

DATC: a multiscale design framework for advanced tailorable composites and hybrid material systems



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There is an urgent need for innovative material concepts for exploration vehicles, space habitats, and other space hardware. Advanced tailorable composites and hybrid material systems (TCHM) are good candidates. To exploit their full potential, suitable theories and design methodologies need to be developed and fully integrated into commercially-available design tools.

TCHM such as laminates with steered tows and variable thickness, and metamaterials, can leverage a broad variety of materials, including metallic alloys, short and/or continuous fibre reinforcements and a variety of matrices. However, the capabilities of existing design tools are greatly lagging behind evolving manufacturing techniques, such as automated fibre placement (AFP) and 3D printing.

The theories underpinning most existing design tools are the classical lamination theory (CLT) for structural analysis and the rule of mixture (ROM) for micromechanical analysis, both of which work for laminates made of unidirectional fibre-reinforced composites (UDFRCs). A design process is usually guided by semi-empirical rules applicable to UDFRCs, e.g. consecutive plies with the same fibre angle should not exceed a certain number, and the fibre angle

difference between two adjacent plies should not exceed a certain value. Some tools idealise composite structures as black aluminium and are only applicable to quasi-isotropic stacking sequences.

The development of the Design Tool for Advanced Tailorable Composites and Hybrid Material Systems (DATC) framework is an effort by AnalySwift, LLC, Purdue University, and the University of Texas at Arlington with funding from NASA. At its core, AnalySwift's SwiftComp software provides constitutive modelling capabilities for these advanced materials. This work was also supported by Elevate Ventures, Inc. and Indiana Economic Development Corporation (IEDC).

Framework overview

This framework is devised to empower engineers in parametrising complex structures, allocating hybrid materials, linking structural analysis to external FEA tools, and systematically seeking out optimal designs. The main capabilities are grouped in four aspects (Figure 1):

- handling spatially-varying microstructural design and different structural models, including solid, plate/shell, and beam;
- using either physical or surrogate models such as neural networks for analysis;
- considering various physical behaviours such as mechanical, thermal, and electrical;
- carrying out a single point design analysis or iterative design evaluations for parametric study or optimisation.

This design tool can be used at three levels, based on the user's need (Figure 2). At the core level, one can use the basic functionality (constitutive modelling) and integrate it into the user's own FEA code and design tool. At the intermediate level, users can form the complete workflow of a point design analysis and make it callable in the user's own optimisation iteration. At the outmost level, everything is done in the present framework by integrating all the necessary ingredients, such as global structural analysis and custom scripts for data processing, for various design studies.

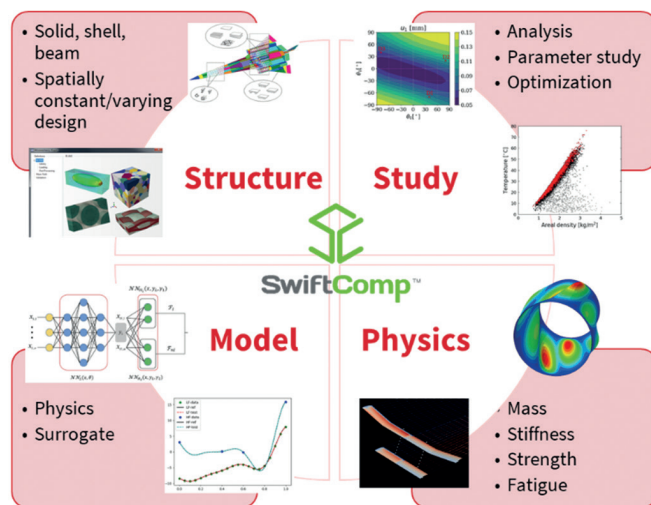


Fig. 1: Main capabilities grouped in four aspects

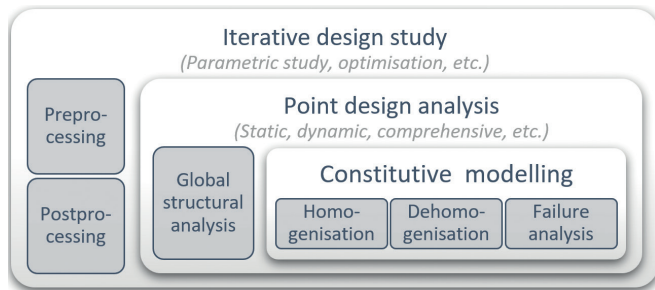


Fig. 2: Three levels of using the tool

The framework comprises the following components:

