is based on the data presented in [36].

on edge-based interactions addresses the relationship between two aggregate particles, assigning a single polygonal face to each pair of adjacent aggregates (Fig. 2.3).

Based on the presented results, the following conclusions are drawn:

- The 6-facet-based interaction scheme results are in all investigated cases almost indistinguishable from the reference simulations with 12-facet.
- The edge-based simulations yield good results in cases where tensile softening or confined compression govern the results.
- The effect of particle distribution on the mechanical response of the LDPM based on 12-facet, 6-facet, and edge-based interactions is found not to depend on the interaction scheme.
- The efficiency and accuracy of the reduced number of interaction surfaces extend to both tensile and compressive loading conditions and reach a speed-up of up to 35% in the investigated cases with no loss in simulation quality. The newly proposed simplified interaction schemes also minimize the memory occupied during execution, which may be significant for extensive structural simulations or multi-physics analyses.

2.3 Material models [3]

Since the interaction of particles is formulated on the facets, corresponding stress and strain vectors are introduced first. The rigid body kinematics is employed to describe the displacement vector, $\mathbf{u}$, associated with the facets [16]

$$\mathbf{u}\left(\mathbf{x}\right) = \mathbf{u}_i + \boldsymbol{\theta}_i \times \left(\mathbf{x} - \mathbf{x}_i\right), \tag{2.1}$$

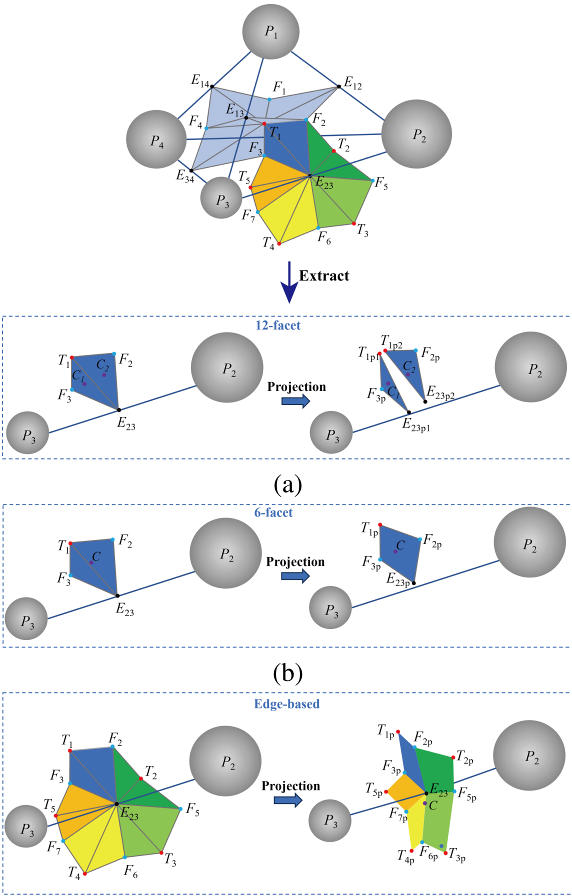
where $\mathbf{u}_i$ and $\boldsymbol{\theta}_i$ are the translational and rotational degrees of freedom of the node i with coordinate vector $\mathbf{x}_i$. For the given displacements and rotations of the associated particles, the relative displacement at the centroid of facet k is determined as

$$\mathbf{u}_{Ck} = \mathbf{u}_{Cj} - \mathbf{u}_{Ci}, \tag{2.2}$$

where $\mathbf{u}_{Ci}$ and $\mathbf{u}_{Cj}$ are the displacements at the k-th facet centroid caused by the translations and rotations of the adjacent nodes i and j, respectively. Displacement vector $\mathbf{u}_{Ck}$ is then employed to define the strain measures and discrete compatibility equations as follows

$$\varepsilon_{Nk} = \frac{\mathbf{n}_k{}^\mathsf{T}\mathbf{u}_{Ck}}{l_{ij}}, \quad \varepsilon_{Mk} = \frac{\mathbf{m}_k{}^\mathsf{T}\mathbf{u}_{Ck}}{l_{ij}}, \quad \varepsilon_{Lk} = \frac{\mathbf{l}_k{}^\mathsf{T}\mathbf{u}_{Ck}}{l_{ij}}, \tag{2.3}$$

[3] The section is based on the data presented in [33, 34].



