



DIGIMAT for ENGINEERING PLASTICS

Document Version 2.0.1, March 2010

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Materials: Engineering Plastics, Reinforced Plastics, PP, PA, PA-MXD6, PPA, LCP.

e-Xstream Technologies: DIGIMAT, Digimat-MF, Digimat-FE, Digimat-MX, Digimat to CAE, Map.

Complementary CAE Technologies: Moldflow, Moldex3D, 3D-Sigma, 3D Timon, Rem 3D, Altair, Abaqus/Standard, Abaqus/Explicit, ANSYS, LS-DYNA, PAM-CRASH, SAMCEF, RADIOSS.

Industries: Material Suppliers, Automotive, Consumer Products.

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EXECUTIVE SUMMARY

e-Xstream engineering is a software and engineering services company, 100% focused on advanced material modeling technologies. We help our customers reducing their development costs and the time needed to bring innovative and high-quality products to the market.

e-Xstream develops the DIGMAT material modeling platform that consists of a complete set of complementary and interoperable software products. Digimat-MF and Digimat-FE are aimed at predicting the nonlinear thermo-mechanical behavior of a large variety of multi-phase materials as a function of their underlying microstructure as described by: 1- the material behavior of each constituent phase; 2- the microstructure morphology defined by the reinforcement weight/volume fraction, shape, length and orientation. These software can be compared to a "numerical material test lab" that one can use to generate a numerical material sample and load it in tension, compression, shear,... Digimat-MF, based on nonlinear semi-analytical homogenization theory, offers accurate and efficient predictions at the macroscopic scale (i.e. at the composite level), as well as averaged results at the microscopic scale (i.e. at the constituent level). Digimat-FE, based on direct nonlinear Finite Element Analysis (FEA) of material Representative Volume Element (RVE), offers accurate local predictions at both the macroscopic and microscopic scales. The time required to build and solve a Digimat-FE model is higher than Digimat-MF.

DIGMAT is strongly coupled to the major injection molding and structural Computer Aided Engineering (CAE) software, to enable an accurate and efficient multi-scale modeling of the end-product, using Digimat-MF as the micromechanical model of the material, at each local point of the product. In this case, Digimat-MF can be seen as the "numerical material" at each integration point of the end-product FEA model.

DIGMAT has a comprehensive set of software tools and capabilities dedicated to the modeling of reinforced plastics and injection molded parts. The software and technologies are backed up by a team of engineers with a strong expertise in nonlinear finite elements, material modeling and multi-scale analysis of reinforced plastics.

CUSTOMER TESTIMONIALS

"DIGMAT is a powerful tool that is giving us a new insight into our composite polymers. Its ability to model thermal expansion as a function of temperature, for instance, has been instrumental in understanding some subtle warpage mechanisms of injection molded parts."

Vito Leo, Principal Scientist, Solvay Advanced Polymers

"The combined use of DIGMAT and Map enables Nokia to combine process and structural simulations in order to take manufacturing into account. In the end, this will lead to a higher confidence in analysis results and a more realistic product optimization."

Niels Lerke, Simulation Specialist, Nokia Mobile Phones R&D

"We believe in the incorporation of fiber orientation from flow simulations into a structural simulation package like Abaqus. DIGMAT is the absolute front runner in that. It is not only a trend but an absolute necessity to make simulations of intrinsically anisotropic material like glass fiber reinforced thermoplastics more realistic and to increase their predictive power. "

Dr. Ir. Harold van Melick, Global CAE manager, DSM Engineering Plastics

Digmat-MF, The Mean Field homogenization software

Digmat-MF is a user-friendly micromechanical material modeling software where the user inputs the material behavior of the phases, the microstructure description and the loading applied to the resulting multi-phase material, guided by a tree data structure.

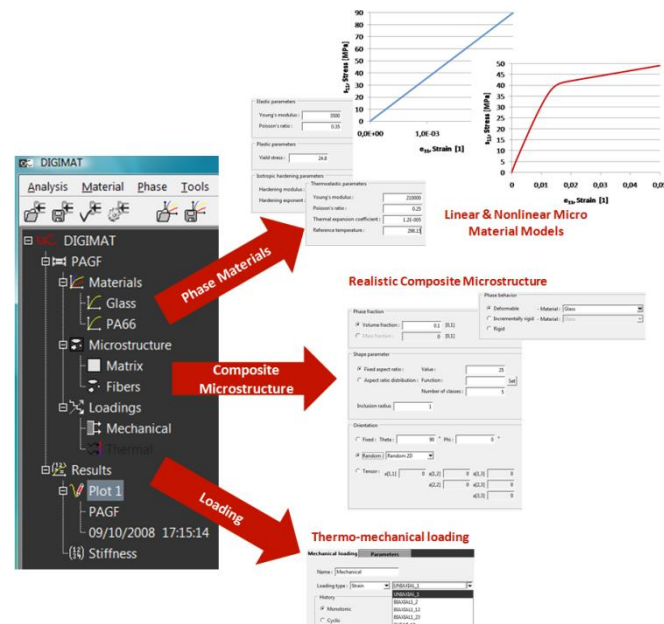


Figure 1: Tree Data Input Structure: Materials, Microstructure and Loadings.

