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TO OUR CUSTOMERS

New release of your MICRESS® software package.

Dear MICRESS® user,

enclosed please find the most recent release of your MICRESS® software package. The present release 6.4 of MICRESS® comprises a number of improvements and new functionalities. Of course, we also attempted to fix all bugs being reported by our user community.

Different variants are provided:

- MICRESS® 6.4 is available with or without TQ coupling. The coupled version uses the TQ library corresponding to Thermo-Calc release TC 2017a. GES5 files created with Thermo-Calc version TC 2015b and above are compatible. A new MICRESS®-TQ license file for TQ 2017a is provided along with the current release mail for all users of MICRESS®-TQ with valid maintenance.

- MICRESS® 6.4 is supplied as serial or as partly parallelized version. The solvers for diffusion, stress, flow, temperature and the newly introduced solver for volume change can be executed multi-threaded based on OpenMP (www.openmp.org).

- MICRESS® 6.4 is supported for Windows (7 and 10) as well as for Linux (Ubuntu 16.04 LTS Xenial, CentOS 7.0, and OpenSUSE 42.2 Leap). All platforms have to be 64 bit.

Along with MICRESS®, we provide the tools:

- DP_MICRESS 7.117
- MICpad 6.400

DP_MICRESS is also freely available from the MICRESS® website (www.micress.de).

News on MICRESS®:

The release 6.4 of MICRESS® comprises a number of new functionalities and features as shortly described in the following:

- *Reading of molar volumes from database*

  MICRESS® now offers to read phase-specific mean molar volume data from a thermodynamic database. Note that some databases do not yet contain volume information. In this case MICRESS® will stop with an error-message.

- *Consideration of volume change during phase transformation:*

  Concentration coupled simulations can now be run with the new option 'volume_change' in order to consider temperature and growth related shrinkage or expansion. The underlying model is based on the assumptions that matter is conserved and the entire simulation domain expands homogenously while always remaining in a stress-free state. Local volume differences are instantaneously homogenized by internal material fluxes being calculated by a newly implemented expansion-relaxation-solver based on a convergence criterion. Note that the volume-change option can be combined with an option for 'interstitial' diffusion which proved to be especially helpful for simulation of spheroidal graphite growth in ductile cast-iron. Three new output files (.mole .molV and .expa) are provided to monitor the evolution of the local number of moles, the molar volume and the local expansion.

- *Zoom of restart-files in 'structure_only' mode*

  The 'restart structure_only' option allows constructing an initial microstructure from the restart output of earlier simulations. Restarted structures can be shifted and rotated before being composed into a newly defined grain structure. As a new feature, an additional zoom factor can now be specified. This zoom factor is especially helpful to bridge multiple length scales in process chains. Note that zooming requires a correction of the concentration fields when contracting diffuse interfacial regions which may cause or amplify numerical artifacts. The zoom factor thus should not be selected too large. By now, only the values 2 and 3 have successfully been tested.

- *Flow-simulation as post-processing tool*

  The MICRESS® output file .frac0, containing the spatial distribution of the liquid phase, can now be used as input for a MICRESS® fluid dynamics computation. This is especially useful to calculate the permeability of a microstructure at a certain stage of solidification.

- *Merging of grain regions with identical properties during initialization*

  Grains are generally defined as regions being separated by interfaces. To avoid that equal, but initially separated grains form interfaces when getting into contact, MICRESS® can now treat regions with identical properties as a single grain. To activate this feature, the user can assign a group number in addition to the phase number. All initial regions with equal phase and group number will be merged during initialization provided they do not differ in orientation or recrystallization energy. Merging of grain regions is not only helpful to avoid unphysical interfaces, but also to improve numerical performance.

- *Temperature-dependent lamellar radius in 'unresolved' mode*

  The 'unresolved' eutectoid model now can treat a temperature-dependent lamella radius having the function to mimic the impact of curvature undercooling.

- *Adoption of chemical mobility data from another phase*

  When using a chemical mobility database, unknown mobility data of one phase can now be adopted from another phase. This is a helpful pragmatic solution, if some required mobility data is missing. If for example the mobility data of the γ'-phase is not available in the database, the new keyword 'switch_diff_data' now allows taking the mobility of the γ-phase as an estimate instead.

- *Improved automatic update of thermodynamic data*

  The automatic selection of updating intervals for thermodynamic data from database for each phase pair has been improved with respect to practical applicability. Note that automatic updating is now purely based on a local temperature deviation criterion. For isothermal processes, the alternative manual selection of updating intervals is recommended.