- a core module for constitutive modelling comprising SwiftComp and a builder for microstructures;
- an assemblage of base microstructure designs stored within a library;
- a parameterisation model, accompanied by a user input syntax organising the overarching structural design and optimisation configuration;
- The Dakota toolkit, providing iterative methods for parametric study and optimisation;
- lastly, Python modules interlinking the aforementioned components and providing interfaces for external codes.

Multiscale microstructural modelling, design and analysis

Mechanics of structure genome (MSG)

MSG is a unified approach to the efficient high-fidelity constitutive modelling of general composite structures and materials. It is based on the concept of structure gene (SG) defined as the smallest mathematical building block of a structure for describing the microstructure. An SG contains both geometry and material information, and acts as the analysis domain of constitutive modelling. Starting from a 3D anisotropic heterogeneous continuum, MSG first identifies the SG and then decomposes the original problem into the constitutive modelling of SG and the global structural analysis, using the principle of minimum information loss (PMIL) (Figure 3). The constitutive modelling is implemented in SwiftComp to compute the effective

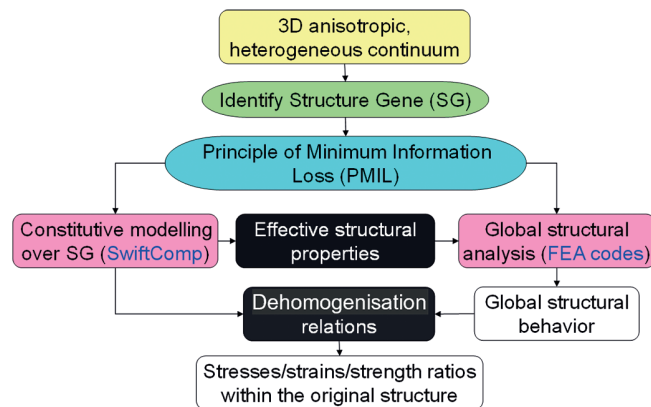


Fig. 3: MSG-based constitutive modelling

structural properties needed by the global structural analysis, and the local stress/strain/strength ratios within the original structure. Global structural analysis, linear or nonlinear, can be easily handled by commercially available FEA packages. All the difficulties associated with composites and modelling approximations are therefore confined in constitutive modelling, whose accuracy is ensured to be the best by PMIL.

Since the effective structural properties are computed in terms of the SG, one set of effective structural properties corresponds to one SG. If the entire structure is composed of multiple different SGs, multiple sets of effective structural properties will be computed. On the other hand, the local stress/strain/strength ratios not only depend on the SG, but also on the global structural behaviour (e.g. structural loads). Since the global behaviour often varies over the entire structure, the local stress/strain/strength ratios will also vary over the entire structure. However, this does not mean that they need to be computed at every point. Such information only needs to be computed at a few critical spots. Furthermore, the stress/strain/strength ratios are computed using simple matrix multiplications. Their calculations only take a few seconds for each SG, even for 3D SGs.

Hierarchical description of microstructural designs

MSG/SwiftComp is an FE-based code, making design parameterisation of structures a challenge. Given the complexity and extensive array of possibilities inherent to microstructural design and the corresponding building tools, this framework uses a combination of base design with specific parameters to precisely define an SG. A base design describes a family of analogous structures, effectively serving as a prescriptive template for a dedicated builder, while the parameters actuate variations within the design family. This approach effectively provides a balance between design adaptability and the dimensionality of parameters. To allow general multiscale modelling and parameterisation, a hierarchical and nested arrangement of SGs is implemented. In addition to raw materials with basic properties, the framework permits the allocation of an SG to a designated region of the global structure, or another SG, accompanied by explicit parameter specifications. In other words, SGs can be stacked or nested to form a complex microstructural design.