Digmat-MF is based on two homogenization schemes: Mori-Tanaka and Interpolative Double Inclusion. The latter is, in some cases, more accurate for handling large volume fractions of reinforcements and higher contrast between the reinforcement and the matrix stiffnesses. First and second order homogenizations are available for both schemes. Second order provides softer composite response and is particularly suited for material response softening induced by matrix damage.

A complete set of material constitutive laws is available to model the behavior of each phase of the reinforced plastics. For the polymer matrix, the following models are of particular interest: Thermo-Elastic (TE), Elasto-Plastic (EP), Damaged Elasto-Plastic (DEP), Visco-Elastic (VE) and Elasto-Visco-Plastic (EVP). The first three models are strain rate independent and are therefore aimed at modeling the quasi-static response of the reinforced material. The TE material can be considered as anisotropic even before considering the anisotropy induced by adding the reinforcements. This is used to model anisotropic polymer matrices such as LCP. The temperature dependency of the polymer matrix can also be taken into account.

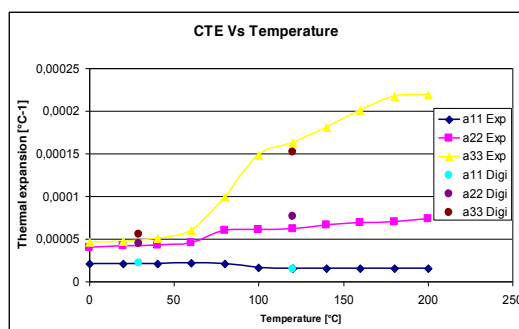


Figure 2: Predicted versus measured coefficient of thermal expansion (CTE) of glass fiber reinforced PPA. Courtesy of Solvay.

Temp. [°C]	E ₁₁ DIGIMAT [MPa]	E ₁₁ Exp. [MPa]	Δ_r
29	12031	11803	-1.91%
120	4073	3740	-8.93%
	E ₂₂ DIGIMAT [MPa]	E ₂₂ Exp. [MPa]	Δ_r
29	7480	7223	-3.57%
120	1281	1257	-1.96%

Table 1: Predicted versus measured Young modulus of glass fiber reinforced PA-MXD6. Courtesy of Solvay.

The VE and EVP material models are used to model the creep, relaxation and the material response under high strain rate solicitations (e.g. crash, drop testing).

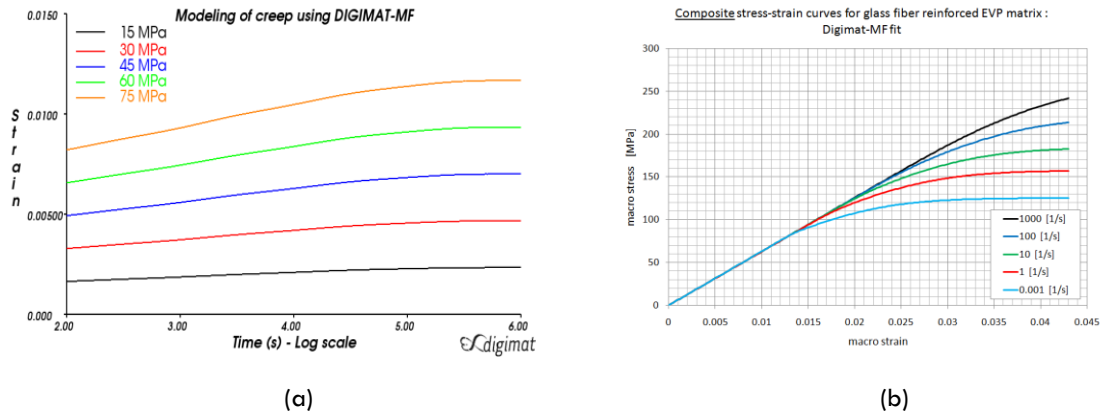


Figure 3: (a) Prediction of the strain evolution with time at different applied stress levels of a glass fiber reinforced plastic using Digimat-MF. (b) Prediction of the nonlinear stress-strain curve of a glass fiber reinforced polypropylene subject to a tension test at different strain rates.

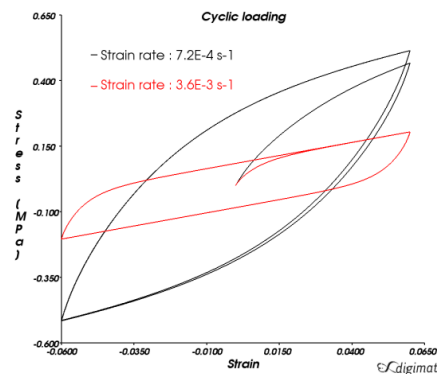


Figure 4: Prediction of the effect of the strain rate on the visco-elastic response of the reinforced material subject to cyclic loading.

Fiber reinforcements are usually modeled as an elastic material either isotropic (e.g. glass fibers) or transversally isotropic (e.g. carbon fibers). Reinforcements are assumed to have an ellipsoidal shape, defined by its aspect ratio ($AR = \text{Length}/\text{Diameter}$). Platelets, spheres and fibers can thus be easily modeled.