- *Constraint for redistribution of phase concentrations*

  The new keyword 'criterion_higher' (or 'criterion_lower') can be used in the phase diagram input section to impose the constraint that the composition of a given element in a specific phase has to be higher (or lower) than the composition in the other phase. This feature helps to prevent switching to the wrong composition set while avoiding the necessity to define a fix concentration limit.

- *Additional composition sets*

  The option 'diff_comp_sets'/vol_comp_sets/enth_comp_sets adds additional composition sets (phases with the same base name, which are already included in the MICRESS® simulation) when calculating single-phase properties like diffusion coefficients, molar volumes or latent heat. An example is: FCC_L12 and FCC_L12#2. This allows equilibration in supersaturated phases. Other phases with different base names can also be added indirectly by renaming them to a "pseudo composition set" (i.e. with the same base name) in the phase diagram input (see: user defined phase names).

- *User defined phase names*

  Phase names from a thermodynamic database can now be user defined. Apart from convenience, it may be important in connection with 'diff_comp_sets' if phases forming a miscibility gap do not have the same base name.

- *New global definitions of the thermodynamic description*

  The new option 'globalG' allows a global definition of the thermodynamic description for each phase interaction. This option typically should be selected in case the system is close to equilibrium and relatively homogeneous (e.g. Ostwald ripening, rafting etc.). Thermodynamic noise is reduced and performance is significantly improved using this option.

  Similarly to 'globalG', the new option 'globalGF' defines a common thermodynamic description for each interaction, but only for interconnected regions.

  The relinearisation options 'global' and 'globalF' have been reformulated for more consistency, while keeping their functionality as before. An additional flag ('database consistency') can further increase consistency of all named relinearisation options by further distinguishing between dual interfaces, triple junctions, quadruple junctions etc.

- *Two-sided 1D-far field extension for composition fields*

  In order to efficiently treat long-range composition far-fields during directional growth, MICRESS® allows the definition of a 1D-far field extension at the top boundary of the simulation domain. Alternatively to this existing one-sided 1D-far-field, the new release now also offers a two-sided 1D-far-field extension for composition fields in East-West direction.

- *Output of maximum grain boundary diffusion coefficients*

  Grain boundary diffusion is defined in MICRESS® by a change in activation energy. For a better control of this feature, the resulting maximum grain boundary diffusion coefficients are now stored in the .diff output file.

- *Improved automatic interfacial mobility for off-diagonal diffusion*

  The simulation of diffusion-controlled growth requires a correction of the interfacial mobility. In contrast to earlier releases, the mobility needs no longer to be calibrated manually, but the option 'redistribution_control' enables an automatic mobility calculation. This feature, being under continuous development during the last years, has now been further improved with respect to off-diagonal diffusion, especially in cases with negative diagonal terms. The use of this option from now is recommended for all well-resolved simulations of diffusion-controlled phase transformations including solid-solid reactions.

- *New options for extrapolation of thermodynamic data*

  'multi_plus': This option adds a default linear extrapolation of non-diagonal terms with respect to the concentration of the flux element. This can be important for cases with strong concentration gradients, possibly leading to unstable diffusion matrices, resulting in chess-patterned concentration fields and/or inf/NAN concentration values. Although "local" extrapolation can sometimes be similar in effect, the new option is much more performant. Note, that off-diagonal diffusion coefficients written to the .diff output are normalized (divided by concentration) when using 'multi_plus'. This option finds applications e.g. for stabilization of diffusion in highly alloyed systems.

- *Definition of extrapolation mode for each element*

  'diagonal' allows switching from multibinary to diagonal extrapolation for individual elements. In earlier MICRESS® releases this was only possible simultaneously for all elements by using "interaction" (without any further parameters).

- *Definition of anisotropy exclusively for special misorientation relationship*

  The new keyword 'special_orientation_anisotropy' allows for the definition of an anisotropy function applying only to interfaces with a special misorientation relationship while all other interfaces of the same kind are treated as isotropic. This option is particularly useful to model e. g. twin boundaries or Widmanstätten growth.

- *New nucleation options:*

  The new nucleation site definition 'front' allows placing nuclei within a defined distance to a phase front. This is not only helpful to simulate nucleation close to a solidification front, but also to model detached melting inside a solid. A typical application is e. g. the formation of liquid phase pockets during soldering. Moreover, the maximum number of nuclei can now easily be set to unrestricted by putting a negative number. A user-defined off-set to the driving force ('dG_offset') is now also considered when calculating the driving force for nucleation.

Improved performance:

A number of measures have been taken to improve performance, resulting in e. g.:

- Strongly reduced memory usage in case of TQ-coupling with many phases and elements
- Improved performance to enable handling of strong anisotropy while using the standard non-faceted anisotropy model.

