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Multiphysics-Lattice Discrete Particle Model: possible strategies for upscaling

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Abstract

The optimization of civil infrastructure maintenance and management is a challenging task, littered of open issues requiring the synergic development of effective structural health monitoring systems and reliable models to be addressed. Relevant to concrete structures, models cannot disregard the multi-physics nature of the problem: moisture and heat transport phenomena in uncracked and cracked conditions, the ingress of aggressive agents, and the ensuing chemical reactions - that the latter may trigger - heavily affect the mechanical performance. Most of the mentioned processes happen at a scale typically smaller than the structural one. Then, it is also necessary to perform multiscale analysis, capable of adapting structural models to the insights resulting from lower scale analyses. In the last decade, Multiphysics-Lattice Discrete Particle Model (M-LDPM) has been successfully adopted to model a wide range of phenomena in civil engineering involving concrete structural members: ageing, environment-induced degradation, shrinkage, creep, and usage of advanced construction materials. Furthermore, the discrete nature of the model has shown the capability of predicting the cracking patterns accurately. However, such a comprehensive and accurate model simulates the material at the mesoscale, and the path towards the exploitation of the insights resulting from lower-scale modelling at the structural level is paved of computational and theoretical burdens. In this work, a review of the state-of-the-art concepts that allow upscaling M-LDPM is presented. The aim is to explore alternatives for the formulation of computationally efficient macroscale models that leverage on both the predictive quality of M-LDPM in capturing and predicting the material constitutive behaviour, and the computational affordability that features the classical Finite Element Method for the structural analysis of complex systems.

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1. Introduction

Transport infrastructures are crucial elements for economic growth and social development. Among them, road and rail bridges play an essential role by creating crossings between countries and regions and facilitating the transport of people and goods. In 2019 only Europe counted more than 1234 km of road bridges over 100 metres. However, most of them were designed and built between the 1950s and 1960s, assuming a service life of 50÷100 years and with material properties, design methods, and knowledge of the probabilistic occurrence of extreme natural events less developed. They are still operational today, in most cases, without a clear assessment of their safety performance. In 2001, the EU-funded project BRIME identified that highway bridges in France, Germany, and the UK presented deficiencies at a rate of 39%, 30%, and 37%, respectively. As a matter of fact, in 2018, a survey by the Organization for Economic Cooperation and Development (OECD) showed that roughly 0.7% of the global GDP was invested in inland transport infrastructures, mainly because of maintenance interventions. In Italy, as an example, in the same year, more than 70% of the total public investment in road transport infrastructures was used for structural repairing and strengthening. The criticalities featuring the EU bridges asset are further exacerbated by the more and more frequent extreme events (e.g., long periods of droughts, intense precipitations, rise in sea levels, hurricanes, and flooding in coastal regions) due to the climate change our planet is currently experiencing. Such global changes require humans to adapt to these new weather patterns by strengthening the resilience of existing infrastructure and designing new ones under evolving service conditions. In addition, the strategies adopted to tackle this challenge must comply with the green transition that our society will realize in the near future. It clearly stands out that the durability of transport infrastructures and the sustainability of both construction and management processes are topics of the utmost relevance and cannot be addressed separately. More durable structures mitigate the need for costly and frequent maintenance. Likewise, sustainable approaches in terms of techniques, technologies and materials lead to a wiser usage of raw materials together with social and environmental beneficial effects.

The optimization of bridge maintenance and management is a challenging task, littered of open issues, which in last decades has been gaining an increasing interest by researchers and practitioners. Due to its complexity, this task requires the synergic development of effective structural health monitoring systems and reliable modelling tools. Regular visual inspections and high-quality data collection allow us to detect the degradation level of the structural members and their response to varying environmental, mechanical, and/or kinematic boundary conditions. However, although on-site investigation serves as an essential cornerstone for the analysis, by itself, it only offers limited insights into the complex time-dependent behaviour. The complexity is due to the multiple coupled hygro-thermo-chemo-mechanical processes, further complicated by the exposition to extreme environmental loads. Sound and accurate physics-based models permit us to interpret the monitoring data, identify the most effective solution to adopt, and, eventually, predict the response in other scenarios of interest. Such models cannot disregard the multiphysics nature of the problem: moisture and heat transport phenomena, such as the ingress of aggressive agents and the ensuing chemical reactions that the latter may trigger, heavily affect the mechanical performance. Most of the mentioned processes happen at a scale typically smaller than the structural one. Because of this, it is also necessary to perform multiscale analysis, capable of adapting the structural and macroscale models relying on the insights resulting from lower scale analyses. The behaviour of structural materials is typically characterized by micro- or mesoscale mechanisms. Therefore, when they are used for either new constructions or the retrofitting of existing bridges, the multiscale approach becomes even more important to properly capture the changes induced by external factors. Nonetheless, the computational performance for highly comprehensive numerical simulations is always limited to a certain specimen size, being hardly exploitable at the structural level.

