

Contributions and challenges on the computational modelling of damage and fracture

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Abstract. Computational modeling of damage and fracture propagation is a challenging problem, still attracting the attention of many research groups throughout the world. Over the years, the Italian community in structural mechanics, gathered in the scientific fori provided by Aimeta congresses and by the meetings of its interest groups (in particular GIMC and, later, GMA), has provided a huge amount of innovative contributions to the subject. The variety and richness of these contributions make it impossible to provide an exhaustive account in this short note. Rather, we want to try retracing the main stages of the evolution of the Aimeta community research in this particular field from the limited viewpoint of the activity carried out in our research group at the Politecnico di Milano, along the last 30 years.

Keywords: Damage · Strain localization · Regularization · Fracture.

1 Introduction

One century has elapsed since the pioneering work of Alan Arnold Griffith [21] on the energy approach to fracture. In 1927, in the fourth edition of his fundamental treatise on the mathematical theory of elasticity [23], at page 121 Love was still writing “. . . The conditions of rupture are all but vaguely understood. . .”. Many things have changed since then and, thanks to the seminal contributions of Westergaard, Irwin, Rice and many others, we have now understood a lot about the mechanics of fracture. The same can be said for the mechanics of damage, starting from the fifties with the early work of Kachanov [22] and the subsequent contributions by Rabotnov, Lemaitre and others, which have made useful and accurate mathematical models available to the engineering community. Despite these progresses, the prediction of the evolution of damage in a structure, up to its final condition of failure, can still be considered a challenging task, attracting the attention of thousands of researchers around the world.

The purpose of this short note is to provide a brief account of the research activities carried out over the last 30 years by our research group at the Politecnico di Milano on the computational modeling of damage and fracture. Since the beginning, these activities have been strongly influenced by the developments taking place within the Aimeta community and have found a natural forum for presentation and discussion in the congresses and conferences of Aimeta and its

Groups of Interests, in particular the Italian Group of Computational Mechanics (GIMC) and the Group of Mechanics of Materials (GMA). The Italian mechanics community has been particularly active and prolific on this subject and it is impossible for us to summarize here the huge variety of important results that have been contributed over the last three decades. What we propose is therefore a survey of the developments in this field, though limited to the particular viewpoint of our contributions.

Many other colleagues in our research lab at the Politecnico have been active and have contributed along these years to the field of damage and fracture. For the same reasons as above, we cannot however go analytically through the details of these contributions. Some of them (Stefano Mariani, Aldo Ghisi, Roberto Fedele) have collaborated with us and will appear in the references. Among the others, we just mention Alberto Corigliano, for his work on the formulation of cohesive models for mixed-mode delamination, [1, 2] and on the multiscale failure of microsensors [25]; Anna Pandolfi, for her work on the simulation of crack propagation and fragmentation, [27, 30, 29]; Attilio Frangi and Giorgio Novati for their work on boundary elements simulation of brittle fracture [26]; Gabriella Bolzon (see, e.g., [4, 5]); Giuseppe Cocchetti (see e.g. [18]); Raffaele Ardito, for damage identification in concrete dams, [3]. Finally, we mention the work of Giulio Maier, scientific father and mentor, whose vast and fundamental contributions to the mechanics of materials and structures cannot be summarized at all.

2 Damage models

2.1 Bi-dissipative model for concrete

Towards the end of the nineties, research was actively in progress on the modeling of concrete failure. Due to the quasi-brittle nature of concrete, linear elastic fracture mechanics tools could not be satisfactorily applied. Other theories, based on cohesive and/or smeared crack approaches and on damage models, were diffusely investigated, a lot of attention being devoted to the issue of pathological mesh dependence in the softening stage of material response. At that time, these different approaches were the object of numerous contributions and intense discussion in the Aimeta community.

