ICME: From academia to industry

By Dr. Issam Doghri, Co-founder and Chief Materials Scientist, e-Xstream engineering, Professor at U.C. Louvain (Belgium)
About ICME and multiscale modeling

The ICME acronym stands for “Integrated Computational Materials Engineering”, and is a modeling chain which links a manufacturing process, a material’s microstructure, its engineering properties and the performance of products made with it. Dr. Roger Assaker lays out his “10x” vision on how ICME can be deployed across industries in order to help design better products in an optimized and cost-effective way. In the present text, I will briefly describe the multiscale approach, which is the cornerstone of ICME and enables to link a material’s response across different length scales. Within the “10x” vision, multiscale modeling plays a crucial role in: virtual material development (1), virtual material testing (2), virtual manufacturing (6), effect of manufacturing process (7), virtual engineering (8), material intelligence (9) and material-centric digital twin (10).
Any material is heterogeneous if the scale of observation is fine enough (e.g., that of molecules or atoms). However, engineering materials are used in solids or structures at a macroscopic scale, which can range from a few millimeters to several meters. At that scale, we can consider materials to be homogeneous (over the whole structure or in subparts) and use continuum mechanics to solve a boundary value problem with appropriate numerical techniques, typically by finite element analyses (FEA). However, a material which is considered as homogeneous at a macro scale might still be heterogeneous at finer scales (called micro or meso) which are much larger than molecular or atomic scales, for instance the scale of the fibers for composite materials, that of the pores for porous materials and the grains for polycrystalline metals. What happens at those micro or meso levels greatly influences the engineering properties at macro scale. For instance, a composite material is made of a matrix phase in which one or more other phases are embedded, each one of them including several fibers, particles, cavities or microcracks. The composite’s macro (or effective) response strongly depends on the material properties of its different phases, and on the geometry, spatial distributions, orientations and volume fractions of the “inhomogeneities” (or “inclusions”).

In order to find the link between the macro response and the “microstructure”, one can carry out an experimental campaign, but this can quickly become tedious, expensive and cannot be predictive, by construction. Another approach is via numerical modeling and computer simulations, based on the notion of “representative volume element” (RVE), which is large enough to statistically represent the microstructure, and small enough with respect to the size of the structural body (e.g., a part) at macro scale. This is the objective of multiscale modeling, a key part in ICME, which will be illustrated in the following example.

**An illustrative example: short fiber reinforced composite (SFRC)**

Short fiber reinforced composites (SFRCs) where a thermoplastic polymer matrix is reinforced with short glass fibers represent a large class of applications. Those SFRCs are usually manufactured using an injection molding process, which results in having in each small volume misaligned short fibers which are more or less randomly dispersed. However, the fibers within a small volume are neither aligned nor randomly oriented, and their orientation can be described by an orientation distribution function (ODF), whose average measure in a RVE is given by a so-called orientation tensor (OT). The fibers’ length is also distributed, although in practice one considers so-called fixed equivalent lengths, with values of ratios of length over diameter in the order of 20 being typical. The manufacturing process also induces some porosity (whose evolution might lead to damage).

The material response is both strongly anisotropic and heterogeneous throughout a part. In addition, the response of a thermoplastic polymer (and thus of a SFRC) is nonlinear and history-dependent. It depends on time, loading rate, temperature, moisture; it exhibits creep, relaxation, ageing. It exhibits permanent (plastic) deformation after removal of external load. Now, we need to capture all these features and their variation with changes in orientation, fiber length, fiber volume fraction, matrix material (e.g., polyamide versus polypropylene). And we need to model all these changes not only at an elementary volume level, but for all such elementary volumes at the structural scale (that of a part). In order to address all the challenging issues listed above, we need an accurate, robust and fast computational modeling procedure. In other words, we need ICME. First, we have to model the manufacturing process, that is injection molding in this case. There are software packages which do this, based mostly on models by Tucker et al. These programs enable to predict the fibers’ OT in each small volume at the end of process.