(c)

Figure 2.3: Visualisation of the lattice system (P=particle, T=tetrahedron centroid, F=face point, E=edge point, solid blue line=tetrahedron edge): (a) 12-facet interaction; (b) 6-facet interaction; (c) edge-based interaction. [36]

where $\mathbf{n} = (\mathbf{x}_j - \mathbf{x}_i)/l_{ij}$, $\mathbf{m}$ and $\mathbf{l}$ are two mutually orthogonal vectors in the plane of the projected facet, i.e., perpendicular to n, and $l_{ij} = \|\mathbf{x}_j - \mathbf{x}_i\| = [(\mathbf{x}_j - \mathbf{x}_i)^\mathsf{T}(\mathbf{x}_j - \mathbf{x}_i)]^{1/2}$. $\mathbf{x}_i$ and $\mathbf{x}_j$ stand for the positions of node i and j, respectively.

The original evaluation of normal and shear stresses at each facet was formulated for concrete by Cusatis et al. [16]. This formulation involves: (i) elastic behaviour; (ii) fracture and cohesion; (iii) compaction and pore collapse; (iv) friction. The material parameters of the model either characterise the concrete mix and are used to generate a concrete mesostructure or describe the material's behaviour. This model was later adjusted to be used for similar materials such as rocks [2], fibre-reinforced concrete [24] or strain-hardening cementitious composites [40].

It was pointed out in [5] that the split mentioned above into the normal and shear components is not able to recover the full Poisson ratio range ($-1 < \nu < 0.5$) and is limited to $\nu < 0.25$, otherwise negative shear modulus is obtained. Therefore, the volumetric-deviatoric split introduced by Carol and Bažant [11] for microplane models is considered. The volumetric-deviatoric split allows the recovery of the full Poisson ratio range needed for alloys. Because of the underlying tetrahedral mesh and corresponding facets Ω_e (see [16]) the volumetric (hydrostatic) strain is calculated as [17]

$$\varepsilon_{Vk} = \frac{1}{3\Omega_{e,0}} \sum_{m \in \mathcal{F}_e} \Gamma_m l_{ij} \varepsilon_{Nm}, \tag{2.4}$$

where $\Omega_{e,0}$ is the initial volume of the tetrahedral element, $\mathcal{F}_e$ is the set of facets belonging to one element, and Γ_m and l_{ij} are the facet area and distance of the adjacent nodes corresponding to the facet m, respectively. The normal deviatoric strain takes the form

$$\varepsilon_{NDk} = \varepsilon_{Nk} - \varepsilon_{Vk}. \tag{2.5}$$

Moreover, the shear (tangential) strain in the plane of the facet is written as $\varepsilon_{Tk} = (\varepsilon_{Mk}^2 + \varepsilon_{Lk}^2)^{1/2}$ and deviatoric strain as $\varepsilon_{Dk} = (\varepsilon_{NDk}^2 + \varepsilon_{Tk}^2)^{1/2}$. The corresponding stress components then read

$$\sigma_V = E_V \varepsilon_N, \quad \sigma_{ND} = E_D \varepsilon_{ND}, \quad \sigma_M = E_D \varepsilon_M, \quad \sigma_L = E_D \varepsilon_L, \tag{2.6}$$

where $E_V = E/\,(1-\nu)$ and $E_D = E/(1+\nu)$ are the volumetric and deviatoric moduli, respectively, related to Young's modulus E. The constitutive material law defined on the facets is described in the following section. By imposing the equilibrium through the principle of virtual work, the internal work and nodal forces associated with the facet can be calculated [16]. Note that subscript k is omitted in the following text for readability.