Within this context, in 1999, at the XII GIMC in Naples and later, in the same year, at the XIV Aimeta Congress in Como, we presented a simple model for concrete [11], intended to be robust and suitable for large scale computations of engineering structural problems, and to reproduce accurately the following main macroscopic features of concrete behavior: stiffness degradation; strength reduction (softening) after peak stress; different behavior, with different fracture energies in tension and compression; apparent strength and ductility increase in compression under increasing lateral confinement; unilateral effect, i.e. stiffness recovery when the loading condition is reversed from tension to compression; degradation of material properties characterizing the behaviour in tension due to previous development of damage in compression. The proposed isotropic damage model considered two separate dissipation mechanisms, depending on two

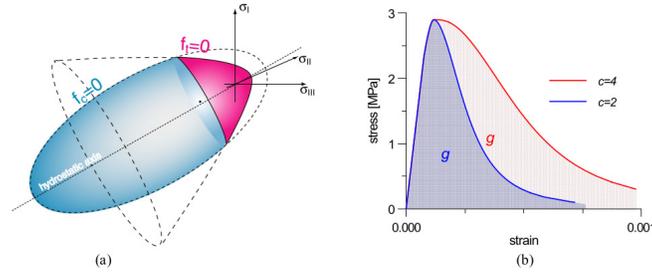


Fig. 1. a) Elastic domain in principal stress space; b) fracture energy scaling.

monotonically increasing scalar damage variables, one in tension and the second in compression (hence the name bi-dissipative, see Fig. 1a). Reasonably accurate and convergent results with a simple computer implementation, avoiding mesh dependence of global results in the presence of strain localization in the softening regime, were achieved by the so called fracture energy regularization technique, as an alternative to the more rigorous, but more complex nonlocal approaches, which were intensively studied at the time. To facilitate the scaling of the material fracture-energy density in the model, a special form of the hardening-softening functions was also proposed (Fig. 1b).

2.2 Model for concrete affected by alkali-silica reaction

Besides mechanical loading, long-term chemical reactions between the different constituents of concrete, possibly in the presence of aggressive environments, can cause the degradation of concrete structures. Starting from 2008, we studied in particular the phenomena of the alkali-silica reaction (ASR) and of the external sulfate attack (ESA). The interest in those phenomena was driven by several research projects on the safety assessment of concrete dams conducted with different Italian groups, active in the Aimeta community.

The ASR is a chemical reaction occurring in concrete between the alkali of the cement paste and non-crystalline silica, which is found in some kind of aggregates. The main product of the reaction is a gel, which expands in the presence of water, initially filling up the pre-existing concrete pores and then causing micro-cracking and overall expansion of the concrete structure. To predict the mechanical effects of this reaction, we formulated a bi-phase chemo-thermo-damage model [8]. The basic idea of the model is shown in Fig. 2: concrete affected by ASR is modeled, according to Biot's theory of porous media, as a heterogeneous material at the meso-scale, constituted by two elastic-damageable phases: the gel produced by the chemical reaction, which expands in time, and the homogenized concrete skeleton, which is subjected to tensile effective stresses causing damage. The response of the homogenized concrete skeleton to effective stresses is described by the model recalled in the previous section.

The model was validated through comparison with experimental tests reported in the literature and applied to the prediction of degradation in dams.



Fig. 2. Scheme of the bi-phase material representing concrete affected by ASR: solid skeleton and pressurized wet gel

Extensions to consider the effects of anisotropy [14] and of partial saturation [9] were proposed and discussed at the XIX, XX, and XXI Aimeta Congresses.

2.3 Model for concrete affected by sulfate attack

The external sulfate attack (ESA) is another important cause of concrete degradation. It consists of a complex set of reactions between sulfate ions (coming from the external environment) and the hydrate calcium aluminates present in the cement paste. The final reaction product is the secondary ettringite that, forming within the hardened matrix, can generate swelling and microcracks formation inside the material.

Figure 3a schematically shows the effect of ESA: when sulfates penetrate, leaching and swelling occur in the zone in contact with the aggressive solution. Beyond this zone, the concrete is intact and swells due to ettringite formation, causing tensile stresses and microcracks formation in the most internal parts.

To simulate the mechanical effects of ESA, similarly to what proposed in the case of ASR, we developed a multi-phase material model, also accounting for partially saturated conditions [6]. A reactive-diffusion model was used to compute the sulfate molar concentration and the amount of formed ettringite. The ettringite formation implies a volume increase and, once the initial porosity is filled, it induces a volumetric deformation. Two phenomenological isotropic damage variables describe the chemical degradation and the stress-induced degradation. The model has been validated by simulating experimental tests under isothermal conditions presented in the literature, and then used to simulate the behaviour of a reduced-scale model of a tunnel lining. Figure 3 shows the chemical and mechanical damage distributions after 2 and 6 months. The chemical damage progressively develops, starting from the surface in contact with the aggressive soil and then spreads through the whole thickness of the tunnel lining. The mechanical damage in tension concentrates at the upper part of the vault and reaches high values already after 2 months of exposure. Another highly damaged part develops at the interface between concrete and soil at one third of the arch.