The climate change exposes road and rail bridges to multiple hazards. While government bodies promote policies to enhance the sustainability of anthropogenic activities, the infrastructure owners are required to field prevention and maintenance actions to prevent disasters from happening. Predictive physics-based models might improve the decision-making process. It would be possible to simulate the infrastructure response to several extreme events accounting for the actual conservation state and eventual maintenance interventions, either to be realized or already accomplished.

In the last decade, the Multiphysics-Lattice Discrete Particle Model (M-LDPM) has been successfully adopted to model a wide range of phenomena in civil engineering involving concrete structural members: aging, environment-induced degradation, shrinkage, creep, and usage of advanced construction materials. The discrete nature of the model has shown the capability of predicting the cracking patterns accurately. However, such a comprehensive and accurate model simulates the material at the mesoscale, and computational and theoretical burdens pave the path toward the exploitation of the insights resulting from lower-scale modelling at the structural level.

This work presents a review of the state-of-the-art concepts that might allow M-LDPM upscaling to explore alternatives for the formulation of computationally efficient macroscale models that leverage the predictive quality of M-LDPM in capturing and predicting the material constitutive behaviour and the computational affordability that features the classical Finite Element Method for the structural analysis of complex systems.

2. Multiphysics-Lattice Discrete Particle Model

The Multiphysics-Lattice Discrete Particle Model (M-LDPM) results from coupling the Lattice Discrete Particle Model (LDPM), a mesoscale model simulating the mechanical behaviour of cementitious materials (Cusatis et al. 2011a,b), and the Hygro-Thermo-Chemical model, which was initially conceived as a macroscale continuum-based model to simulate the moisture and heat transport phenomena in reactive cement-based materials (Di Luzio and Cusatis, 2009a,b).

LDPM simulates concrete at the mesoscale (length scale 10^{-2} m), as a two-phase material (mortar and coarse aggregate). The geometrical configuration is generated by a trial-and-error random procedure, in which the aggregate particles are assumed to have a spherical shape and are randomly placed within the volume. Then, zero-radius particles are located along the external surfaces to facilitate the imposition of boundary conditions. Based on the Delaunay tetrahedralization of the generated system of points, a three-dimensional domain tessellation is carried out, and linear segments, namely tetrahedra edges, are generated to connect all particle centres. The outcome is a system of lattice-connected cells interacting through triangular facets: the mechanical interaction among particles is based on four particle-subsystems, in which the spheres (nodes) are connected by struts (edges), having cross section (triangular facets) resulting from the volume tessellation. The lattice particle system's deformation is described by the rigid body kinematics. In this perspective, the displacement step $[\![\boldsymbol{u}_C]\!]$ at the centroid of the *k-th* projected facet, C_k, is used to define the strain measures: $\varepsilon_N = (\boldsymbol{n}^T[\![\boldsymbol{u}_C]\!])/l$, $\varepsilon_L = (\boldsymbol{l}^T[\![\boldsymbol{u}_C]\!])/l$, and $\varepsilon_M = (\boldsymbol{m}^T[\![\boldsymbol{u}_C]\!])/l$, where $\boldsymbol{n}$, $\boldsymbol{l}$, and $\boldsymbol{m}$ are the unit vectors identifying a local reference system on each facet in normal and shear directions, respectively. The subscripts N, M, and L indicate the strain components along the mentioned directions. At the centroid of each projected facet, vectorial constitutive laws are defined. They are hence defined at the mesoscopic scale and govern the mechanical behaviour of concrete. In the elastic regime, normal and shear stresses are proportional to the corresponding strains. Then, stresses are computed as $\sigma_N = E_N\varepsilon_N^*$, $\sigma_L = E_T\varepsilon_L^*$, and $\sigma_M = E_T\varepsilon_M^*$, where ε_N^*, ε_L^*, and ε_M^* are the strain components net of mesoscale eigenstrains that might arise due to thermal expansion, creep, and shrinkage (Abdellatef, et al., 2015; Wan et al., 2016; Alnaggar et al., 2017; Boumakis et al., 2018). The normal and tangential moduli, E_N and E_T, are equals to E_0 and αE_0, respectively, where E_0 is the effective normal modulus, whereas α represents the shear-normal coupling parameter. In a facet under tension, the mesoscale crack opening, occurring when the strain goes beyond the tensile elastic limit, is expressed by the vector $w_c = w_N\boldsymbol{n} + w_L\boldsymbol{l} + w_M\boldsymbol{m}$, where $w_N = l(\varepsilon_N - \sigma_N/E_N)$ is the opening/closure of the crack along the direction orthogonal to the facet, while $w_L = l(\varepsilon_L - \sigma_L/E_T)$ and $w_M = l(\varepsilon_M - \sigma_M/E_T)$ are two sliding components, catching shear displacements at crack surfaces. In the mesoscale model, three non-linear phenomena govern the material response beyond the elastic limit: (i) fracture and cohesion, (ii) compaction and pore collapse, and (iii) friction. Modelling the inelastic behaviour relies on the definition of effective strain $\varepsilon = \sqrt{\varepsilon_N^2 + \alpha(\varepsilon_L^2 + \varepsilon_M^2)}$ and stress $\sigma = \sqrt{\sigma_N^2 + (\sigma_L^2 + \sigma_M^2)/\alpha}$, which are employed to formulate damage-type constitutive laws. The interested reader may refer to (Cusatis et al. 2011a,b).