Figure 4 (next page) is an illustrative example portraying the two-level SG modelling of a composite laminate. In Level 1, a 1D SG depicts a bi-layer structure made of homogeneous laminae, while in Level 2, SGs characterised by a square packing represent the fibre-matrix system of UDFRC, providing homogenised lamina constants needed by the Level 1 SG. This modelling strategy also breaks down the design parameters into each of the two levels. Material choices for fibre and matrix and fibre volumes go to Level 2 while fibre angles and layer thicknesses go to Level 1.

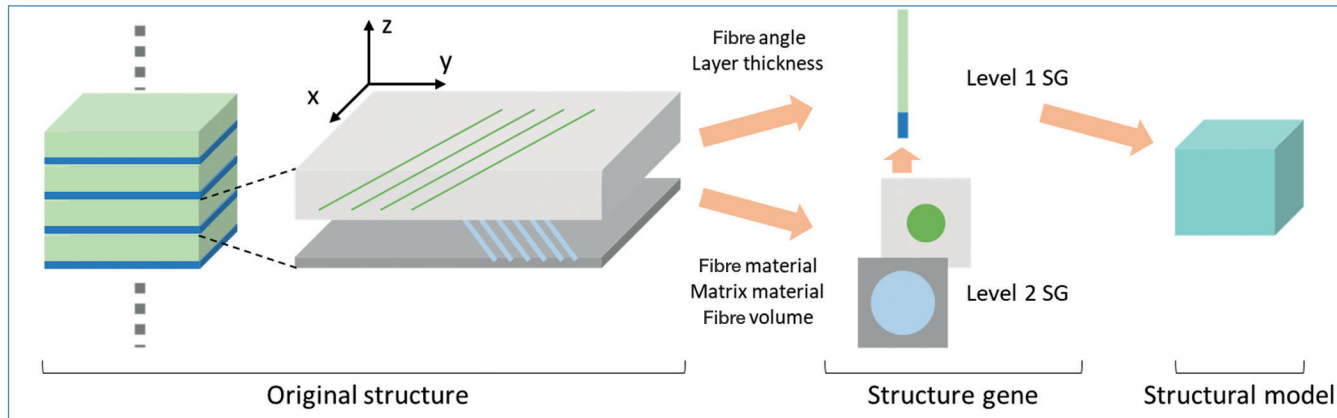


Fig. 4: Example of a two-level SG decomposition of a composite laminate

Automated analyses of SGs

Accompanying the multi-level modelling is a recursive function traversing through the hierarchical structure of SGs. Once the multi-level SG structure is well defined, this function will automate the execution of SG building and analyses, including homogenisation, dehomogenisation and failure analysis. Specifically, an SG database will be checked for the desired structure-property relationship. If such relationship is absent, indicating that certain regions are assigned to an SG but remain unanalysed, the function initiates a descent to the lower-level SG analysis stage. This involves the propagation of design parameters to the subordinate level, subsequently returning outcomes for effective property calculations before ascending to the higher-level SG.

Spatially-varying microstructural design

In pursuit of achieving a high degree of design customisation, alongside diverse microstructures and multi-level modelling, the present framework employs an additional approach: the definition of spatially-varying parameters. Instead of assigning constant values to SG design parameters, this functionality allows defining distribution functions of parameters that will vary with respect to spatial coordinates. These

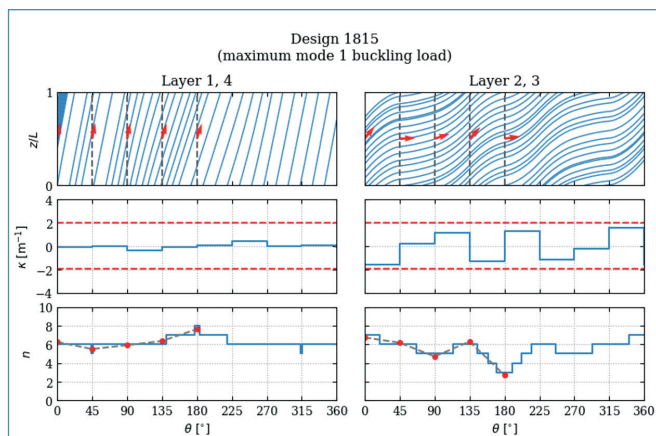


Fig. 5: Example of a spatially-varying laminate design with steered fibre tows and non-uniform layer thicknesses

distribution functions are defined at the global structural level. Consequently, during homogenisation, they will be assessed at designated positions, leading to the construction of specific SGs. Four types of functions have been established within the framework: built-in functions, one-line expressions, linear interpolation, and Python scripts. Notably, users retain the freedom to employ continuous and smooth functions to define distributions of discrete-type parameters, with the tool automatically converting calculated values into integers. Figure 5 shows an example of a four-layer laminate with curved fibre tows and spatially-varying layer thicknesses (number of plies).