3 Strain localization and regularization methods

In parallel with the formulation of complex damage models intended to describe with high accuracy various degradation phenomena, in the 90s an important in-

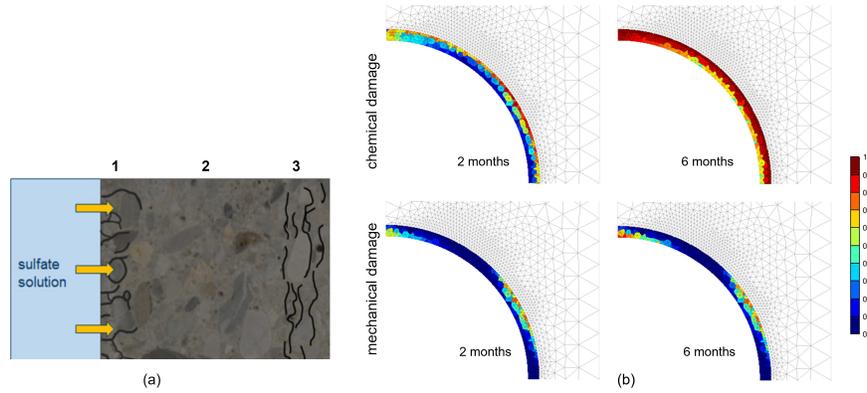


Fig. 3. (a) Schematic view of the degradation and formation of three zones in a specimen affected by ESA; zone 1: leaching and ettringite formation, zone 2: expansion due to ettringite formation, zone 3: microcracking due to tensile stresses. (b) Chemical and mechanical damage evolution in a tunnel lining due to ESA.

ternational scientific debate started about the localization phenomena occurring in damageable materials and softening models, with the consequent ill-posedness of the boundary value problem. To restore well-posedness, different regularization strategies were proposed and discussed in the forum provided by Aimeta and GIMC Congresses, starting from the XII Aimeta Congress of Naples in 95. Here we briefly account of gradient-dependent and non-local formulations.

3.1 Gradient-dependent models

In local continuum damage model or in plasticity models with softening, when localization occurs, damage or plastic strains grow in a band whose thickness tends to zero, leading to the wrong prediction of material failure without dissipation. To avoid this un-physical behavior, a characteristic internal length, which characterizes the material micro-structure, must be introduced in the model. In [15], an isotropic gradient-enhanced damage model is proposed in which the loading function not only depends on the damage value, but also on its Laplacian. The coefficient of this latter term depends on the material internal length and fixes the width of the localization zone. Due to the presence of the gradient term in the loading function, in finite element analysis, not only the displacements, but also the damage field must be modeled and proper boundary conditions on damage must be added. The finite element mixed formulation of the finite-step was obtained through the Hu-Washizu variational principle. This strategy proved to be effective to regularize the problem.

From the computational point of view, the gradient regularization is quite demanding due to the coupling between different points in the corrector phase. However, for particular forms of the loading function, the corrector phase can be recast in the form of a linear complementarity problem, which can be solved

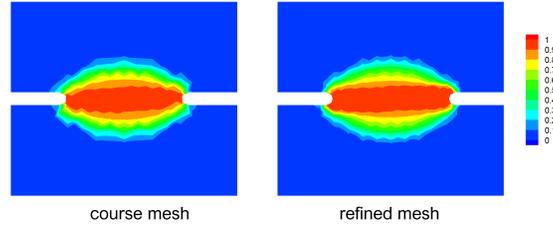


Fig. 4. Notched tension test: damage distribution for coarse and refined meshes

very efficiently e.g. by the Mangasarian’s algorithm. The more recent phase-field approach to quasi-brittle and ductile fracture can be seen a more rigorous formulation of the same type of approach.

3.2 Nonlocal models

Another popular approach to introduce an internal length is the nonlocal integral formulation. The key idea is to consider in the definition of the constitutive behavior of a point its interaction with other points inside a proper neighborhood defined by the material length. Different formulations are obtained by different choices of the non-local variable, which is replaced by its averaged mean over the neighborhood. The resulting models should ensure the well-posedness of the initial boundary value problem and possibly be not too computationally demanding. The choice of replacing the strain invariants with their non-local counterparts in the loading functions proposed in [7] proved to comply with the above requirements and effectively regularized the model described in 2.1. Figure 4 shows the mesh independence of the damage pattern in a tension test.