Different fiber lengths can be modeled by acting on the aspect ratio, from short fibers (e.g. $1 < AR < 20$), to long ($20 < AR < 1000$) and continuous ones (e.g. $AR > 1000$). Fiber orientation can be either fixed, random or described by a second order orientation tensor that can be predicted by injection molding software or measured experimentally. DIGMAT includes proprietary technology to handle orientation tensors accurately. Different polymers like elastomers can also be used to "reinforce" a polymer matrix and to predict the response of the end material like Thermo-Plastic Elastomer (TPE).

The interaction between the reinforcement and the matrix phases can be modeled by considering a coating phase which is defined by a relative or an absolute thickness with respect to the reinforcement dimensions.

Finally, a series of failure indicators can be defined at the composite (i.e. macro) and at the phase level (i.e. in the matrix and/or in the reinforcing phases).

Digmat-FE, Finite Element modeling of Representative Volume Elements (RVE)

Digmat-FE is a micromechanical material modeling software using a direct finite element representation of a realistic representative volume element of the reinforced plastic microstructure. Digmat-FE is complementary and fully interoperable with Digmat-MF. The main advantages of Digmat-FE with respect to Digmat-MF are:

1. the possibility to generate very complex RVE with ellipsoidal and/or non-ellipsoidal inclusions (e.g. semi-crystalline microstructure morphology);
2. take into account geometrical effects such as inclusion clustering and percolation;
3. compute the actual distribution of the local fields at the micro scale (i.e. in each phase of the reinforced polymer) in addition to the macroscopic thermo-mechanical response of the multi-phase material.

The CPU time needed to set-up and run a Digmat-FE model is much higher than the equivalent Digmat-MF with comparable macroscopic response predictions. Digmat-MF should then be used whenever possible and when the material needs to be modeled at each integration point of a structural FEA model.

Digmat-FE operates following a tree input data structure very similar to that of Digmat-MF, with only a limited amount of additional data required to control the actual RVE geometry generation.

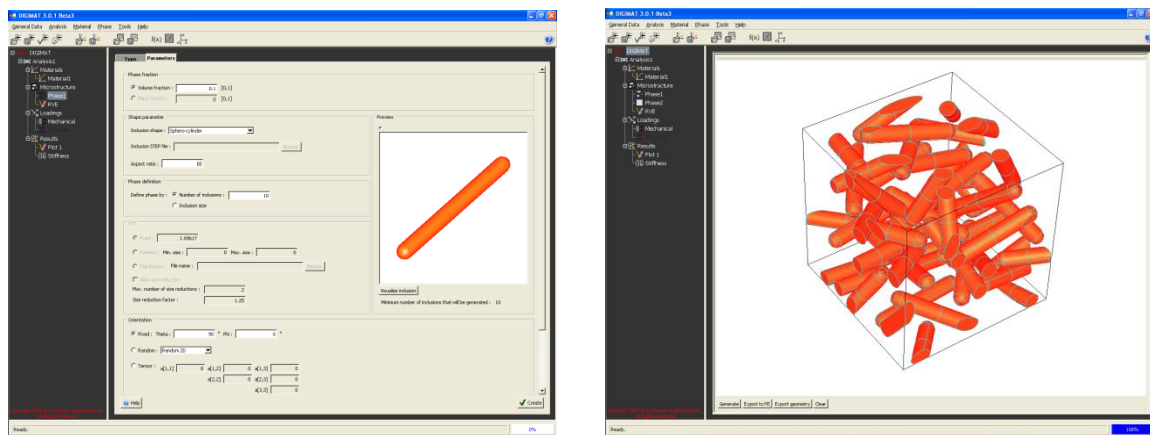
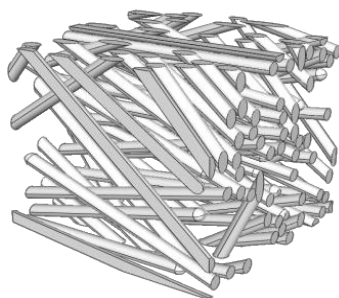
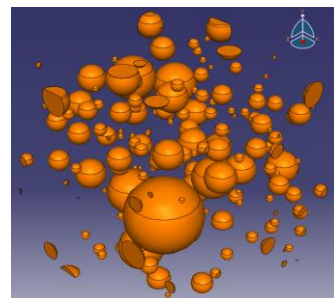


Figure 5: Digmat-FE uses a tree data structure similar to that of Digmat-MF. It is fully interoperable with Digmat-MF.

Digmat-FE can be used to generate very realistic RVE microstructure geometries such as glass fiber reinforced polymers, where the fiber orientations are specified by an orientation tensor, or a polymer matrix filled with coated or uncoated spherical inclusions of various sizes. These geometries can be exported in *step* or *iges* formats.