The new models for particulate polymers and metals are defined based on the aforementioned volumetric-deviatoric split that was introduced. With the extensive use of polymer-based composites, especially their increased use in critical load-bearing structures, there is a growing need to predict their behaviour, including, e.g., the deformation under general loading conditions [20] and the evolution of material properties often related to ongoing cross-linking and physical aging [31]. The rapid growth of computing power and advanced finite element software availability also enables progress in accounting for different polymer phenomena. The current formulation combines viscoelasticity to capture the time-dependent behaviour, fracture and plasticity. Moreover, utilising LDPM allows the simple formulation of material law in the vectorial form on each facet. In particular the formulation includes [33]: (i) viscoelastic beahaviour captured by Leonov model; (ii) fracture; (iii) material compaction; (iv) frictional behaviour. Moreover, the material law for metals, inspired by the definition studied and described in [10], is introduced in [34]. This material model based on the LDPM formulation is meant to be utilised to investigate and design 3D-printed alloys.

2.4 Model calibration and parameters evolution [4]

The calibration procedure employed for the lattice models is often based on hand-fitting and deep expert knowledge of the model. Such an approach requires already experienced users to be able to calibrate the required properties based on multiple experimental data satisfactorily. Moreover, the inherent variability of the results caused by the random generation of the particle configuration also presents another limitation for the calibration process. The probabilistic calibration process was examined in [23] to improve the calibration procedure. The identification method presented is general, computationally feasible, and automated, thus allowing for comprehensive model utilisation. The core of the calibration procedure for the model is Bayes' theorem for probabilistic parameter identification, which allows uncertainties connected to the available experimental data and the model inaccuracy to be considered. However, this probabilistic formulation requires a high number of LDPM simulations. Therefore, an approximation of LDPM based on a polynomial chaos expansion is employed to reduce the related computational costs. This substitution is convenient because it reduces computational time and overcomes the obstacle of LDPM stochasticity since the polynomial chaos expansion can be considered a rough approximation of the mean LDPM response. The calibration of the model is thus turned into fitting the mean LDPM response to the mean observed stress-strain diagram for a concrete mix with given material

[4] The section is based on the data presented in [23, 30].

parameters. The Bayesian inference results in a posterior probability distribution of deterministic values of material parameters corresponding to a given concrete mix, and this distribution expresses uncertainty due to the insufficient information contained in the experiments conducted, measurement error, and estimated model stochasticity. The proposed identification strategy is robust and precise enough to fit the synthetic stress-strain diagrams representing ten different concrete mixes. Since only uniaxial compression and three-point bending tests were utilised in the identification procedure, many parameters played similar roles, and more independent data would be needed to separate their effect.

It is also essential to understand the material's behaviour over time to ensure high safety levels and functionality over the lifespan of concrete structures (50-100 years). As widely known, concrete changes its performance over time, typically leading to enhanced material properties if deterioration mechanisms are neglected. In [30], the evolution of material properties is studied numerically and experimentally. The experimental data includes calorimetric and shrinkage tests, internal humidity and temperature measurements, and mechanical tests. The numerical framework developed in [39] is utilised with minor changes in the ageing laws to capture the experimental data.

3 SELECTED PROBLEMS

From the engineering point of view, the accurate prediction of the response of structures, or more specifically, structural members, is one of the essential problems and can be decisive for an efficient and safe design. Modelling is gaining importance as the civil engineering community moves from purely prescriptive experience-based design to performance-based design concepts [21, 38]. To efficiently and adequately design new or perform rehabilitation and strengthening of existing concrete structures, the need for a reliable material model appropriate for the scale of the structural elements is paramount. As mentioned in the previous sections, the LDPM is a computationally expensive approach. Thus, numerical analysis is usually limited to structural elements rather than to the simulation of whole structures. The following sections use the LDPM to study selected civil engineering problems.