- Improved consistency of extrapolated diffusion coefficients (using option 'l') leading to less numerical instabilities, especially in case of strong composition gradients.

- Improved performance of the diffusion solver, especially in cases without temperature gradients and without local extrapolation (depending on application).

- New criterion for diffusion solver time stepping of cross-terms often improves speed (depending on application).

- Retrieval of local diffusion coefficients ('l') from database has become much faster.

Examples:

The number of examples included in the MICRESS® distribution has been substantially increased while some old examples have been updated and improved. Furthermore, a classification into "application", "training" and "benchmark" type examples has been made to help users selecting an appropriate entry point for their work.

News on DP_MICRESS:

DP_MICRESS (version 7.117) is included into the present distribution of MICRESS® 6.4. This powerful postprocessor contains following new functionalities being included since the last release:

Look and Feel:
- Navigation
    - Stepping by time step IDs enables stepping in results with multiple entries for the same simulation time (as result of restarted simulations with appending results).
    - Keyboard shortcuts: Pos1 (first), PageUp (backward), PageDown (forward), End (end).
- Window tile arrangement and sorting order can now be set either by row or by columns
- Color Scales
    - Font and size can be set individually for each color scale.
    - Redesigned method to switch between continuous and discontinuous customized color scales.
    - While scripting, annotations (Color Scale, Length Scale, Infobox) and animations can now be controlled individually for each window by adding the window ID as a command parameter.
- MICRESS® version, compilation time, simulation time, and operating system are displayed in the tool tip of result window titles.

Import/export filters:
- Data Export
    - Result fields (e.g. '.korn') and orientations tabulated in the TabO file (e. g. orientation in Euler angles for each grain) can now be exported to Dream3D/HDF5 files.
    - ASCII export with line breaks analog to the geometry can now be performed analogue to the import 2D of initial grain structures from file.
    - Data can be specified as cell or point data when exporting to VTK.
    - In potential overwriting situations warnings are given. Overwriting of loaded results is always denied to prevent loss of original simulation results.
- Import/Export of color scales especially for use along with Paraview
    - Color map name for listing/identifying a map in Paraview.
    - Import/export as a JSON file (standard export format) or as an XML file.

New types of data analysis:

- Histogram view of value distributions as a new display mode of the data properties
- Segregation analysis
- Morphology analysis (work in progress, beta state)
    - After defining a minimum and maximum value (i. e. two contour lines), data cells having values between these bounds and being neighbored are condensed into a single object.
    - The number of cells, the perimeter and area in 2D, and the surface and volume in 3D are given as a table with entries for each object per time step.
    - FEM surfaces of identified objects are represented as triangular elements and can be exported as combined surface to a single STL file.

Optimizations:

- When handling large compressed result files in native MICRESS® format, especially the stepping in such data sets has been optimized. To benefit from this optimization, uncompressing to temporary files at startup has to be disabled in the memory settings.

News on MICpad:

MICpad allows for editing driving files. Its version number from now on is aligned with the MICRESS® version number. Bookmarks, colored comments and input strings largely facilitate navigating and editing especially large driving files. MICpad further acts as a control center allowing starting and monitoring the simulations as well as monitoring and organizing the results. The new features in MICpad 6.4 comprise:

Look and Feel:
- More stable update mechanism for bookmarks which is done by text parsing only, replacing the former 'reset to standard bookmarks'. User bookmarks can be added by underlining in the text.
- Movable tabs via drag&drop in the tab title bar
- Modified 'Running simulation warning' while closing a file: Options: "run detached simulation in background", "kill simulation", "cancel" (also window cross).
- Saving a driving file of an ongoing simulation raises a warning. Possible actions are 'save anyway', 'create a copy' or 'cancel'.
- Block commenting: shortcuts added (select: ctrl+B; comment: ctrl+D; uncomment: ctrl+shift+D).

New functionalities:
- Phase diagram plots per component can be visualized for driving files using "linear" and "linearTQ" descriptions.
- 2D anisotropy plots can be displayed per phase interaction.

Documentation:

The distribution of MICRESS® 6.4 comprises the following 5 volumes of the manual, which have been updated to include descriptions for all new features and options:

MICRESS® manual Vol.0: MICRESS® - phenomenological background
MICRESS® manual Vol.1: MICRESS® installation
MICRESS® manual Vol.2: running MICRESS®
MICRESS® manual Vol.3: MICRESS® post processing

We do hope that these improvements will assist you in solving your problems and will continue to make MICRESS® 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.

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Global Marketing, Sales & Support MICRESS®