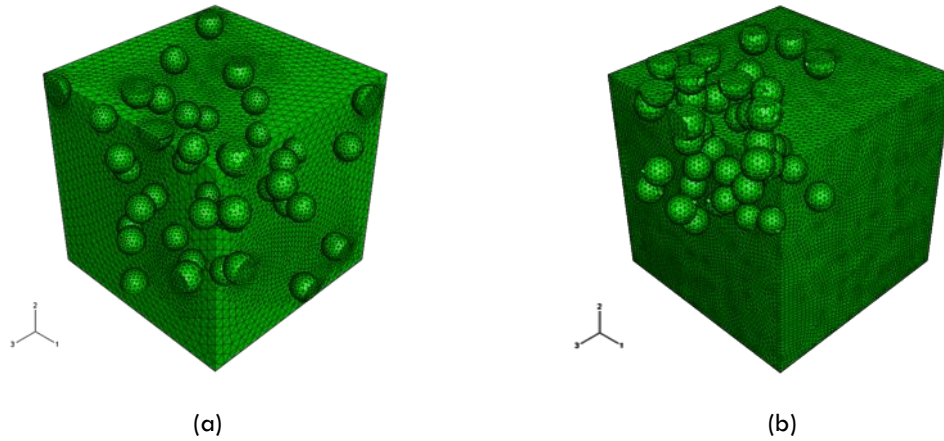
(a)



(b)

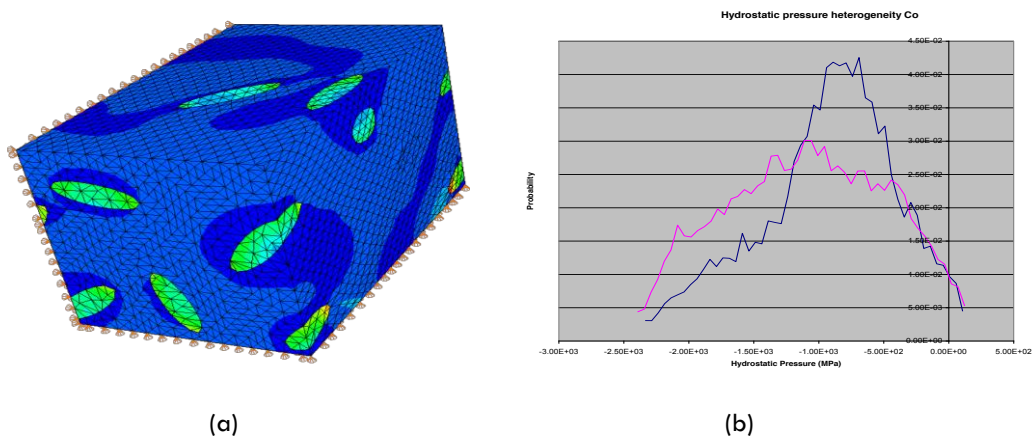
Figures 6: (a) RVE geometry of a glass fiber reinforced polyamide. (b) RVE geometry of a nanofilled polycarbonate.

Digmat-FE is interfaced with Abaqus/CAE for the semi-automatic meshing of the RVE microstructure and for the preparation of the Abaqus finite element model to solve.



Figures 7: (a) and (b) Semi-automatic meshing of a polymer matrix reinforced with randomly distributed and clustered nanofillers.

Abaqus/Standard is then used to solve the nonlinear RVE model. The final results can be post-processed as a regular Abaqus FEA solution and within Digimat-FE for the micromechanical related results (e.g. computation of the stress, strain or failure indicator distribution in a given phase of the reinforced polymer).



Figures 8: (a) Regular post-processing of the microstructure FEA. (b) Hydrostatic pressure distribution in the matrix phase. Courtesy of Solvay.

Reverse engineering using Digimat-MX

As DIGIMAT relies on a micromechanical approach to model the macroscopic material response, the material behavior of each constitutive phase must be described using the appropriate material model. Although the mechanical properties of the reinforced plastic are often known, these are the measured ones; the user may lack data about the in-situ behavior of the composite phases. To compensate for this lack of data, reverse engineering can be used. This inverse method consists of determining some of the micromechanical model parameters, typically material parameters of the matrix phase, based on the composite response computed by DIGIMAT and the experimentally measured composite response.

Digmat-MX, with its built-in optimization engine, automates the reverse engineering process and facilitates the identification of material parameters from measured composite responses. As it deals with multi-objective optimization problems, calibrating material models based on several microstructures and/or loading rates now becomes much easier and straightforward.

Figure 10 illustrates the results of a multi-curve reverse engineering, based on composite experimental tensile responses obtained with test specimens parallel and perpendicular to the injection flow of a material sample plate. The elasto-plastic parameters of the matrix phase constitutive material model have been identified from the composite responses at 0° and 90° degrees with respect to the injection direction. The automated reverse engineering procedure carried out by Digimat-MX took less than three minutes for this specific case and lead to an accurate identification of the material parameters.