LDPM has been later extended to simulate the behaviour of fibre-reinforced cementitious materials, showing promising results (Schauffert et al., 2012a,b). Also noteworthy is the capabilities that LDPM showed in simulating the response of reinforced concrete structural elements, as demonstrated by several authors (Lale et al., 2018; Feng, et al., 2018; Alnaggar et al., 2018; Bhaduri et al., 2021). In these works, the mechanical model was able to accurately capture and, once properly calibrated, predict the crack patterns featuring the path to failure of RC members in compression, bending, and when exposed to exceptional events, such as a projectile penetration. The steel reinforcement is therein

modelled through discrete elements, whose interaction with the surrounding matrix is modelled with a penalty contact law.

The simulation of complex phenomena occurring in concrete structures, such as (i) strength and stiffness build-up from casting onwards (Wan et al., 2016; Cibelli, 2022), (ii) crack self-healing (Cibelli et al., 2022; Cibelli et al., 2024), (iii) creep and autogenous and drying shrinkage (Abdellatef et al., 2015; Boumakis et al., 2018), (iv) damage induced by alkali-silica reactions (Alnaggar et al., 2017), (v) spalling and mechanical decay at high temperatures (Shen et al., 2020, 2021), (vi) chloride penetration in cracked conditions (Zhang et al., 2021; Cibelli et al., 2023), and (vii) corrosion-driven damage, requires LDPM to be two-way coupled with a model simulating both moisture and heat transport phenomena, as well as the chemical reactions featuring the afore-mentioned phenomena. To this purpose, LDPM has been coupled with the Hygro-Thermo-Chemical (HTC) model.

The HTC formulation, recently improved by Pathirage et al. (2019) and Cibelli (2022), draws on two state variables, the relative humidity h and temperature T, and the associated field equations, which read

$$\nabla \cdot \left(D_h \nabla h \right) = \frac{\partial w_e}{\partial h} \frac{\partial h}{\partial t} + \frac{\partial w_e}{\partial \alpha_c} \dot{\alpha}_c + \sum_{k=1}^{n} \frac{\partial w_e}{\partial \alpha_k} \dot{\alpha}_k + \dot{w}_n \tag{1a}$$

$$\nabla \cdot (\lambda \nabla T) = \rho \, c_t \frac{\partial T}{\partial t} + \dot{\alpha}_c c \tilde{Q}_c^{\infty} + \sum_{k=1}^{n} \dot{\alpha}_k k \tilde{Q}_k^{\infty} \tag{1b}$$