The numerical aspects related with the non-local formulation were further discussed in [12] and [13] and presented in 2000 at the GIMC meeting in Brescia.

4 Modeling of crack propagation and delamination

4.1 Finite element models for crack propagation

The finite element modelling of crack propagation is a complex problem in view of the necessity to follow the evolution of the displacement discontinuity. Smeared crack, or continuum damage approaches, as those discussed in the previous section, remove the evolving discontinuity, at the cost of the necessity to resolve the evolving band, with the ensuing computational cost.

In the Extended Finite Element Method (XFEM), the difficulty connected with the finite element modeling of an evolving discontinuity is overcome by augmenting the displacement interpolation basis through ad hoc assumed local functions, incorporating a displacement discontinuity. In addition, local known

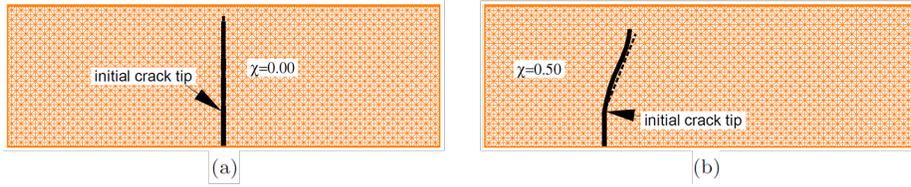


Fig. 5. Mixed-mode Three-point-bending test: comparison between available experimental (dashed lines) and numerical (continuous lines) crack paths for different position χ of initial notch: (a) $\chi = 0.00$; (b) $\chi = 0.50$.

features of the exact solution can be explicitly added to the standard FE approximation fields, as in the case of brittle fracture. In the case of quasi-brittle fracture, the tractions transmitted between the two sides of the discontinuity in the process zone avoid the stress singularity in the tip region, eliminating the need of this latter enhancement. Rather, they require considering a cohesive behavior along the propagating discontinuity in the process zone. This has been achieved in [24] by enhancing the approximation fields via quadratic polynomials, discontinuous across the fracture surface, using in 2D three-node constant strain triangles. Figure 5 shows the results for a three-point-bending test and for varying position of the initial notch. A similar approach has been successfully implemented in [16] for the simulation of fracture processes in quasi-brittle weakly functionally graded materials (FGMs), endowed with elastic and toughness properties gradually varying in space. These XFEM approaches have also been presented and discussed at the XV and XVII Aimeta Congresses, in Taormina 2001 and Firenze 2005, respectively.

A particular type of problems in fracture mechanics is represented by the blade cutting of thin shells. The process of cutting is a highly nonlinear and complex problem, dominated by the co-existence of several geometric scales. The first one is the scale of the thickness of the thin-walled structure, which is usually orders of magnitude smaller than the in-plane global dimensions. The second is given by the material critical size of the process zone, where the in-elastic phenomena preceding crack propagation take place. Another small scale is determined by the curvature radius of the cutting blade, which can be of the order of microns, or even less, in the case of a sharp blade.

In cutting problems, the main crack propagation direction is dictated by the blade movement, so that the mesh can be a priori adjusted to follow the correct propagation path, without the need to use extremely refined meshes. A new type of cohesive interface element, to be interposed between adjacent separating solid-shell elements, the so-called “directional” cohesive element, has been proposed in [20, 28, 17] and discussed at several Aimeta Congresses (XX, Bologna 2011, XXI Turin 2013, XXII Genoa 2015) and GIMC/GMA conferences (XVIII GIMC Siracusa 2010, XXI GIMC/VIII GMA, Lucca 2016).

When a suitable fracture criterion is met at a given node, this is duplicated and a massless string is introduced in the model in correspondence of each pair

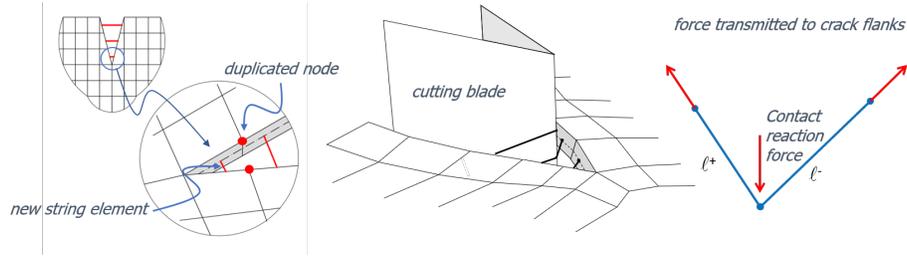


Fig. 6. Insertion procedure for directional cohesive elements: node duplication, string insertion, contact detection, cohesive force definition.