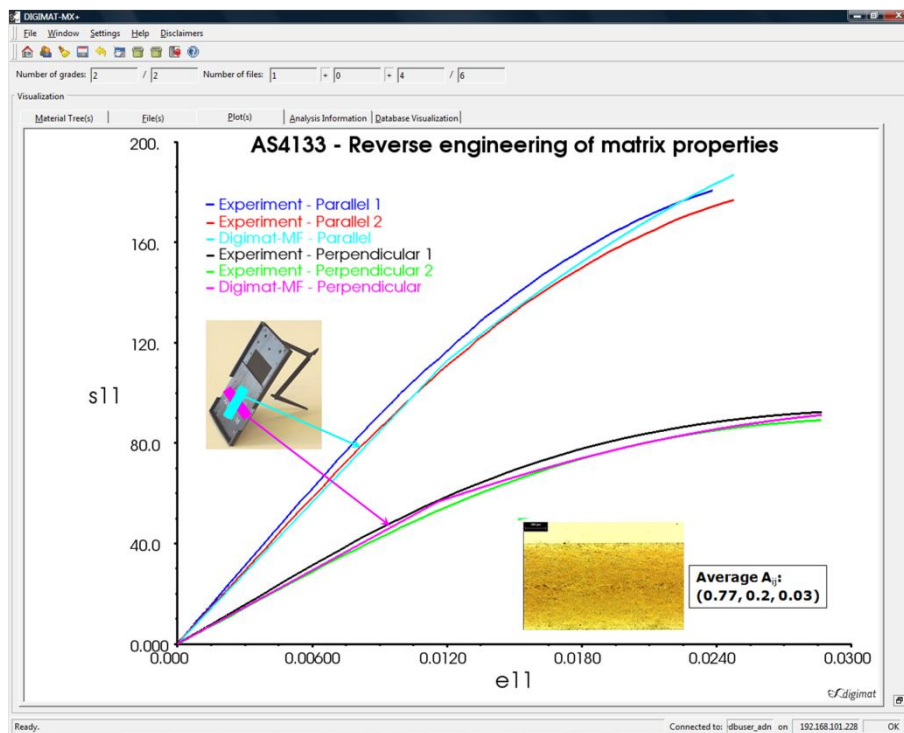


Figure 10: Reverse engineering of Solvay's Amodel AS-41 33 glass reinforced polyphthalamide (PPA) using Digimat-MX.

DIGIMAT Interfaces to CAE Software

DIGIMAT is seamlessly and strongly interfaced upstream and downstream to the major injection molding and structural CAE software used in the engineering plastics industry. The accurate and efficient nonlinear multi-scale modeling process based on DIGIMAT is illustrated below.

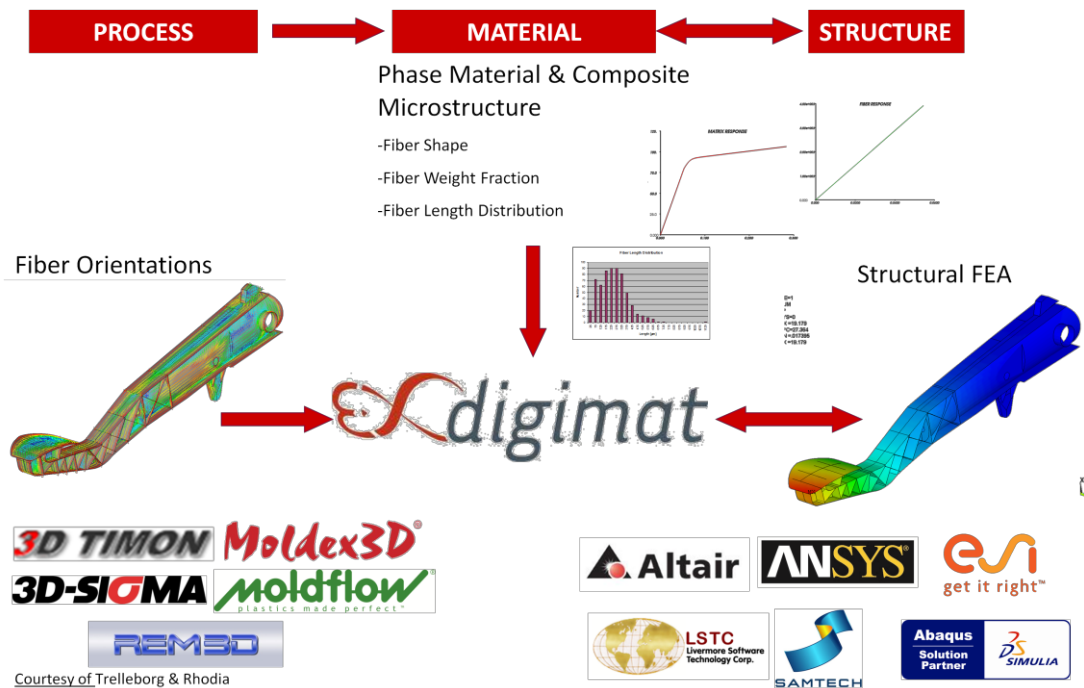


Figure 11: Illustration of the multi-scale modeling process using Digimat to CAE interfaces for the reinforced plastics industry.

The process flow can be described as follows. The structural FEA model is defined as usual (i.e. optimal structural mesh refinement and element type, boundary conditions,...) except for the material definition where DIGIMAT is used. In DIGIMAT, the reinforced material is described by defining the behavior of the constituent phases (i.e. the polymer matrix phase and the reinforcing phase(s)) and the microstructure morphology. The latter is notably characterized by local fiber orientations as predicted by the injection molding software using the injection molding mesh. The mapping of fiber orientations and other relevant properties such as temperatures and initial stresses is carried out from the injection molding mesh onto the structural analysis mesh using Map.