Eq. 1a describes the water mass conservation. In the left-hand term, the moisture flux divergence $\partial w/\partial t = \nabla \cdot \boldsymbol{J}$, is combined with the first Fick's law $\boldsymbol{J} = -D_h(h,T) \cdot \nabla h$, with $D_h(h,T)$ moisture permeability coefficient. In the right-hand side, instead, the effects of (i) sorption/desorption isotherm ($\partial w_e/\partial h \cdot \partial h/\partial t$), (ii) cement hydration ($\partial w_e/\partial \alpha_c \cdot \dot{\alpha}_c$), and (iii) variation of chemically bound water in time ($\dot{w}_n$) on the moisture balance are considered. The sum term, looping over the index k, refers to non-conventional supplementary cementitious materials, if any, whose chemical activity does have an impact on the water mass balance. Previous works showed the potential of successfully simulating the effect of silica fume (Wan et al., 2016) and slag (Cibelli, 2022). Eq. 1b represents the heat balance. The heat conduction in concrete is described for temperatures lower than 100°C by means of Fourier's law: $\boldsymbol{q} = -\lambda \nabla T$, in which $\boldsymbol{q}$ is the heat flux and λ the heat conductivity. Likewise, for moisture, also the enthalpy balance is affected by the chemical reactions occurring from early age onwards. The interested reader can refer to (Di Luzio et al., 2009a; Pathirage et al., 2019; Cibelli, 2022) for further details about the HTC formulation.

The HTC-LDPM coupling is based on the definition of Flow Lattice Elements (FLEs): flow channels installed within the LDPM tetrahedra-based mesh, which make up a 3D network, referred to as transport lattice system (Hao et al., 2023). This strategy allows for having two frameworks numerically aligned, anchored to each other, and ready to be directly connected and coupled. The dual lattice system for transport/diffusion is constructed as follows: in the 3D mesh of tetrahedra generated during the construction of the LDPM geometry, a Flow Lattice Element (FLE) connects two points inside two adjacent tetrahedra (tet-points), which are also vertices of the corresponding polyhedral cells. The FLE describes the transport between these two adjacent tetrahedra. Then, the diffusion across the entire computational domain can be represented by a network of FLEs connecting all the tetrahedra. In addition, a thin layer of edge elements orthogonal to the external surface of the domain is generated to enable the boundary conditions application and simulate the discontinuous drop between the sample surface and the surrounding environment, see Hao et al. (2023) for details. The resulting lattice system is often referred to as a dual lattice system in order to emphasize the specular nature of its construction as compared to the one adopted for the mechanical mesh (Bousikhane et al., 2018; Hao et al., 2023).

3. Upscaling approaches for M-LDPM

Concrete is a heterogeneous material whose microstructure significantly affects the response to both mechanical and environmental actions. Though a large scientific production has flourished since the early 1950s, the numerical modelling of concrete structures remains a field gathering the interest of many researchers worldwide. This likely stems from the complexity of the phenomena involved, on the one hand, and the will to improve the existing theories

and models to result in more accurate tools able to capture the reality and provide reliable predictions of the structural performance in a wide range of civil engineering applications.

Concrete is a multiscale system whose numerical modelling derives from the observation scale of interest. Cusatis et al. (2014) proposed 6 scales for concrete, ranging from the *cement paste scale*, from 10^{-9} m to 10^{-3} m, where the interfacial transition zone (ITZ), internal structure, and mineral composition play a significant role, to the *full structure scale*, from 10^{0} m to 10^{2} m, at which the analysis is done through well-established structural theories implemented in robust and efficient software. Each length of observation requires a different modelling approach in order to properly capture the phenomena occurring at the given scale. As a general rule, disregarding the affordability of the computational cost, accurate modelling at a lower scale should enable the simulation of the phenomena featuring the behaviour at larger scales. However, this is only partially true since the size effect might be not automatically captured (Bažant and Planas, 1998). In the mesoscale (10-2 m) model LDPM, the effect of the major material heterogeneities is modelled in order to capture the intrinsic material characteristic length associated with fracture and the consequent reduction of the structural strength as a function of the structural size. This section aims to present the principal approaches available in the literature to take advantage of LDPM accuracy at the full structure scale.

3.1. Mathematical homogenization

Mathematical homogenization was first formulated by Babuska (1975) and later exploited by several authors to derive constitutive equations stemming from fine-scale models, in most cases based on the principles of the classical continuum mechanics. Moving from the Generalized Mathematical Homogenization (GMH) developed by Fish et al. (2007), Cusatis et al. (2014) proposed an improved version to adopt for the two-scale LDPM homogenization, in which, differently from previous works, also the rotational equilibrium equation of the particles were considered.