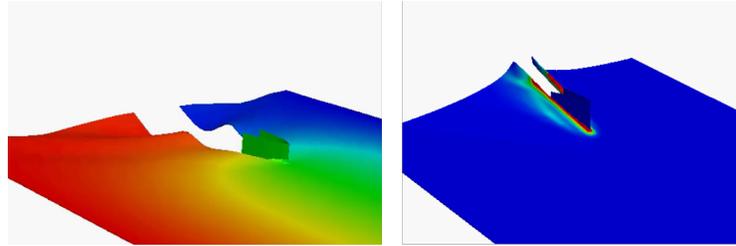


Fig. 7. Blade cutting of a rubber sheet (left) and of a steel plate (right).

of separating nodes (Fig. 6). The string is a straight segment, naturally endowed with a length coinciding with the distance between the nodes and transmitting a cohesive force defined by the specific cohesive traction-separation law adopted. The string element is a well defined geometric entity and its contact against the cutting blade can be checked throughout the analysis duration. When a point of a string element is detected to be in contact with the blade, the string is subdivided into two string elements (Fig. 6). In this way, the cohesive forces are transmitted between the crack flanks along directions taking into account the presence of the cutter. When the current total length of the string exceeds the limit value, the string is removed. The proposed method with directional cohesive elements has been applied to blade cutting simulation of a number of different configurations and materials (Fig. 7) with excellent accuracy of results.

4.2 From regularized damage to cohesive-crack

Continuum approaches prove efficient in the first stage of spreading of damage in localized regions. However, the width of the band of growing damage tends to reduce, making the computational costs excessive for real-life structures. If the mesh is adaptively refined during the analysis, a significant computational burden is still due to the continuous convection of current results from the old mesh to the new one. Another important drawback of the non-local continuum

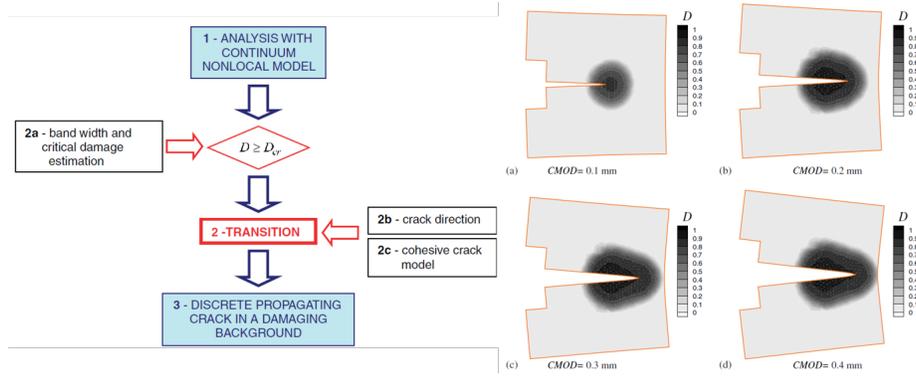


Fig. 8. Left. Schematic flow of the procedure. Right. Wedge-splitting test: damage evolution and transition to fracture.

approach is that non-local interaction remains active also when damage tends to one, leading to an unrealistic spread of the fully damaged band. These difficulties suggested to consider the possibility of a transition from a continuum damage model, in the early stage of loading, to a discrete description of crack evolution, as in the XFEM approach. In this way, the advantages of both formulations could be retained, avoiding their main drawbacks.

The debate on this issues has been intense, in particular at the beginning of the 2000s, at the III Joint Conference of the Italian Group of Computational Mechanics and the Ibero-Latin Association of Computational Methods in Engineering, in Giulianova, 2002, and at the XVI Aimeta Congress, in Ferrara, 2003. On these occasions, we presented an integrated strategy to model the transition from a continuum description of damage evolution to a discrete model for cohesive crack propagation [10].