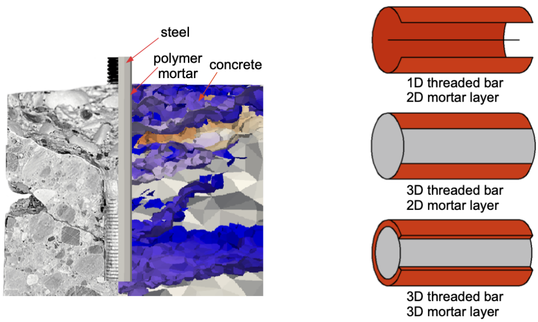
3.1 Adhesive anchors [1]

In recent years, post-installed anchors have been frequently used to fasten appliances to load-bearing elements and link structural members. A threaded

[1] The section is based on the data presented in [9, 27].

rod inserted into a borehole filled with adhesive mortar is commonly called a bonded anchor. Due to the many different materials and failure mechanisms involved, the topic is highly complicated, necessitating numerical support for the experimental analysis. A trustworthy model capable of simulating a system's short-term behaviour must be established before creating a more intricate framework to study the lifespan of fasteners exposed to different deterioration processes. Such a model is developed and validated in [27]. Fig. 3.1(a) shows a typical pull-out test utilised for the bonded anchor characterisation, together with numerical simulation results, presented in [27]. Three different materials are involved, i.e., concrete (base material), steel (reinforcement) and polymer mortar (adhesive). Therefore, to successfully simulate the behaviour of this and also other structural problems, a combination of different material models has to be employed. The level of detail that we want to meet according to the scope of investigation also determines appropriate simplifications of fastening systems which can be made. For instance, a bonded anchor pull-out problem could be modelled with 2D axisymmetric or 3D elements.

Moreover, each material component of the setup can also undergo different dimensionality reduction, see Fig. 3.1(b). In [27], the threaded bar is modelled employing 1D beam elements and the concrete part using the LDPM. The prescribed stress-slip law represents the interaction between the steel and concrete through the mortar layer.



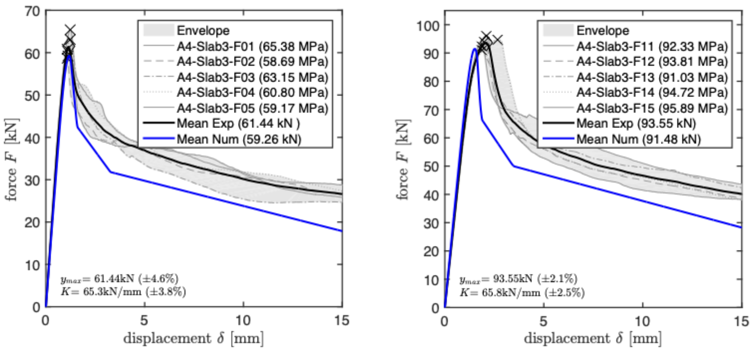
(a) (b)

Figure 3.1: Bonded anchor: (a) pull-out test, experiment vs. numerical simulation; (b) numerical simplification of steel-bond interaction. [27]

The results presented in [27] can be summarizes as follows:

- The proposed numerical framework captures the pull-out tests of bonded anchors precisely, Fig. 3.2;

- The numerical results also capture the crack propagation, which differs based on the embedment depth and bond strength. The failure can range from complete concrete cone to combined concrete cone-bond failure to bond failure.