The governing equations of the LDPM framework, mentioned in the previous sections, are completed by the equilibrium equations of each individual particle P^I:

$$M_u{}^I\ddot{\boldsymbol{U}}^I - V^I\boldsymbol{b}^0 = \sum_{\mathcal{F}_I} A\boldsymbol{t}^{IJ} \qquad M_\theta{}^I\ddot{\boldsymbol{\Theta}}^I = \sum_{\mathcal{F}_I} A\boldsymbol{w}^{IJ} \tag{2}$$

where V^I and $M_u{}^I$ represent the cell volume and mass, respectively, whereas $M_\theta{}^I$ is the cell rotational inertia, $\boldsymbol{b}_0$ the body forces, A the facet area, $\boldsymbol{w}^{IJ} = \boldsymbol{c}^I \times \boldsymbol{t}^{IJ}$, and $\boldsymbol{t}^{IJ} = t_\alpha \boldsymbol{e}_\alpha$.

In the homogenization process, a periodic discrete system, i.e. a number of adjacent RVEs, and two separate lengths scales are considered. $\boldsymbol{x}$ and $\boldsymbol{y}$ are the coordinate systems at the two different scales, linked by the relationship $\boldsymbol{x} = \eta\boldsymbol{y}$, where η is a very small positive scalar ($0<\eta<<1$). The displacement field $\boldsymbol{U}^I = \boldsymbol{u}(\boldsymbol{x}^I, \boldsymbol{y}^I)$ of a generic particle P^I is approximated as $\boldsymbol{u} \approx \boldsymbol{u}^0 + \eta\boldsymbol{u}^1$, where only terms up to order $\mathcal{O}(\eta)$ are considered. The functions $\boldsymbol{u}^0(\boldsymbol{x},\boldsymbol{y})$ and $\boldsymbol{u}^1(\boldsymbol{x},\boldsymbol{y})$ are continuous with respect to $\boldsymbol{x}$ and discrete (i.e. defined only at finite number of points) with respect to $\boldsymbol{y}$. Similarly, for rotations it is possible to write: $\boldsymbol{\Theta}^I = \boldsymbol{\theta}(\boldsymbol{x}^I, \boldsymbol{y}^I)$ and $\theta \approx \eta^{-1}\omega^0 + \varphi^0 + \omega^1 + \eta\varphi^1$. Thus, ω^0 and ω^1 are interpreted as rotations in the fine scale, whereas φ^0 and φ^1 as the corresponding coarse scale rotations. Unlike the expansion of displacements, the asymptotic expansion for rotations features a term of order $\mathcal{O}(\eta^{-1})$ and two distinct terms of order $\mathcal{O}(1)$. Since the distance between the particles P^I and P^J can be considered as infinitesimal in the macroscopic reference system $\boldsymbol{x}$, the Taylor series expansion of both displacement and rotation at the node P^J around the node P^I is adopted in order to derive the asymptotic expansion of the strains. Finally, the discrete equilibrium equations in Eq. 2 are rescaled as follows:

$$\overline{M}_u{}^I\ddot{\boldsymbol{u}}^I - \overline{V}^I\boldsymbol{b}^0 = \eta^{-1}\sum_{\mathcal{F}_I} \overline{A}t_\alpha \boldsymbol{e}_\alpha{}^{IJ} \qquad \eta\overline{M}_\theta{}^I\ddot{\boldsymbol{\theta}}^I = \eta^{-1}\sum_{\mathcal{F}_I} \overline{A}\eta^{-1}w_\alpha \boldsymbol{e}_\alpha{}^{IJ} \tag{3}$$

where all the following quantities are $\sim\mathcal{O}(1)$.

$$\overline{M}_u{}^I = M_u{}^I/\eta^3, \quad \overline{V}^I = V^I/\eta^3, \quad \overline{A}^I = A/\eta^3, \quad \overline{M}_\theta{}^I = M_\theta{}^I/\eta^5 \tag{4}$$

Further details about the formulation can be found in Cusatis et al. (2014). For the purpose of this work, it is worth highlighting that the same authors proposed promising preliminary results showing that the technique accurately captured the alkali silica reaction-induced damage when a coarse finite element was adopted for a 200 mm hexahedral finite element with one Gauss point at which one RVE was attached. In addition, the authors studied the effect of the RVE size by running the same numerical simulations employing 5 different RVE sizes. During each time step, the FE strain tensor was transferred to the RVE, and the homogenized stress tensor was calculated and transferred back to the FE level to derive nodal forces and displacements. The results showed that the distance between LDPM-based RVE and FE responses was negligible and not affected by the RVE size during the elastic branch, whereas it increases when smaller RVEs are adopted. However, acceptable error (<10%) is obtained when RVE much smaller than the specimen size is used. Elias and Cusatis (2022) recently explored the mathematical homogenization through asymptotic expansion also for the upscaling of mass transport phenomena coupled with concrete mechanical behaviour as an extension of previous works which focused exclusively on the mechanical problem (Rezakhani and Cusatis, 2016; Rezakhani et al., 2017; Rezakhani et al., 2019). The results confirmed that the approach ensures an accurate match between the outcomes achieved by means of LDPM and those ones obtained through the homogenized model.

