



Dr. Georg J. Schmitz
+49 241 80-98014
G.J.Schmitz@micress.de

Aachen, 20. August 2020



TO OUR CUSTOMERS

Dear HOMAT user,

compared to the previous version 5.3, the new HOMAT version 6.0 constitutes a major revision of the program suite HOMAT. It contains several improvements and novel features, which are briefly presented below.

1. The major difference between version 6.0 and the previous versions 5.x is the new treatment of the periodic boundary conditions (B.C.) via a master-slave projection algorithm, which does not need any penalty factor. No additional stiffness at periodic surface nodes are thus introduced, leading to larger fluctuation displacements or velocities and to larger corrections of the volume averaging material property. Therefore, the effective material properties predicted by version 6.0 are more accurate as former predictions, because pure numerical penalty terms for periodicity are avoided.
2. All documentation of the HOMAT suite is now available online under <https://docs.micress.rwth-aachen.de/homat/>
3. New capabilities:
 - Stokes flow homogenization is implemented in HOMAT v6.0 allowing to predict the Darcy permeability tensor, its principal directions and values and an anisotropy factor. The new Stokes flow homogenization option, however, cannot be combined with the two other types of homogenization (thermal, mechanical).
 - In order to model accurately the quasi-incompressibility of phases like the melt or the amorphous phase of a semi-crystalline polymer, several mixed element types have been newly implemented:
 - equal order linear displacement and pressure elements, stabilized or not by a double Gauss point integration of the pressure term,
 - mini elements, where the linear displacement field is enriched by a volume bubble term and eventually
 - “bubLi” elements, with the same enriched displacement field as the mini element variant, but additionally stabilized by the double Gauss point integration of the pressure term.

All these mixed elements can be used in thermo-elastic homogenization or localization analyses and are mandatory in Stokes flow homogenization problems to model fluid domains.

- Curved geometries inside the RVE can now be better approximated using quadratic volume elements having either 10, 15 or 20 nodes.
 - Effective material properties can now be printed not only in the RVE coordinate system but also in a user-specified local coordinate system.
 - In thermos-elastic homogenization runs, HOMAT v6.0 can now calculate and store the microscopic strains induced by the microscopic displacements on the RVE. In the presence of mixed elements, the pressure field is recorded and can be visualized.
 - If cubic effective behavior is detected, the elastic constants, the Zener anisotropy factor are stored in the *.hres file in addition to the anisotropic Hooke matrix.
4. New numerical features in HOMAT v6.0:
- At the interface between two material domains, a tied contact is now realized. The slave nodes are condensed and only the master nodes are retained in the linear system. This reduces the system to be solved and saves computational time. After solving the system, the master results are duplicated on the slave nodes.
 - The number of degree of freedoms (“DOF”) per node can now be varied in the RVE model. In presence of a mixture of incompressible and compressible phases, a 3D model will have some nodes with 4 DOFs as well as other nodes retaining classic 3 DOFs.
 - The sparse matrix format is used in HOMAT 6.0 to store the global system matrix. In this format, a flexible number of DOFs per node can be treated more easily..
 - A new symmetric preconditioning, based on the square root of the diagonal terms, is applied on the system matrix. The linear system of equations for the thermal, mechanical or flow problem is solved by an enhanced iterative BiCGstab solver.
5. Mesh2HOMAT in HOMAT version 6.0 generates a new XTUPLE list in the *.hgeo file.in case of presence of n-tuple nodes, i.e. at nodes where more than 2 materials are present at the same geometric location, Old hgeo files (without XTUPLE list) being generated with earlier HOMAT versions will not work with HOMAT v6.0. It is recommended to re-perform meshing of your original mesh using the Mesh2HOMAT being implemented in HOMAT 6.0
6. In Mesh2XXX several new features have been introduced:
- The new parameter *neper-gmsh* is added to the keyword *input_format*. In this way, Mesh2XXX can now also handle .inp files being generated either by the polycrystal generator **Neper** or by the FE mesh generator **Gmsh** (<https://gmsh.info>).
 - *-output*: this new parameter allows the user to specify *the base name*, common to the command and geometry output files, written by Mesh2XXX.
 - Mesh2XXX version 6.0 introduces *named placeholders* instead ‘...’ for the name of an unknown material: NAME=material_<no.> on the keyword /MATERIAL of HOMAT or *MATERIAL of ABAQUS.
7. Specific features have been added to Mesh2HOMAT V 6.0:
- The new option *-all_free_surfaces* permits to write not only the periodic surfaces but also all other outer surfaces in the *.hgeo file.
 - An additional parameter *no_clones* can be specified by the user in combination with the keyword *-write_vtk*. In this case, an unstructured mesh is written in VTK format without storing the newly generated nodes and elements at the material interfaces. In this way, a simple Abaqus2Vtk mesh converter has been obtained and now is available as part of HOMAT 6.0.
 - The new option *-discre* permits the user to specify the desired mixed element formulation per material. Please refer to the online manual for a detailed description of this new option.