(a) (b)

Figure 3.2: Experimental and numerical results for different bonded lengths: (a) 70 mm; (b) 110 mm. [27]

Furthermore, the safe design of fastening systems depends on a detailed understanding of the mechanisms and processes that cause excessive deformations or even failure over time, especially considering multi-decade performance. The uniform bond model, a key concept in adhesive anchor system design, is based on existing standards and guidelines. It typically approximates the real stress distribution for loads near the system's pull-out capacity and during short-term testing well. On the other hand, noticeable time-dependent deformation is a feature shared by mortar and concrete, particularly at high temperatures. As a result, significant shear stress redistributions are anticipated due to creep over a structure's lifetime. Critical stress levels may be achieved locally depending on the degree of stress redistribution. Therefore, understanding bond stress redistribution events in adhesive anchor systems under long-term load is essential. Unfortunately, the combined impacts of adhesive creep and concrete cannot be separated experimentally. This phenomenon is studied in [9], where the creep of the concrete and visco-elastic mortar is evaluated. The presented conclusion can be summarised as:

- The investigation showed the antagonistic effects of concrete and adhesive creep;

- Concrete creep tends to load the upper part of the anchor while unloading the bottom part, leading to a stress redistribution that diverges from the uniform bond law model. Mortar creep tends to unload the upper part of the anchor while loading the bottom part, leading to a stress redistribution that approaches uniform bond stress distribution.

3.2 Prestressed/post-tensioned concrete beams [2]

The serviceability limit states of reinforced concrete buildings are primarily determined by design considerations related to time-dependent deformations, including shrinkage and creep. This research emphasizes the practical implications of poor design, which can lead to large cracks that speed up steel corrosion and severe deformations that affect the structure's serviceability, as highlighted by Benboudjema et al. [7]. The coupling of the LDPM for concrete with the Hygro-Thermo-Chemical (HTC) model, as demonstrated in [1, 35], has direct applications in capturing the evolution of the internal structure of concrete and its mechanical properties, creep, and shrinkage. Including steel relaxation in these effects is crucial for determining the prestress loss and simulating the behaviour of beams in shear or three-point bending, making the research findings highly relevant and applicable.

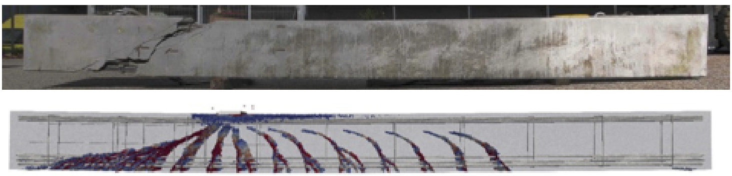


Figure 3.3: Comparison of prestressed beam shear failure by experiment and predicted simulation. [35]

The conclusion made may be summed up as follows:

- The lattice discrete particle model can accurately show the behaviour of prestressed concrete beams, both in load level and failure mechanism, Fig. 3.3;
- The coupling among shrinkage, concrete creep, and steel relaxation is crucial for the accurate modelling of prestressed beams.

[2] The section is based on the data presented in [1, 35].

3.3 Viscoelastic behaviour of macro-synthetic fibre reinforced concrete [3]

Due to the expansion of their structural applications, developing predictive models and assessing the mechanical short and long-term performance of fibre-reinforced concretes (FRCs) are becoming increasingly important. Long-term behaviour is a challenging topic even though numerical and analytical models have been proposed, and their short-term behaviour has been extensively researched.

Creep deformations can be predicted for concrete, but their interaction with the cementitious matrix must be considered when fibres are added to concrete. Such interaction strongly depends on the type of fibre. It is affected by microcracking at the fibre-concrete interface, non-linear bond behaviour, and the creep of polymeric fibres, which influences the long-term behaviour of structural elements, particularly in cracked conditions. The work presented in [18] introduces a unique computational approach for modelling the long-term behaviour of polymeric fiber-crack FRC elements. The framework is based on the LDPM, which has demonstrated the ability to forecast the short-term deformations of fiber-reinforced concrete [29]. However, including fibre-viscoelastic behaviour is necessary to capture the long-term response adequately. Fig. 3.4 compares experimental and numerical results for the creep tensile tests on notched cylinders with varying temperatures over time. Based on the results of FRC with polypropylene macro-fibers presented in [18], the following conclusions are drawn:

- The definition of viscoelastic behaviour of fibres allows to simulate the response of cylinders in uniaxial tension with sufficient accuracy at the temperatures of 20°C and 30°C;
- The proper definition of fibre volume in the numerical model is crucial for an accurate prediction.

