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# TO OUR CUSTOMERS

Dear MICRESS® user,

enclosed please find the most recent release of your MICRESS® software package. The present release 7.1 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® 7.1 is available with or without TQ coupling. The coupled version uses the TQ library corresponding to Thermo-Calc release TC 2020b. GES5 files created with Thermo-Calc version TC 2015b and above are compatible. A new MICRESS®-TQ license file for TQ 2020b is provided along with the current release mail for all users of MICRESS®-TQ with valid maintenance.

- MICRESS® 7.1 is supplied as serial or as partly parallelized version. The solvers for diffusion, stress, flow, temperature, solver for volume change, and phase-field solver (new) provide a performance benefit when executed multi-threaded. The OpenMP (www.openmp.org) programming paradigm is used.

- MICRESS® 7.1 is supported for Windows (10) as well as for Linux (Ubuntu 20.04 LTS, CentOS 7.9, and OpenSUSE 15.2). All platforms have to be 64 bit.

Along with MICRESS®, we provide the following tools:

- DP_MICRESS 7.132
- MICpad 7.100

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

**News on MICRESS®:**

In detail, the release 7.1 of MICRESS® comprises a number of new functionalities and features as shortly described in the following:

*Improvements in input:*

- New - more transparent - keywords have been defined for selecting the scope of linearization parameter sets for treating thermodynamic phase interactions:
    - "global" (formerly "globalG") addresses the entire phase interaction.
    - "interface" (formerly "global") distinguishes individual grain interactions.
    - "fragment" (formerly "globalGF") distinguishes interconnected regions of a phase interaction.
    - "local" (unchanged, but no longer default) performs calculation of linearization parameters in each individual interface grid cell.

- "sumlimits \[k2…kn\]" (Numerical Parameters for Concentration Solver) allow setting limits for the sum of the phase compositions over certain elements which are specified as a list after input of the phase number. A typical application is checking the identity of $\gamma$- or $\gamma$'-phase using the sum of the compositions of the $\gamma$' formers (in case there is only one substitutional sublattice and "ordered" cannot be used). There is no corresponding "penalty" function available.

- "independent_sublattice \[k3..kn\]" (Numerical Parameters for Concentration Solver, TQ only) allows defining that the given list of elements form an own closed sublattice (without VA) and therefore impose an extra restriction of their compositions (their sum is fixed). k1 is used as submatrix component. Linearisation parameters are obtained with respect to the submatrix component instead of the main matrix component. Thus, redistribution is calculated inside the independent sublattice, and the sum condition is applied to the submatrix element.

  The option is automatically applied to phases with corresponding sublattices (e.g. ALPHA phase) if the corresponding elements are not defined manually as stoichiometric (which was the standard approach up to now). Manual definition in this case allows for choosing the numerically most favourable submatrix element, which should have good solubility and sufficient concentration in other interacting phases. In cases where defined sublattices are not really independent the option may nevertheless help to provide composition exchange during extrapolation (which otherwise would only work through relinearisation).

*Improvements in output:*

- The new output ".refR" shows the reference number of the relinearisation parameter set, making the different linearisation scopes more transparent, which can also be identified in the new .TabLin output format.

- The .numR output, which shows the logarithm of the number of iterations used for relinearisation activity since the last output, displays this information now on the whole interface region where it belongs to (depending on local or global scope).
- The .TabLin output file has been amended by the information of the reference number for the linearisation data, which is also graphically shown in the new .refR output. After the conventional output section for each output time (per grain interaction), a second block shows this information sorted by its linearisation reference number. This allows the user to control the linearisation parameters for a given location at the interface.