Multi-physical analysis

Thermomechanical analysis

In addition to mechanical properties, MSG can also handle multi-physical analysis. A typical application is using thermo-mechanical analysis to identify materials with near-zero thermal sensitivity for use in structures deployed in space.

In the Figure 6 example, two types of hybrid material systems are considered: a layered binary structure and a UDFRC. Comparisons are also made among different types of constituting materials, including metallic alloys, ceramics and polymers. This tool is used to homogenise these material systems and output effective material properties. The UDFRC is modelled using a 2D square-packed SG representing the long fibre-matrix system (lamina). This microstructure has three design variables: matrix material choice, fibre material choice and fibre volume fraction. The latter is measured using the radius of the ideal circular fibre cross-section. The layered binary structure contains two types of laminae stacking in the thickness direction alternatively. This system has not only the variables mentioned in the UDFRC but also three new ones including fibre angles and the layer thickness ratio of the two laminae. This microstructure utilises a two-level modelling strategy as mentioned previously, where random samples are drawn from the design space and effective properties (CTE vs specific modulus) are compared. This study can help engineers quickly identify the specific properties of different types of composites in an early design stage.

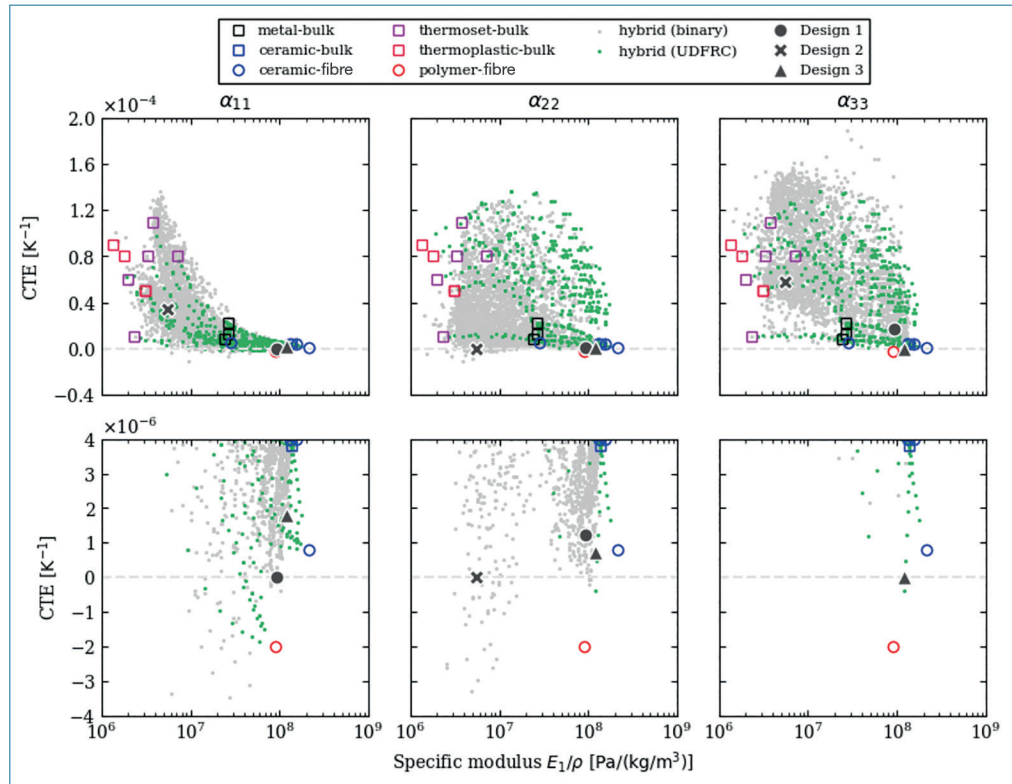


Fig. 6: Comparison of the effective thermomechanical properties of two microstructural designs with different constituent materials (top row); zoom-in view of the top row near the zero CTE (bottom row)

Open architecture

This framework is developed as an open architecture. Users can link this program with custom tools to achieve more complex and advanced design studies that cannot be done using DATC only. Currently, this includes four interfaces: global structural analysis, custom analysis using Python script, a custom builder for microstructure, and GUI plug-ins.