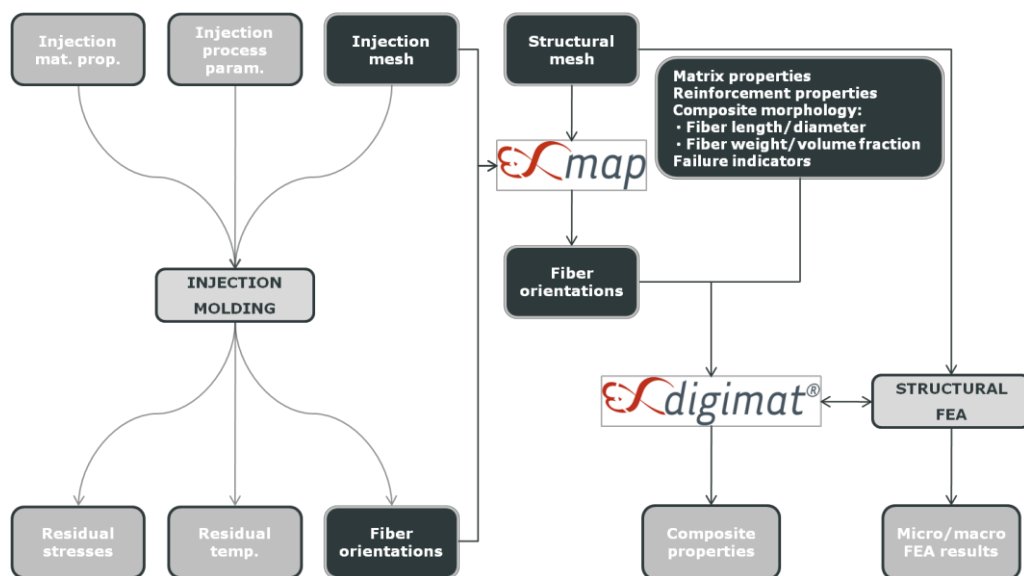


Figure 12: Flow chart of the nonlinear multi-scale modeling process based on DIGIMAT software.

DIGIMAT Interfaces to Injection Molding Software

DIGIMAT is interfaced to the major injection molding software (i.e. Moldflow (Midplane and 3D), Moldex3D, 3D-Sigma, 3D Timon and Rem3D). These interfaces enable DIGIMAT users to take into account the effect of local fiber orientations, residual stresses and temperatures that are induced by the injection molding process on the local material behavior in the final product.



Figure 12: Illustration of the interface between Moldflow Midplane, DIGIMAT and ANSYS Mechanical. The material is a glass fiber reinforced polyamide where the matrix is modeled as a nonlinear elastoplastic material reinforced with elastic fibers. The effect of the local fiber orientations predicted by Moldflow is taken into account by DIGIMAT at each integration point of the ANSYS model. Courtesy of Trellborg & Rhodia.



Figure 13: Illustration of the interface between Moldex3D, DIGIMAT and Abaqus/Standard. The material is a nonlinear polyamide reinforced with elastic fibers. Fiber orientations predicted by Moldex3D are used by DIGIMAT to compute the composite mechanical behavior.

DIGIMAT Interfaces to Structural Finite Element Analyses (FEA)

DIGIMAT is strongly coupled to linear and nonlinear structural FEA software through the Material User Subroutines(s) of the correspondent FEA software. Digimat-MF to structural FEA interfaces are provided as pre-compiled libraries to enable accurate and efficient nonlinear multi-scale structural modeling where Digimat-MF acts as the micromechanical material model that takes into account the behavior of the material constituents and the morphology of the underlying microstructure at each element/integration point.

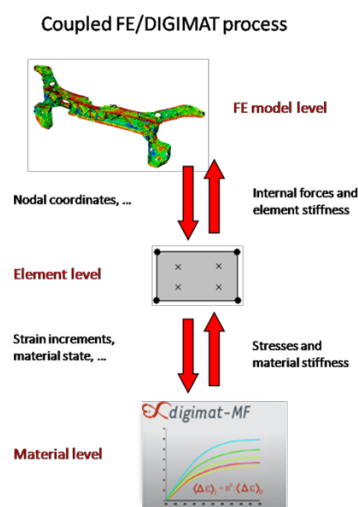
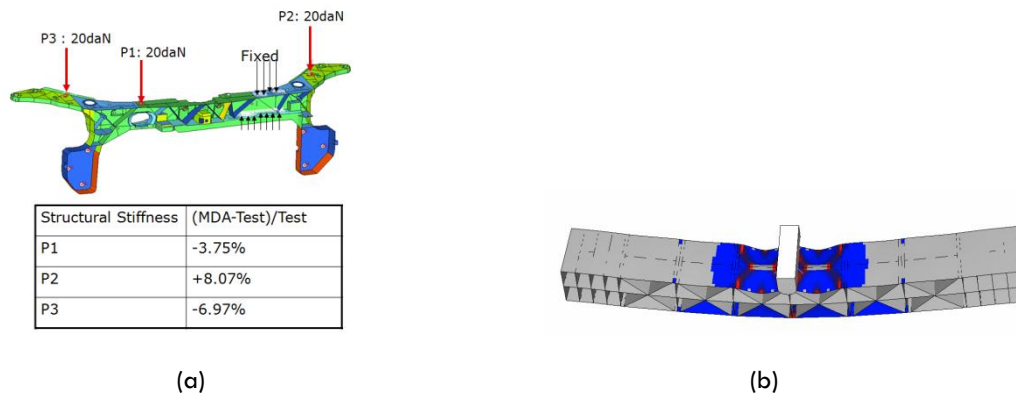


Figure 14: Coupled FE / DIGIMAT Process.