3.4 Fibre-reinforced polymer-concrete joints [4]

Fibre-reinforced polymer (FRP) composites have been extensively used in civil engineering over the last three decades [3]. Externally-bonded FRP strips can increase the load-carrying capacity of reinforced concrete structures. The premature debonding phenomenon of FRP composites, when externally applied to a reinforced concrete structure, is a practical challenge. The work in [37] focuses on the use of the lattice discrete particle model (LDPM) to

[3] The section is based on the data presented in [18].
[4] The section is based on the data presented in [37].

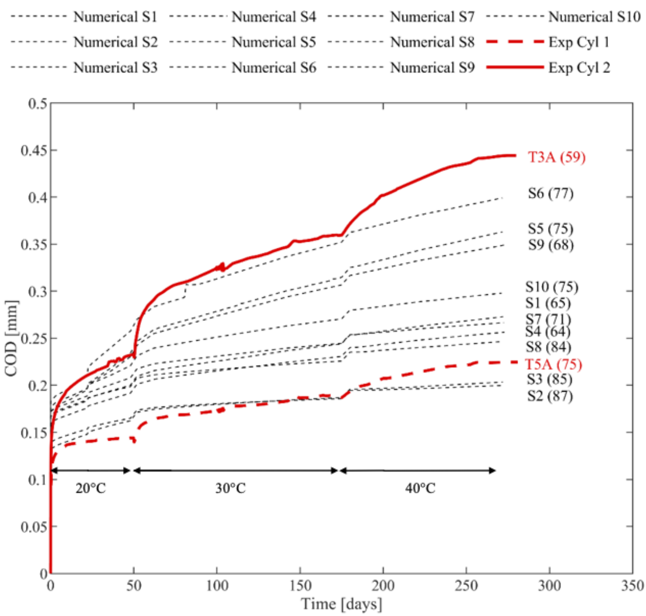


Figure 3.4: Uniaxial tensile creep experimental tests - comparison of numerical and experimental results. [18]

simulate the bond behaviour of FRP-concrete joints tested using a single-lap direct shear test. The mesoscale LDPM parameters are calibrated against companion tests carried out for material characterisation of the concrete used in the FRP-concrete joints, thus removing any bias in selecting the parameters. A comparison between the numerical simulations of direct single-lap shear tests (Fig. 3.5) and the experimental responses indicates that LDPM can model the bond behaviour of FRP-concrete joints and provides insight into the width effect observed, which has significant practical implications for the field of civil engineering and materials science.

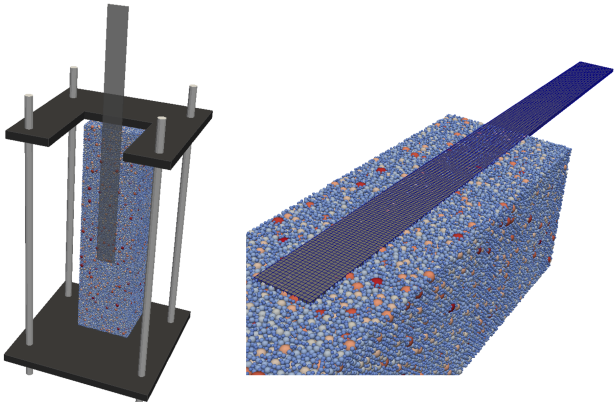


Figure 3.5: Numerical model of direct single-lap shear test. [37]

Numerical simulations of single-lap shear tests of FRP strips attached to concrete prisms were carried out. The concrete parameters were calibrated using the same experimental campaign's compressive and fracture tests. Six different bonded widths were tested and modelled to study the width effect. Based on the presented results in [37], the following conclusions are drawn:

- The proposed model accurately depicted the debonding behaviour of the FRP strip from concrete without additional cohesive law between concrete and FRP. Utilising a master-slave formulation between the elastic FRP strip and the concrete surface particles, the LDPM model was able to simulate the interfacial crack propagation beneath the concrete surface realistically;
- Good agreement between the numerical simulations and experimental results was obtained for all investigated bonded widths ($b_f = 15$, 30, 40, 50, 75 and 90 mm) utilising the same material parameters, see Fig. 3.6.