*New functionalities:*

In view of the very dynamic evolution of the field of "additive manufacturing", own intense work on modelling SLM processes and a strong demand from our customers for microstructure evolution modelling during additive manufacturing, quite a number of new functionalities leading to a *"SLM-Package"*, which however is not a separate MICRESS module, but part of the MICRESS Basic Module:

- In order to account for high spatial gradients (e.g. in case of SLM), the scope of "global", "interface" and "fragment" can be further limited by specification of a maximum distance (given in the same input line).
- For improving the usability of MICRESS for simulation of large domains with strong thermal gradients (e.g. entire layers in SLM), the temperature range used for TQ-operations can be restricted, avoiding numerical issues with very high and/or very low temperatures. Where needed, values are extrapolated (e.g. enthalpy, molar volume), while linearisation parameters, diffusion data and driving forces are restricted according to the selected temperature. The option is activated using the keyword "temp_limit_tq" in section "Numerical Parameters" for the concentration solver, followed by a minimum and maximum value. A further option "temp_limit_tq_phase" allows for a phase-specific temperature limitation which helps avoiding e.g. problems with $\gamma$'-phase in Ni-alloys which should no be used at higher temperatures. The latter option also prevents adding corresponding composition sets to single-phase equilibria with "diff_comp_sets", "enth_comp_sets", "vol_comp_sets".
- The averaging scope of the thin-interface correction ("tic") models (atc, mob_corr) can now be either aligned with the relinearization scope (see above) or with the diffusion segments, thus avoiding averaging of linearisation data, compositions and diffusivities over large temperature ranges. The corresponding options "tic_tq_segments" or "tic_z_segments" are thus relevant in case of high temperature gradients – as occurring in SLM - and should be activated in the section "Numerical Parameters" for the concentration solver.
- The 1d_temp field can now also be used with a combination of heat-flux condition and cylinder or polar coordinate system, which is absolutely necessary for SLM simulations with intrinsic temperature field coupling. Using 1d_temp with non-cartesian coordinate systems now allows (and requires) the definition of the origin of the coordinate system, which must be located above the 1d-domain (i.e. outside of the 1d-temperature field). This

is achieved by entering a distance from the top boundary condition in the "Model" section of the input file and also defines indirectly the length/area on which the flux is applied.

  - For efficient use of the .dTLat output when defining the thermophysical properties of the 1d-domain, a position inside the 2D/3D-microstructure simulation domain can now be specified, where the output refers to (averaged over the length of one grid cell of the 1d-temperature field). In earlier versions, the position was automatically taken to be the center of the 2D/3D-domain, which turned out to be insufficient for SLM applications.

- Nucleation
  - The effect of substrate curvature on nucleation-undercooling can be activated for nucleation on interfaces (option: substrate_curvature)
- Numerical Parameters for Concentration Solver
  - The dysfunctional option “dependent” has been finally depreciated and removed.
  - “diagonal_full” (Numerical Parameters for Concentration Solver, TQ only): When calculating the diagonal partition matrix for diagonal extrapolation, the full thermodynamic factor matrices are used, leading to a better consideration of cross dependencies. Caution: “Demixing” problems, which are typical for multi-binary extrapolation, may reoccur!
- Phase interactions
  - Phase interaction data (TQ only): When using phase-pair wise relinearisation option “manual” for choice of the updating interval, a temperature range can be given as optional parameters in the same line after the value of the interval (which now always must be in the same line with "manual").
- Diffusion
  - Interstitial elements are automatically detected and treated correspondingly
  - When using “diagonal” extrapolation, the partition matrix is written to the log-file instead of a “reduced” partition matrix.

*Improved functionalities:*

- Phase field
  - Improved consistency in n-tupel points. The former ‘first come first serve’ approach was neither symmetric nor consistent with forbidden phase interactions.
  - Improved thin-interface correction (“tic”) in case of anti-trapping current (“atc”). The prefactors of the atc-currents and the mobility correction were adjusted in order to improve accuracy. The evaluation of the mobility is now identical for ‘normal mob_corr’ and ‘atc mobcorr’. Though first tests revealed increased accuracy, the convergence behavior has still to be tested.
  - Profile stabilisation: The profile stabilisation and its criteria was improved. The future goal is to enable automatic profile stabilisation without (or with reduced) user input.
  - Extrapolation of quasi-equilibrium with TQ-coupling has been considerably improved. This is mainly due to two modifications:

- When calculating the linearization parameters for the backward direction, a Gibbs energy addition is made to phase beta to keep the chemical potentials exactly identical as in the forward direction. This addition corresponds to the driving force per formula ("DGF"). This matters only in case of interstitial elements, because then changes of the chemical potential also correspond to changes of the diffusion potential. As a consequence, linearisation parameters for phase beta (and also dS-) are substantially different from the prior (wrong) values, if the driving force is not small (i.e. e.g. directly after nucleation).
- As consequence of the Gibbs energy addition described above, the chemical potential can now be used as a condition for stoichiometric elements which is kept constant during calculation of the linearisation parameters. This improved treatment leads also to major differences in the linearization parameters (on the side of the stoichiometric elements) and thus to differences during extrapolation, even if small driving forces are present.