Global structural analysis

This framework supports the connection to Abaqus or Nastran third-party software tools for structural FEA. The structural model created in these commercial tools can be used by DATC for defining a microstructural design. It could be spatially varying, evaluating specific SG designs, and exporting effective structural properties and merging the data with the main global structural model.

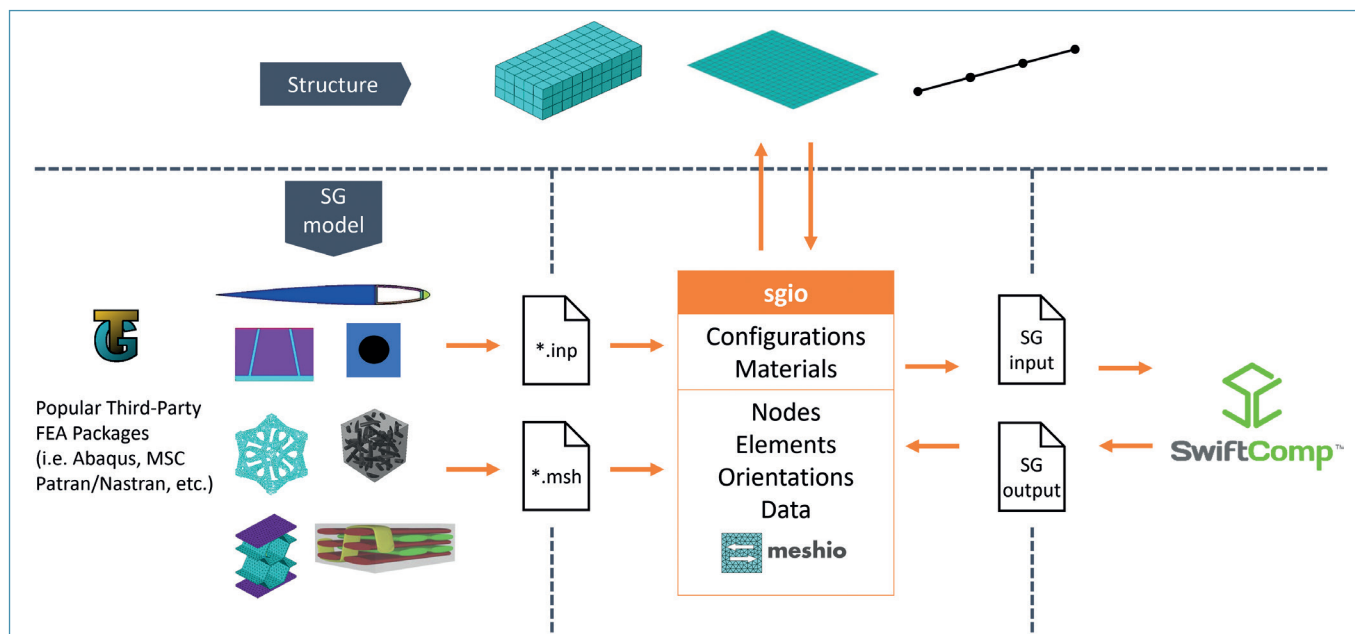


Fig. 7: Interface for creating custom microstructures

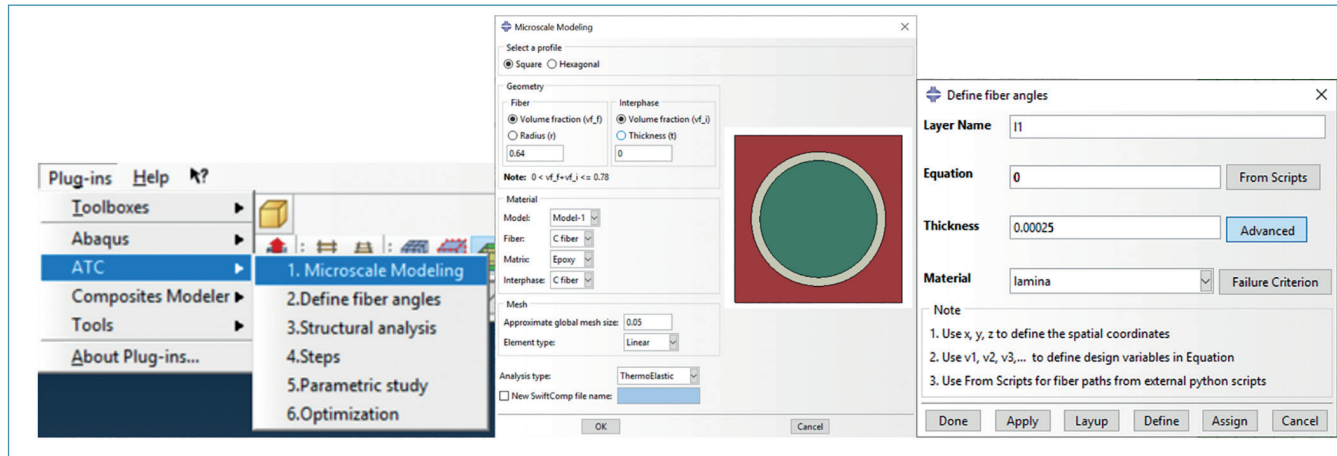


Fig. 8: Abaqus/CAE plug-in: main menu, "Microscale modelling" window, and "Define fibre angles" window

Custom analysis using Python script

In addition to the built-in analysis steps including SG analysis and global structural analysis (Abaqus and Nastran), users can do all kinds of other things using Python scripts. The framework provides instructions on how to access data from DATC as inputs and send returned values to DATC. This custom step can be used for data processing of design inputs and analysis outputs, executing other analyses not supported by Abaqus and Nastran, etc.

Custom builder for microstructure

To expand the design space of microstructures, it may not be enough to use the built-in SG builder, which supports 1D and some 2D SGs only. An interface is provided for users to import custom microstructures with arbitrary complexity. This interface is mainly achieved by a "sgio" independent Python module, developed based on a "meshio" third-party module, which supports and converts many meshing data formats. Figure 7 gives an overview of the "sgio" interface. Essentially, it acts as a central data structure for meshing data in different formats, SwiftComp input/output, and effective properties used by the global structural model.

GUI plug-in