Next, the resulting OT file must be mapped between two meshes: from the process simulation mesh to the one of the solid part for structural FEA. Now, each integration point in the solid mesh at macroscale is considered to be the center of a RVE which contains the microstructure, that is a large number of misaligned fibers embedded in a thermoplastic polymer matrix. The effective response of each RVE needs to be computed. It can be shown that by imposing appropriate boundary conditions (BCs) on the RVE’s surface (e.g., periodic or kinematic BCs) the RVE’s response is obtained by relating volume averages of micro stress and strain fields (inside the RVE). This is called homogenization or scale-transition or two-scale or multiscale modeling.

There are two approaches to obtain the homogenized response of a RVE: full-field and mean-field. In the former, one solves for the detailed micro fields and then computes the RVE averages of stresses and strains. However, full-field RVE simulations with FEA are very costly, especially for nonlinear behavior. Another full-field method, based on
using regular grids, transforming and solving the problem in Fourier space, enables to reduce the FEA cost by at least one order of magnitude. However, the cheapest homogenization method by far is mean-field (MF) homogenization, which is based on assumed relationships between mean values of strain or stress fields in each phase of a RVE. The extremely low CPU cost of MF is due to analytical solutions in linear elasticity, and to approximate semi-analytical extensions of those solutions and MF models to the nonlinear regime. The tradeoff however being that MF does not give access to detailed microfields (which are of interest for strength analyses) and its accuracy might be insufficient for inelastic behavior.

Finally, we are interested in the deformation of the actual part, manufactured with injection molding, and made of SFRC materials. Each integration point at the macroscale hides a heterogeneous microstructure. From one point to another, this microstructure changes (due to the change in OT) and of course the strain field changes also. For nonlinear materials, the pointwise strains also change with time, and also iteratively within each time step. If for each integration point of the macro mesh, we solve the RVE problems with a full-field method (in FEA at RVEs, this is called a FE2 approach) then the computational cost will be prohibitive, and not for engineering use.

If we use MF at the RVE level, then the CPU cost will be much more reasonable, but still too high in practice (this was the first approach in coupling Digimat with FEA solvers). Another alternative is called hybrid in Digimat. It is a semi-coupled approach where the RVEs are homogenized in pre-processing mode, then an appropriate number of macro and anisotropic material models are identified and used in the FEA analysis of a part at macro scale.

A few remarks about the history, the present and the future of ICME

Although the ICME acronym is recent, and despite the topic being very modern, the origins can be traced back to the rules of mixture and the models of Reuss (uniform stress) and Voigt (uniform strain) more than one hundred years ago. Other historic milestones are the Taylor model for polycrystalline metals (1930’s) and Eshelby’s solution in linear elasticity for a single ellipsoidal inclusion in an infinite body (1957). After that, homogenization and multiscale modeling really took off, and every decade since then has seen some important contributions, starting with linear elasticity and then nonlinear problems, either with theoretical models or computational methods. Now, ICME has achieved a maturity level which enables it to be used fruitfully at the industrial scale, and solve problems which were a dream only a decade ago. On a personal level, I was attracted to the topic of homogenization around 1995, and I was truly in admiration with what other researchers had accomplished already. However, I found that most of the literature only showed academic examples on idealized situations, typically monotonic tension tests on a composite with spherical inclusions or aligned fibers.

However, if homogenization is to be used in practice for actual problems, we need to be able to simulate more general loadings (e.g., multiaxial, non-monotonic), more complex microstructures (e.g., SFRCs), general inelastic material behavior (e.g., nonlinear, hereditary) and model actual parts, not just RVEs. That was the motivation behind my academic research on homogenization and multiscale modeling, which led to the development of the first version of Digimat (for “Digital materials”) and to the foundation with Roger of e-Xstream engineering (“extreme modeling for streamlined engineering”) in 2003, but this is another story.

There are still some “hot” issues in ICME, which are the subject of intensive efforts, both in academia and in software development. Examples are: applications of data science and artificial intelligence (data mining, machine learning); working on other kinds of materials (e.g., bio-materials, soft materials, geologic materials, ceramics, new composites, new bio-inspired and other architectured materials, meta-materials, etc.); multi-physics multiscaling (e.g., linking molecular dynamics with continuum micromechanics); renewable energies; electric vehicles; new space homogenization models; computational high cycle fatigue for non-metallic heterogeneous materials; modeling damage and failure at multiple scales; taking into accounting process-induced uncertainties.

Dr. Issam Doghri

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