*Examples:*

- The training examples have been reviewed and categorized by alloy and/or feature. Most of them include a header with a short description.
- New Benchmark example B018_1D_Zener_Diffusion_Control_dri for validation of diffusion-control and anti-trapping against analytical solution from Zener
- Two examples for SLM settings have been added to the application examples for SLM of superalloys.

**News on DP_MICRESS:**

The post-processor DP_MICRESS in version 7.1 brings the following new functionalities:

- Data export
  - Interpolate/average according to ratio between actual dataset and output geometry If a customized geometry with a lower resolution is specified, the actual data will be averaged to fit the lower resolution. Otherwise interpolated.
  - Cut dataset functionality according provided min/max coordinates for a region. This allows the export of 3D regions. Scripting possible.
  - Export of mirrored/repeated views (region). 2 export steps are required for full 3D mirroring.
- Operations: new variables available
  - Direct cell neighbours are accessible by adding a direction (E,W,N,S,B,T) to the field variable, e.g. aW, bN, etc. Not available values at the boundaries will be denoted as NANs. Arithmetic operations with such an NAN in it will be evaluated to NAN. Comparisons will be false.
- View: 3D to 2D projection (X-Ray)
  - This 2D projection feature has been reviewed and now presents a 3D dataset in which each layer contains the average of the values lying behind it. Applying a gray-value color scale, it looks like an X-ray image of the dataset.
- Settings

- Default is not to uncompress to temporary files. Storing compressed stream positions and reading compressed large files while navigating through time steps seems to be more efficient.

**News on MICpad:**

MICpad allows for editing driving files. Bookmarks, colored comments and input strings largely facilitate navigating and editing especially large driving files. MICpad further acts as a control center allowing starting (locally) and monitoring the simulations as well as monitoring and organizing the results. The new features in MICpad 7.1 comprise:

*New functionalities:*

- Homat integration
  - load and run input files for HOMAT and converter tools (Mesh2ABAQUS, Mesh2HOMAT)
- Look & Feel
  - Dark mode (i.e. a different color scheme) introduced. Default is a light color scheme as before. View->Color Scheme can be used to switch (restart necessary).
  - Results button to switch view between driving file/results and results only view
  - Refresh result button
  - View menu: views for driving file and results can be activated individually
  - View of tabular files (.Tab) as tables
    - Hide and show columns
    - Plot diagrams of selected columns
    - Export selected columns as CSV files
  - Long text output can stale the normal text editor scrolling mechanism. Such output will be divided into 3000 lines pages which can be switched with new buttons in the result editor view (top, page up, page down, bottom).
- Syntax checking
  - New and moved keywords in version 7.1
  - Convert from 6.4 to 7.1
- Use real phase and component names in phase and anisotropy plots
- Confirmation dialog for Stop/Kill button to prevent unintended killing of long running jobs

**Documentation:**

The distribution of MICRESS® 7.1 has a full-online documentation, which can be accessed via the documentation tab on the MICRESS website or by calling the help function in either MICpad or DP_MICRESS.

**Outlook:**

For the next release of MICRESS we currently target a topical release on Integrated Computational Materials Engineering ICME focusing on the interoperability of MICRESS with experiments and other software tools as also on the integration of MICRESS into open simulation platforms.

We do hope that all 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). As a service for our customers we compiled all

publications being related to the use of MICRESS® we became aware of since the last release in the appendix. Please notify us about your own publications to allow their inclusion as a reference into our website.

Yours sincerely
ACCESS e.V.