3.2. Proper orthogonal decomposition

The proper orthogonal decomposition (POD) method was applied to the LDPM-based simulation of the concrete behaviour by Ceccato et al. (2018). The authors demonstrated that POD is a powerful tool for building reduced-order approximations of the response of large systems, both linear and non-linear, solved with explicit dynamics algorithms.

As the first step, the method requires the extraction of the characteristic spectral modes by collecting snapshots of the full-order response in certain time intervals, chosen to be representative enough of the actual structural behaviour. The spectral modes are intended to be used as shape functions, applied to global support approximating the actual system deformation. The latter features a significant reduction in the number of degrees of freedom with respect to the full LDPM system. The spectral modes limit the high-frequency deformation modes of the full-order system, allowing for a larger stable time step in explicitly integrating the reduced-order equations of motion. However, the full advantage of this increased time step is mostly observed when only a few spectral modes are utilized.

The accuracy and efficiency of the reduced-order model depend on the number of snapshots used to construct the reduced-order space and the number of spectral modes employed in the simulations. Yet, employing a large number of snapshots raises the computational cost of building the reduced-order space, quickly offsetting the computational benefits of reduced-order integration. Homogeneous essential boundary conditions are automatically transferred from the full-order to the reduced-order system, while non-homogeneous essential boundary conditions can be enforced through a penalty algorithm. A significant reduction in computational cost can be achieved by combining POD with classical mass-scaling approaches. Spectral modes need to be updated when non-linear behavior causes significant changes in the system's deformation characteristics, which is particularly important in 3D applications with softening and characterized by complex crack patterns. The best results are obtained by periodically updating the spectral modes during simulations. For 3D cases, improved results are anticipated when mass scaling is combined with POD, a subject currently under investigation by the authors in ongoing studies.

3.3. FE^2 multiscale approach

Oliver et al. (2014) introduced a multiscale approach to computationally model material failure in concrete structures. Framed into the classical homogenization framework, the proposed approach introduces a length scale associated with both RVE size and mesoscale failure mechanism into the resulting macroscopic homogenized model. This microscopic length scale is conceived to be representative of the actual width of the fracture process zone, defining the bandwidth of the macroscopic localization band that captures cracks at the structural level. This concept has been widely acknowledged in modelling concrete materials (Bazant and Jirásek, 2002) and is automatically obtained through the homogenization process. At the macroscopic scale, this microscopic length scale is locally utilized within the context of the Continuum Strong Discontinuity Approach to material failure (Oliver and Huespe, 2004) and is introduced as a regularization parameter in a new technique (Oliver et al., 2014) for capturing the macroscopic propagation of cracks using finite elements with embedded discontinuities. The outcome is a multiscale approach that

maintains correct dissipation and objectivity with respect to both the macroscopic size of the finite element mesh and the size of the failure cell, which can be easily related to recent proposals for similar purposes (Sánchez et al., 2013).

Oliver et al. (2014) applied the proposed techniques to the modelling of concrete-like materials (i.e., materials consisting of aggregates and mortar at the mesoscopic level). Although the complexity of the mesoscale morphology is constrained by the computational cost of combined multiscale computations, some preliminary examples demonstrated the potential of the approach.

4. Conclusions

This work highlights the need for reliable models to predict the performance of concrete structures and infrastructures in terms of durability and response to extreme events. Due to the wide variety of phenomena involving a heterogenous material such as concrete, the goal can be achieved only through multiphysics models, coupling mechanical and hygro-thermo-chemical constitutive laws.

In the last decade, the Multiphysics-Lattice Discrete Particle Model has been proven to be a valuable tool to simulate the response of plain and reinforced concrete not only against mechanical actions but also in civil engineering applications involving transport and chemical phenomena, such as chloride penetration and fire exposure. However, the mesoscale nature of the model represents a huge limitation in its exploitation for structural analyses. In this perspective, the authors are currently trying to identify the most efficient strategy for upscaling. In this contribution the result of a painstaking literature screening has been reported.