The strategy proposed in this work consists of three steps, as shown in the left part of Fig. 8. In a preliminary step, a critical value of damage is computed for each element, based on its size and on the minimum number of elements considered necessary to resolve the localization band. In step 1) a finite element analysis with standard finite elements and a non-local continuum damage model is carried out to avoid mesh dependence. Step 2) consists of three substeps: in step 2a) the current localization bandwidth corresponding to the accumulated value of damage is estimated based on a perturbation analysis; in step 2b), when the critical damage is exceeded in an element, a discrete cohesive crack is introduced in the element according to an ‘extended’ finite element approach, by enriching the displacement interpolation with discontinuous functions satisfying the partition of unity concept; in step 2c) the cohesive law of the crack is defined through an energy balance, in such a way that the energy not yet dissipated in the damage band is transferred to the cohesive interface. In step 3) the cohesive crack is let to propagate. The result of the application of the methodology to the simulation of a wedge-splitting test is shown in the right part of Fig. 8.

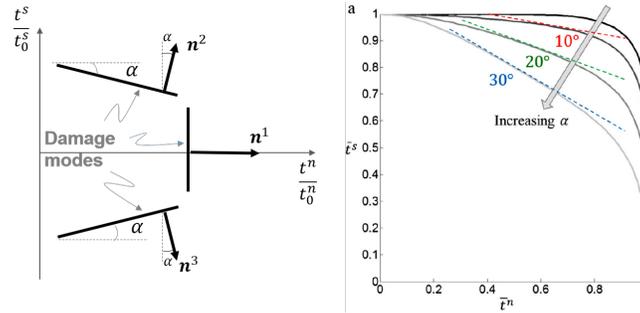


Fig. 9. Damage modes identification in normalized tractions space (left). Activation domain in normalized tractions space (right).

4.3 Interface models for mixed-mode delamination of composites

For layered composites or adhesive junctions, delamination or debonding are typical failure modes, where the delamination front is forced to propagate along the low toughness interface, rather than realigning along a mode I direction, so that mixed mode is the most frequent loading condition. An important feature of mixed-mode delamination is that the fracture energy depends on the active fracture mode and may be significantly different in mode I and mode II. Experimental evidences show that the higher complexity of the fracture surface, with a resulting greater effective area, accounts for the increasing fracture energy in passing from mode I to mode II delamination. The debate on how to treat the fracture energy variation with the mode ratio has been particularly intense over the years, with the proposal of many different approaches.

A new, thermodynamically consistent framework for the formulation of cohesive interface models has been proposed in [19] and presented and discussed at Aimeta Congresses (XXIII, Salerno 2017, XXIV, Rome 2019). While a free energy decomposition in terms of normal and shear components is usually considered, in the proposed model the damage activation locus is obtained by a decomposition driven by the identification of three damage modes (Fig. 9).

In contrast to the majority of available models, the definition of equivalent opening displacements and tractions is not required and the framework is particularly suited for the simulation of complex, non-proportional loading paths. The model requires only few parameters, which can be identified based on tests in pure mode I and II and in mixed mode, for varying mode-ratio.

A new, rigorous and exhaustive validation protocol for delamination models has also been proposed, based on three different types of tests: consistency tests, whereby the model is tested at material point level on intentionally complex loading paths; accuracy tests, whereby the model is applied to estimate the fracture energy evolution with the mode ratio; evolutionary tests, whereby the model is used for the simulation of experimental tests. The proposed model has been shown to provide excellent results in all these test types.

5 Conclusions and perspectives

The computational modeling of damage and fracture can be considered to a certain extent to be a mature field. However, a number of different factors call for more advanced analysis tools, driving the research efforts in new, still not completely explored research directions. A growing worldwide demand for safe and durable products calls for refined design and verification concepts, capable to account for possible defect growth at different scales and for a variety of extreme loading conditions, in a multiphysics, coupled context. From the environmental point of view, a growing attention and consciousness towards the depletion of natural resources calls for extreme design in terms of weight and material consumption, with new bio-inspired and engineered materials, requiring mechanical models capable to span across a multitude of scales. On the other hand, growing competition in the global market calls for new paradigms in design, for innovative and less expensive engineering realizations, requiring design and analysis tools that are robust, fast, accurate and easily usable in an engineering context. Finally, computer architectures are steadily evolving towards distributed computing models (not to mention the still to come quantum computing), calling for highly parallelizable algorithms, to be combined with artificial intelligence tools to manage data-driven material models at different scales.

We are confident that the Aimeta community, with the value of the expertise matured along its history and the growing richness of new talents joining its community will be able to match these challenges and to continue to provide valuable contributions to science and society.

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