- The new optional parameter *-problem* permits the user to specify the desired homogenization or localization analysis already during pre-processing with Mesh2HOMAT. This way, not only the parameter TYPE of keyword /PROBLEM is specified but also the type of analysis per solid section and the output files are preselected.
8. In Mesh2ABAQUS, the new parameter *-maxincsize* allows the user to adapt the maximal allowed increment size per step to the nonlinearity of the virtual test.
 9. The python script ***aba2hom.py*** has been significantly reworked. As outlined in its documentation, the effective equivalent plastic strain and effective von Mises stress are computed, per default using the corresponding volume averaged stress or strain tensors. This evaluation differs from the fast calculation in earlier versions of the script, where the equivalent strain or stress are averaged over the RVE as done in version 5.3. The new option *-f* or *-FastCalculation* permits to retain these - less accurate - equivalent stress-strain curves.

Further, the user can now specify the base name for the output files via the option *-o*. Specifying new option *-MatrixOnly* the user omits the elastic inclusion regions in the volume averaging evaluation process. It is strongly recommended to use this option very carefully.

The specific command /FREQUENCY has received two new options: DROP and TABLEX. DROP is similar to the ALLFRAMES option except it drops only a specified number of frames following one being read. However, the last frame of every step is always stored. Similarly, TABLEX corresponds to the option TABLE except here also the last frame is always written.

10. The post-processing Python script ***Prop2Plot.py*** has been entirely rewritten. This script allows the post-treatment of several homogenization result files of hres type. The scope of this script is to extract all or a selection of effective properties from all the available homogenization result files in the working directory and to write , per property, the extracted effective values as function of the simulation time or of the set temperatures. The respective file format is either a single or several ASCII files suitable for plotting purposes. Please refer to the online manual where the different new optional arguments are further detailed. In addition to classical materials properties, the user can now generate quantities in the local coordinate system, components of the full tensors or the principal values and directions of 2nd order tensors - Individual base names for the different output files can be specified in HOMAT 6.0
11. A new python script named ***makeTabO*** has been integrated to the HOMAT v6.0 release. HOMAT or ABAQUS analysis of a polycrystal microstructure needs phase (material) and orientation data of the individual grains. This new python script covers following cases and generates a TabO file:
 - For MICRESS simulations without orientation output (no_TabO) but available grain data output (TabGD), the makeTabO script enriches the grain data by random orientations according to the Halton sequence.
 - For a synthetic polycrystal microstructure, generated by ***Neper***, the makeTabO script will convert the data given in the *.stcell file of Neper to the TabO format of MICRESS®. Phases can be assigned to groups of grains by various algorithms. Please refer to the online manual for details. Grain orientations are either taken from a given Neper file (*.ori), randomly generated using a Halton sequence or provided as user specified orientation classes.
<https://sourceforge.net/projects/neper/>
12. Several examples have been added to HOMAT 6.0 illustrating the new possibilities and options. Each example is dotted with its own ***Def_example.txt*** file, where the different simulations are outlined and some homogenization or localization results are commented. All examples cover different categories, going from basic benchmark tests to more complex and advanced applications. To get a quick overview of the categories and the corresponding examples, please refer to the README file in the 'Examples' directory. New users are recommended to start from the basic benchmark tests in the recommended order. The new capabilities in HOMAT 6.0 (Stokes flow homogenization, modeling quasi-incompressible material behavior via mixed finite element formulations) are accompanied by several new examples like *cylBL_r2*, *crossWires* as simple Stokes flow homogenization examples. Existing examples for porous structures (*hollow_grid*, *S30-F*) and the solidification example *solidif_A356* have been extended to also predict the effective Darcy permeability tensor. Eventually, the example *SphIncom* of a silica sphere in a quasi-incompressible rubber matrix has been added to demonstrate the procedures, the quality of the implemented mixed element variants and the impact of the sphere geometry on the thermo-elastic homogenization and localization results.

We do hope that these improvements will assist you in solving your problems and will continue to make HOMAT a valuable tool for your research. For more details, please don't hesitate to ask us, preferentially via the MICRESS®-Forum (www.micress.de/forum).

Yours sincerely
ACCESS e.V.

A handwritten signature in blue ink, consisting of a long horizontal stroke followed by a series of loops and a final flourish.

Dr. Georg J. Schmitz
Global Marketing, Sales & Support MICRESS®

A handwritten signature in blue ink, featuring a prominent 'G' followed by a series of loops and a horizontal line at the end.

Dr. Gottfried Laschet
HOMAT developer