The available studies for upscaling are mostly related to the mechanical problem, and promising results show that a multiscale analysis in which the Lattice Discrete Particle Model is used as a fine-scale model might be feasible. However, to the best of the authors' knowledge applications of such approaches to complex structural systems seem to be still lacking. In addition, it is worth highlighting that further investigations are necessary to identify an approach able to scale up the multiphysics implementations today available for the mesoscale model. In the near future, the two above-mentioned aspects will be subject of research efforts.

References

Abdellatef, M., Alnaggar, M., Boumakis, G., and others. 2015. Lattice Discrete Particle Modeling for Coupled Concrete Creep and Shrinkage Using the Solidification Microprestress Theory. 10th Conf. on Mechanics and Physics of Creep, Shrinkage and Durability of Concrete and Concrete Structures (CONCREEP 10), 21–23 September 2015 Vienna, Austria, (pp. 184–193).

Alnaggar, M., Di Luzio, G., Cusatis, G. 2017. Modeling Time-Dependent Behavior of Concrete Affected by Alkali Silica Reaction in Variable Environmental Conditions. Materials, 10.

Alnaggar, M., Pelessone, D., Cusatis, G. 2018. Lattice Discrete Particle Modeling of Reinforced Concrete Flexural Behaviour. Journal of Structural Engineering, 145(1), 04018231.

Babuska, I. 1975. Homogenization and its application. Mathematical and computational problems. 3rd Symposium on the Numerical Solution of Partial Differential Equations, SYNSPADE 1975 (pp. 89-116). University of Maryland, College Park: Academic Press.

Bažant, Z. P., Jirásek, M. 2002. Nonlocal integral formulations of plasticity and damage: survey of progress. J. of Eng. Mech., 128(11), 1119-1149.

Bažant, Z., Planas, J. 1998 (1st ed.). Fracture and Size Effect in Concrete and Other Quasibrittle Materials. New York: Routledge.

Bhaduri, T., Gomaa, S., Alnaggar, M. 2021. Coupled Experimental and Computational Investigation on the Interplay Between Discrete and Continuous Reinforcement in Ultra-High Performance Concrete Beams. II: Mesoscale Modeling. J. of Eng. Mechanics, 147(9), 04021050.

Boumakis, I., Di Luzio, G., Marcon, M., and others. 2018. Discrete element framework for modeling tertiary creep of concrete in tension and compression. Engineering Fracture Mechanics, 200, 263–282.

Bousikhane, F., Li, W., Di Luzio, G., and others. 2018. Full coupling between diffusion and mechanical analysis in a discrete computational framework. In G. Meschke, B. Pichler, & J. G. Rots (Ed.), 5th Int. Symp. on the Chemistry of Cement (p. 305). Bad: CRC Press.

Ceccato, C., Zhou, X., Pelessone, D., Cusatis, G. 2018. Proper Orthogonal Decomposition Framework for the Explicit Solution of Discrete Systems With Softening Response. Journal of Applied Mechanics, 051004.

Cibelli, A. 2022. Computational Modelling of Ageing, Healing and Degradation of Ordinary and Ultra High Performance Concrete. Ph.D. dissertation, Politecnico di Milano, Milan.

Cibelli, A., Di Luzio, G., Ferrara, L. 2023. Numerical Simulation of the Chloride Penetration in Cracked and Healed UHPC via a Discrete Multiphysics Model. Journal of Engineering Mechanics, 149(12), 05023001.

Cibelli, A., Ferrara, L., Di Luzio, G. 2024. Multiscale and multiphysics discrete model of self-healing of matrix and interfacial cracks in fibre reinforced cementitious composites: formulation, implementation and preliminary results. Cement and Concrete Composites, 148, 105465.

Cibelli, A., Pathirage, M., Cusatis, G., and others. 2022. A discrete numerical model for the effects of crack healing on the behaviour of ordinary plain concrete: Implementation, calibration, and validation. Engineering Fracture Mechanics, 263, 108266.

Cusatis, G., Pelessone, D., & Mencarelli, A. 2011a. Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. I: Theory. Cement and Concrete Composites, 33, 881–890.

Cusatis, G., Mencarelli, A., Pelessone, D., & Baylot, J. 2011b. Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. II: Calibration and validation. Cement and Concrete Composites, 33, 891–905.

Cusatis, G., Rezakhani, R., Alnaggar, M., and others. 2014. Multiscale computational models for the simulation of concrete materials and structures. In Bicanic et al. (Ed.), Computational Modelling of Concrete Structures EURO-C (pp. 23-38). Taylor & Francis.