The following interfaces are currently available:

- ✓ Digimat-MF to Abaqus
 - Digimat to Abaqus/CAE
 - Digimat to Abaqus/Standard
 - Digimat to Abaqus/Explicit
- ✓ Digimat-MF to ANSYS
 - Digimat to ANSYS Mechanical
- ✓ Digimat to LS-DYNA
- ✓ Digimat to PAM-CRASH
- ✓ Digimat to SAMCEF
- ✓ Digimat to RADIOSS

DIGIMAT interfaces to nonlinear implicit FEA software like Abaqus/Standard and ANSYS Mechanical are used to predict thermo-mechanical quasi-static load cases such as plastic part cool down and warpage, stiffness, modal response, creep and relaxation.



Figures 15: (a) Quasi-static stiffness prediction of a PPGF automotive technical front end carrier using Digimat to Abaqus/Standard Interface. Courtesy of Renault. (b) 3-point bending of a structured beam made of glass fiber reinforced polyamide. Courtesy of DSM.

Impact and failure can be modeled using DIGIMAT to explicit FEA solvers like Abaqus/Explicit or LS-DYNA as illustrated below. For such analyses, failure criteria can be specified at both the composite and/or the constituent phase levels.



Figure 16: Drop test of a mobile phone cover using Digimat to Abaqus/Explicit with a strain rate dependent model for the polymer matrix. Courtesy of Nokia.

In addition to that, coupled analyses (Injection molding software/DIGIMAT/FEA code) also enable the user to identify the influence of the processing parameters on the structural response of reinforced plastics. These parameters strongly affect the local microstructure of the part, and, as a consequence of this, impact on its structural response to mechanical loading. Figures 16 and 17 illustrate the power of DIGIMAT multi-scale modeling approach to capture such influence. The first example illustrates how the location of the injection points of the molding process influences the structural response (internal energy) of the crashbox, while the second one shows the capability of DIGIMAT multi-scale approach to capture microstructure changes without redefining material properties, see gray and red response curves.

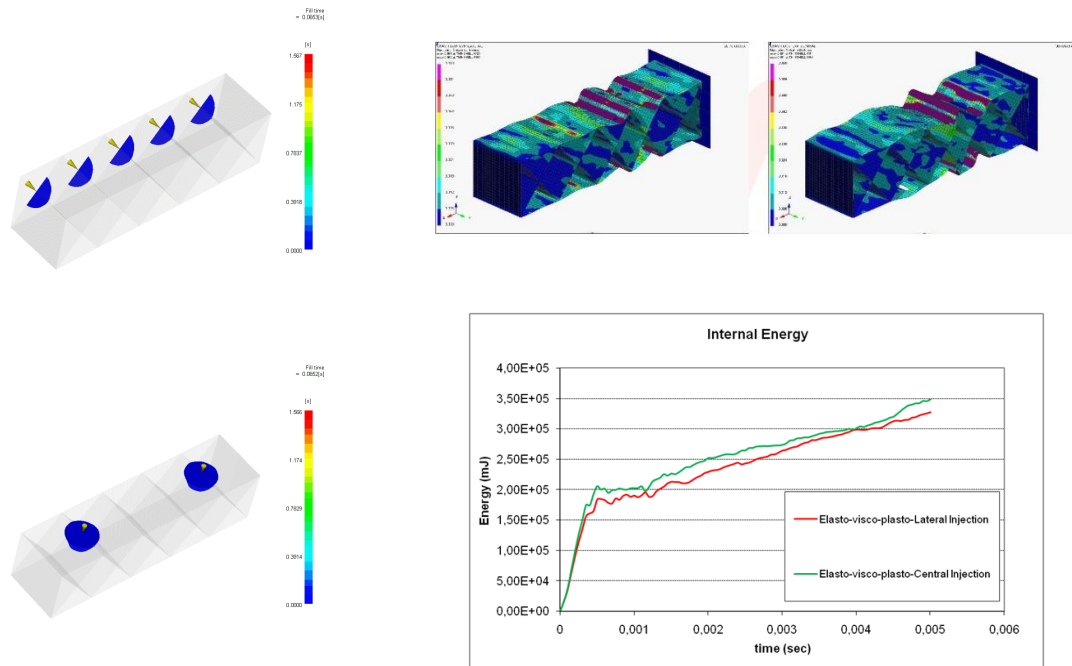


Figure 17: Influence of the injection point location on the internal energy stored up by a crashbox during a crash simulation. Results were obtained by performing a coupled analysis Moldflow/DIGIMAT/PAM-CRASH.