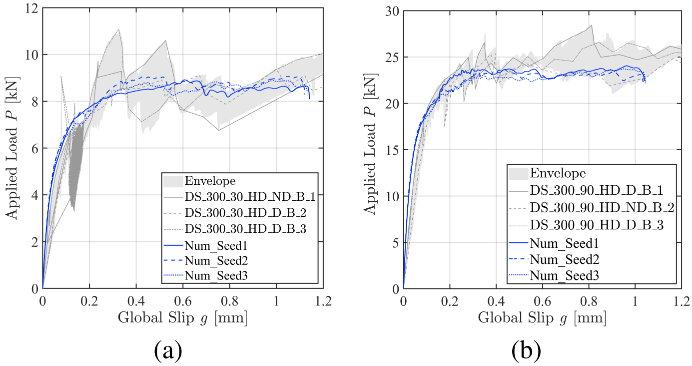


Figure 3.6: Representative comparison between numerical and experimental results of direct single-lap shear tests: (a) $b_f = 30\,\text{mm}$; (b) $b_f = 90\,\text{mm}$. (P=applied load on the free end, g=displacement of the beginning of bonded region) [37]

3.5 Framework for tertiary creep of concrete [5]

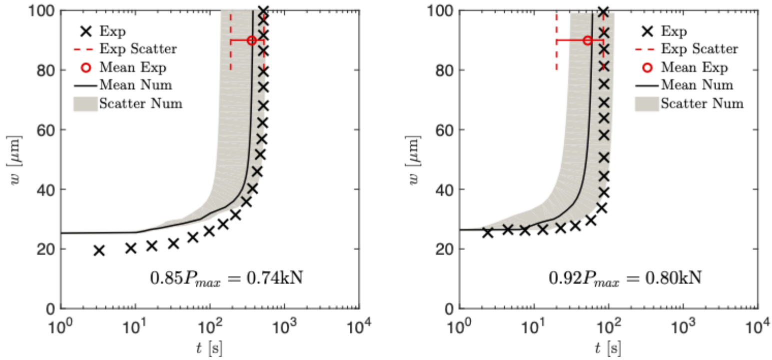
A computational framework for analysing tertiary concrete creep is presented in [8]. It is a comprehensive approach that combines a discrete element framework with linear visco-elasticity and rate-dependency of damage. While ageing visco-elasticity is implemented using the Micro-Prestress-Solidification (MPS) theory, which links the mechanical response to the underlying physical and chemical processes of hydration, heat transfer, and moisture transport through a multi-physics approach, the Lattice Discrete Particle Model acts as a constitutive model. The framework mentioned above is calibrated using a wide range of literature data, including tensile and compressive creep tests and tests at various loading rates. This comprehensive approach ensures the framework's reliability. Subsequently, the approach is rigorously validated against time-to-failure flexural and compression tests, i.e., notched and unnotched beams and dog-bone-like specimens under compression, further supporting its credibility.

Folowing conclusions were made in [8] based on the presented data:

- The numerical framework can predict the time-dependent evolution of concrete creep deformations in the primary, secondary, and tertiary domains and provides very accurate estimates of the times to failure, see Fig. 3.7;
- The independent calibration of all driving mechanisms, i.e., long-term creep, mechanical properties and fracturing rate dependence, has to

[5] The section is based on the data presented in [8].

be performed to obtain a real predictive tool. These tests are rarely available altogether, which might limit the practical application of the proposed framework.