Di Luzio, G., Cusatis, G. 2009a. Hygro-thermo-chemical modeling of high performance concrete. I: Theory. Cem. and Conc. Comp., 31, 301–308.

Di Luzio, G., Cusatis, G. 2009b. Hygro-thermo-chemical modeling of high-performance concrete. II: Numerical implementation, calibration, and validation. Cement and Concrete Composites, 31, 309–324.

Elias, J., Cusatis, G. 2022. Homogenization of discrete mesoscale model of concrete for coupled mass transport and mechanics by asymptotic expansion. Journal of Mechanics and Physics of Solids, 105010.

Feng, J., and others. 2018. Numerical study on the hard projectile perforation on RC panels with LDPM. Const. and Build. Mat., 183, 58-74.

Fish, J., Chen, W., Li, R. 2007. Generalized mathematical homogenization of atomistic media at finite temperatures in three dimensions. Computer Methods in Applied Mechanics and Engineering, 196(4-6), 908-922.

Hao, Y., Cibelli, A., Brown, S.-A., and others. 2023. Flow Lattice Model for the Simulation of Chemistry Dependent Transport Phenomena in Cementitious Materials. European Journal of Environmental and Civil Engineering, 0.

Lale, E., Rezakhani, R., Alnaggar, M., Cusatis, G. 2018. Homogenization Coarse Graining (HCG) of the Lattice Discrete Particle Model (LDPM) for the analysis of reinforced concrete structures. Engineering Fracture Mechanics, 259-277.

Oliver, J., Caicedo, M., Roubin, E., and others. 2014. Multi-scale (FE^2) analysis of material failure in cement/aggregate-type composite structures. In Bicanic e. al. (Ed.), Computational Modelling of Concrete Structures EURO-C (pp. 39-49). Taylor & Francis.

Oliver, J., Huespe, A.E. 2004. Theoretical and computational issues in modelling material failure in strong discontinuity scenarios. Computer Methods in Applied Mechanics and Engineering, 193(27-29), 2987-3014.

Pathirage, M., Bentz, D. P., Di Luzio, G., and others. 2019. The ONIX model: a parameter-free multiscale framework for the prediction of self-desiccation in concrete. Cement and Concrete Composites, 103, 36–48.

Rezakhani, R., Cusatis, G. 2016. Asymptotic expansion homogenization of discrete fine-scale models with rotational degrees of freedom for the simulation of quasi-brittle materials. Journal of Mechanics and Physics of Solids, 320-345.

Rezakhani, R., Alnaggar, M., Cusatis, G. 2019. Multiscale homogenization analysis of alkali-silica reaction (ASR) effect in concrete. Eng., 1139-54.

Rezakhani, R., Zhou, X., Cusatis, G. 2017. Adaptive multiscale homogenization of the lattice discrete particle model for the analysis of damage and fracture in concrete. International Journal of Solids and Structures, 50-67.

Sánchez, P. J., Blanco, P. J., Huespe, A. E., Feijoo, R. 2013. Failure-oriented multi-scale variational formulation: micro-structures with nucleation and evolution of softening bands. Computer Methods in Applied Mechanics and Engineering, 257, 221-247.

Schauffert, E. A., Cusatis, G. 2012a. Lattice Discrete Particle Model for Fiber-Reinforced Concrete. I: Theory. J. of Eng. Mech., 138, 826–833.

Schauffert, E. A., Cusatis, G., Pelessone, D., and others. 2012b. Lattice Discrete Particle Model for Fiber-Reinforced Concrete. II: Tensile Fracture and Multiaxial Loading Behavior. Journal of Engineering Mechanics, 138, 834–841.

Shen, L., Li, W., Zhou, X., and others. 2020. Multiphysics Lattice Discrete Particle Model for the simulation of concrete thermal spalling. Cement and Concrete Composites, 106, 103457.

Shen, L., Lo Monte, F., Di Luzio, G., and others. 2021. On the moisture migration of concrete subject to high temperature with different heating rates. Cement and Concrete Research, 146, 106492.

Wan, L., Wendner, R., Liang, B., Cusatis, G. 2016. Analysis of the behavior of ultra high performance concrete at early age. Cem. and Conc. Comp., 74, 120–135.

Zhang, Y., Di Luzio, G., Alnaggar, M. 2021. Coupled multi-physics simulation of chloride diffusion in saturated and unsaturated concrete. Construction and Building Materials, 292, 123394.