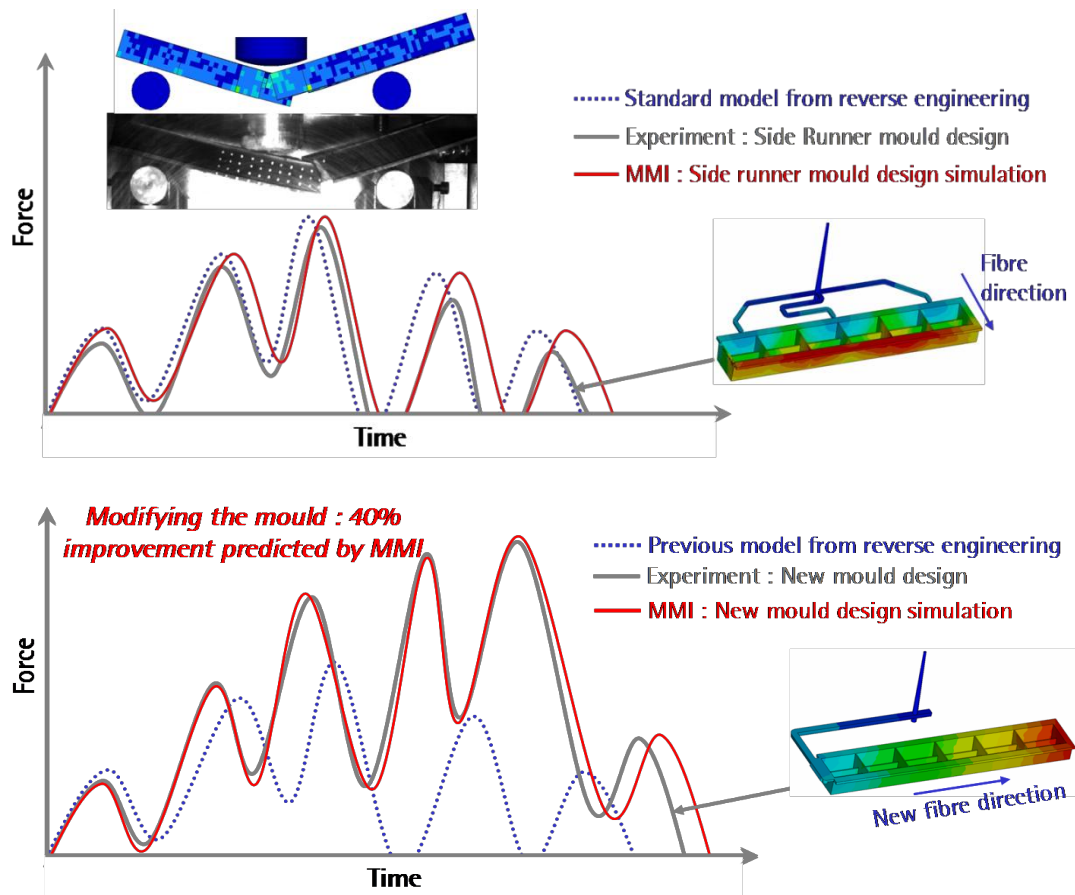


Figure 18: Illustration of the macroscopic response dependency on the process parameters using Digimat to LS-DYNA. MMI, denotes the Digimat to Moldflow and LS-DYNA solution process. Courtesy of Rhodia.

Map

Map offers the capability to transfer fiber orientations, residual stresses and temperatures from the injection molding mesh onto the optimal structural analysis mesh, where they can be used by Digimat-MF to FEA interfaces to perform state-of-the-art nonlinear multi-scale analysis.



Figure 19: (a) Mapping of fiber orientations from triangular mid-plane mesh to quad shell mesh. (b) Mapping of fiber orientations from a 3D injection molding tet mesh to a hybrid hex/tet structural mesh.

Map also features an error computing functionality that allows the user to observe global and local error distributions after mapping. This way, the user can assess the mapping quality.

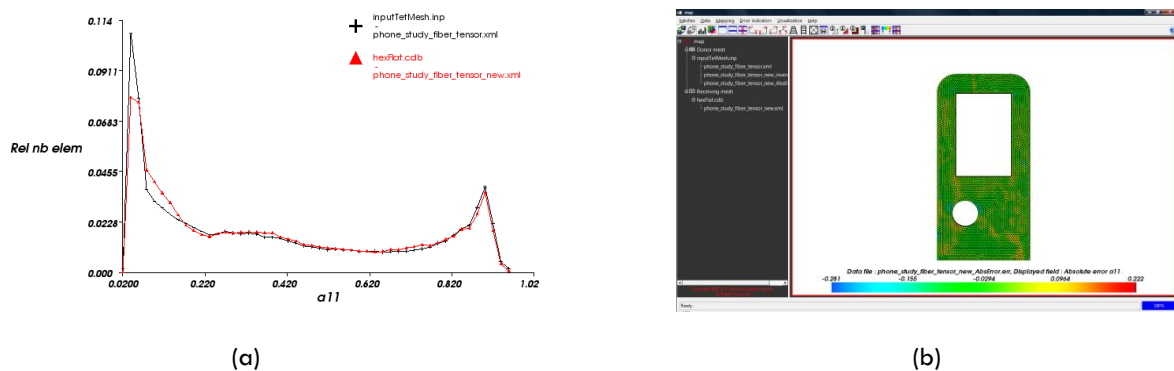


Figure 20: (a) Global error indicator, comparison of the orientation distributions prior and post mapping. (b) Local error indicator, representation of the absolute and relative errors on the mapped geometry.