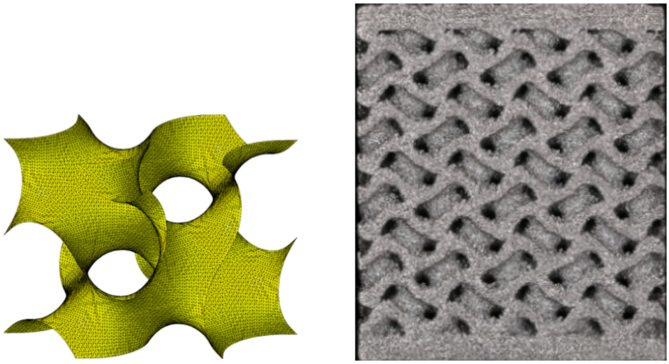
(a) (b)

Figure 3.7: Notched prism tests, comparison of experimental and numerical crack opening vs. time curves for different load levels: (a) $0.85P_{max}$; (b) $0.92P_{max}$. (P_{max} = peak load of quasi-static test)) [8]

4 CONCLUSIONS AND FUTURE WORK

The thesis presents the latest developments in the Lattice Discrete Particle Model and its applications in Civil Engineering. These new developments are a significant step forward in the field, showcasing the LDPMs' potential to consistently deliver accurate results in various loading scenarios and for different materials and structural elements. The main work and conclusions can be summarized as follows:

- The Lattice Discrete Particle Model is computationally expensive, and multiple simulations have to be done for different particle placements;
- The reduction of interaction surfaces (i.e., facets) can reduce the computational cost;
- The LDPM proved to be a suitable tool for simulation of the material behaviour of structural elements under various stress states;
- The LDPM represents well the crack patterns;



(a) (b)

Figure 4.1: Gyroid structure: (a) example of one-cell surface; (b) basic cells.

- Multi-physics simulations are necessary if more complex behaviour is studied.

In the engineering problems presented, the LDPM model was mainly employed to simulate concrete behaviour. However, the preliminary studies presented in [33, 34] also show the great potential of the LDPM formulation to capture the behaviour of various materials well. These developments, currently under investigation, particularly the simulation of bonded anchors using the LDPM for polymers or the LDPM for the simulation of 3D-printed alloy structures (Fig. 4.1), demonstrate the adaptability and versatility of the LDPM in diverse applications. Moreover, to further reduce the computational cost, the adaptive LDPM formulation switching in the area of interest from computationally less demanding edge-based to a more demanding 12 or 6-facet interaction scheme is studied.

ACKNOWLEDGEMENTS

The financial support provided by the GAČR grant No. 23-04971S is gratefully acknowledged.

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Activities

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2019-2021	CTU IN PRAGUE, Faculty of Civil Engineering, Dept. of Mechanics, Czech Republic. Project topic: *Time dependent behavior of thermoset polymers with application to anchor*, GAČR 19-15666S. Principal Investigator, amount granted 4,875,000 CZK (equivalent to app. 190,000€)
2018-2020	CTU IN PRAGUE, Faculty of Civil Engineering, Dept. of Mechanics, Czech Republic. Project topic: *Fire resistance of glued laminated timber beams including uncertainties*, GAČR 18-05791S. Team member, amount granted 4,583,000 CZK (equivalent to app. 178,000€)
2018-2020	CTU IN PRAGUE, Faculty of Civil Engineering, Dept. of Mechanics, Czech Republic. Project topic: *Probabilistic identification of material transport parameters based on non-invasive experimental measurements*, GAČR 18-04262S. Team member, amount granted 5,208,000 CZK (equivalent to app. 202,000€)
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Selected publications

[1] J. Vorel, M. Marcon, G. Cusatis, F. Caner, G. Di Luzio, and R. Wan-Wendner. A comparison of the state of the art models for constitutive

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