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**Appendix: Recent publications related to MICRESS:**

The following section provides a selection of recent (since last release) publications using MICRESS® and its features and/or the software ecosystem being built around MICRESS®. These articles provide some impressions about state of the art MICRESS simulations being performed by our customers and current topics being investigated using MICRESS®:


Chuanqi Zhu, Yuichiro Koizumi, Akihiko Chiba, Koretaka Yuge, Kyosuke Kishidad, Haruyuki Inuid
Pattern formation mechanism of directionally-solidified MoSi2/Mo5Si3 eutectic by phase-field simulation
Intermetallics; Volume 116, January 2020, 106590

L. Koschmieder, S. Hojda, M. Apel, R. Altenfeld, Y. Bami, C. Haase, A. Vuppala, G. Hirt, G.J. Schmitz
AixViPMaP® -an operational platform for microstructure modelling workflows; Integrating Materials and Manufacturing Innovation (2019) 8:122–143 https://doi.org/10.1007/s40192-019-00138-3

G.J. Schmitz: Materials Modelling: past, present, future (in German), RWTH Themen 1(2019) 8-15

G.J. Schmitz: Materials in an ICME framework: From composition and processing of materials to properties and applications of components, Proceedings NAFEMS World Congress 2019 Quebec, Kanada

G.J. Schmitz, G. Goldbeck, E. Ghedini, A. Hashibon, J. Friis: Towards an ICME Methodology in Europe – Nomenclature, Taxonomies, Ontologies, and Marketplaces, Proceedings NAFEMS World Congress 2019 Quebec, Kanada

G. Goldbeck, E. Ghedini, A. Hashibon, G.J. Schmitz, J. Friis: A Reference Language and Ontology for Materials Modelling and Interoperability; Proceedings NAFEMS World Congress 2019 Quebec, Kanada

A. Nicholas Grundy, S. Münch, S. Feldhaus, U. Hecht, J. Bratberg: Continuous Casting of High Carbon Steel: How Does Hard Cooling Influence Solidification, Micro-and Macro Segregation? IOP Conf. Series : Materials Science and Engineering 529 (2019) 012069 https://doi.org/10.1088/1757-899X/529/1/012069

G. Boussinot, M. Apel, J. Zielinski, U. Hecht, J.H. Schleifenbaum: Strongly Out-of-Equilibrium Columnar Solidification During Laser Powder-Bed Fusion in Additive Manufacturing Physical Review Applied. 11. (2019) https://doi.org/10.1103/PhysRevApplied.11.014025

C. Kumara, A. Segerstark, F. Hanning, N. Dixit, S. Joshi, P. Nylen and J. J. Moverare
Microstructure modelling of laser metal powder directed energy deposition of Alloy 718
Additive Manufacturing; Volume 25, January 2019, Pages 357-364
https://doi.org/10.1016/j.addma.2018.11.024

B. Böttger, B. Daniels, L. Dankl, T. Göhler, T. Jokisch
Systematic Phase-Field Study on Microstructure Formation During Brazing of Mar-M247 with a Si-Based AMS4782 Filler; Metallurgical and Materials Transactions A (2019) Pages 1-16
https://doi.org/10.1007/s11661-019-05113-3

Na Ta, Lijun Zhang, Yong Du

A trial to desgin γ/γ' bond coat in Ni-Al-Cr mode TCBs aided by phase-field simulation

Coatings 8 12 (2018) Pages 421-440, https://doi.org/10.3390/coatings8120421

G. Agarwal, A. Kumar, H. Gao, M. Amirthalingam, S.C. Moon, R.J. Dippenaar, I.M. Richardson, and M.J.M. Hermans: Study of Solidification Cracking in a Transformation-Induced Plasticity-Aided Steel Metallurgical and Materials Transactions A; Volume 49, April 2018, Pages 1015-1020 https://doi.org/10.1007/s11661-018-4505-7

B. Böttger, R. Altenfeld. G. Laschet, G. J. Schmitz, B. Stöhr, B. Burbaum
An ICME Process Chain for Diffusion Brazing of Alloy 247
Integrating Materials and Manufacturing Innovation 7 2 (2018) Pages 70-85
https://doi.org/10.1007/s40192-018-0111-1

Ming Wei, Lijun Zhang, Mingjun Yang, Kai Li, Shuhong Liu, Pizhi Zhao, Yong Du
Phase-field simulation of the solidified microstructure in a new commercial 6xxx aluminum alloy ingot supported by experimental measurements: Int. J. Mater. Res. (formerly Z. Metallkd.) 109 (2018) 2 , Pages 91-98 https://doi.org/10.3139/146.111584