A GUI plug-in is developed for Abaqus and MSC Patran/Nastran to perform design optimisation of advanced tailorable composites using the API languages (i.e. Python in Abaqus and Patran Command Language (PCL) in MSC Patran/Nastran). Abaqus and MSC Patran/Nastran are third-party software and not involved in the development of DATC. Users can define all the design setups

and carry out constitutive modelling, structural analysis, and optimisation in an integrated environment within a commercial FEA package. The GUI plug-in generates the main design file and calls external Python scripts to execute the design framework. The main modules in the developed GUI plug-in are shown in Figure 8 (Abaqus version), where ATC stands for Advanced Tailorable Composites. Each item in the menu ("Microscale modelling", "Define fibre angles", "Structural analysis", "Steps", "Parametric study" and "Optimisation") opens a window for users to provide all the inputs needed for a design study.

Conclusion

DATC, a framework developed for the multiscale modelling, analysis, and design of advanced tailorable composites, is a tool based on MSG, an efficient high-fidelity constitutive modelling method for structural models including solids, plates/shells and beams. Functionalities were developed on top of MSG to achieve multiscale parameterisation, spatially-varying design, and automated hierarchical (de)homogenisation of microstructures. In addition to mechanical performance, coupled multi-physical analyses are also available. The open architecture of this framework allows the integration of custom tools and hence even broader design requirements, including global structural analysis by commercial tools, complex microstructural designs, custom analysis and data processing steps, and user-friendly GUI plug-ins in Abaqus and Nastran. □

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