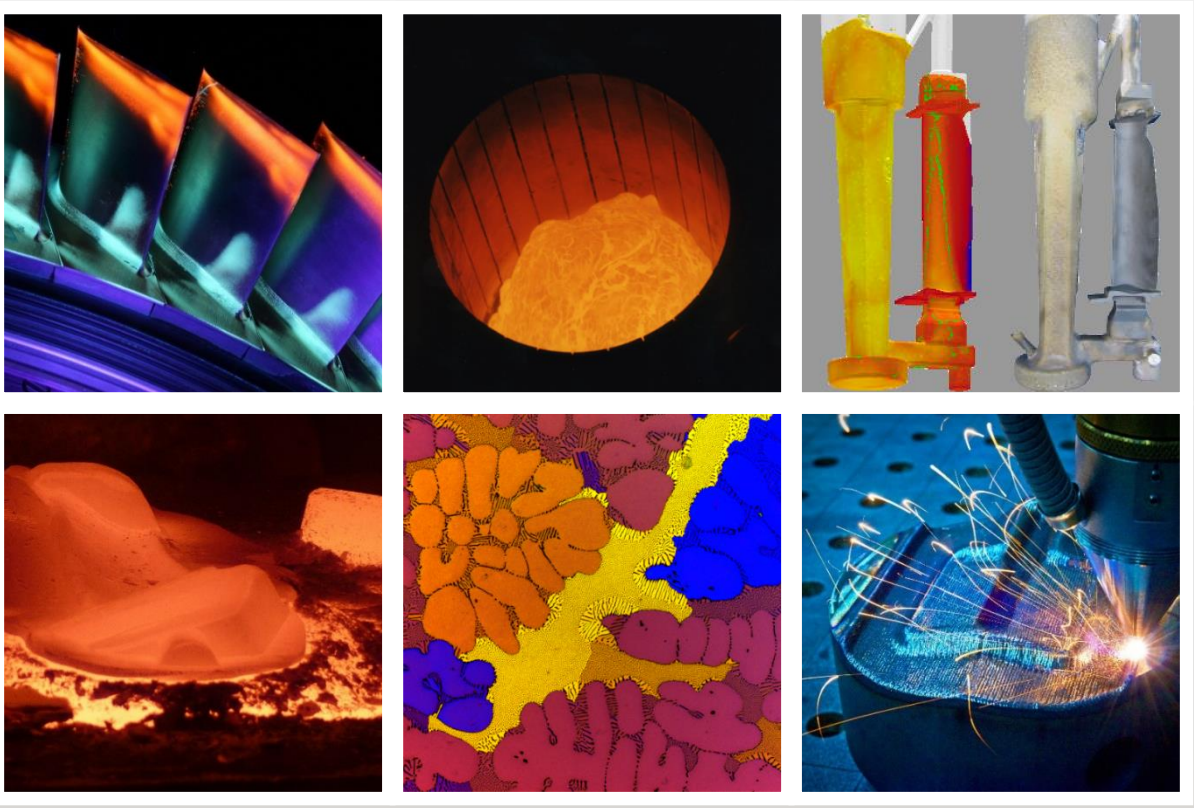

Tutorial
Creation of GES files

access

This presentation

Group A	Group B	Topics
15:45-16:00	08:45-09:00	**Registration**
16:00-16:30	09:00-09:30	8a **Coupling to thermodynamics** Plenary – *GJS* • Thermo-Calc equilibrium and Scheil-Calculation as a basis for MICRESS simulations • Creating a GES5 thermodynamic database with Thermo-Calc
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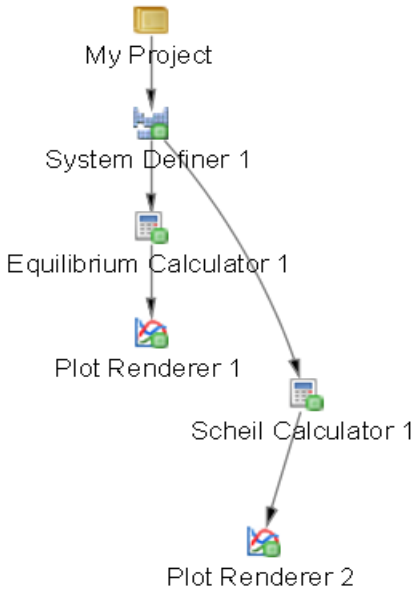
Some useful considerations

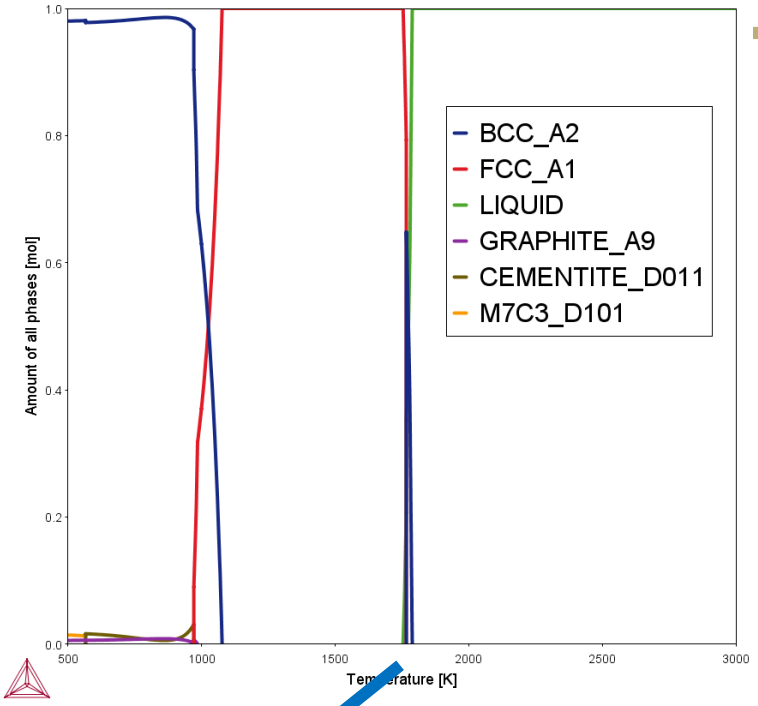
- Before setting-up a MICRESS simulation for a new alloy system:

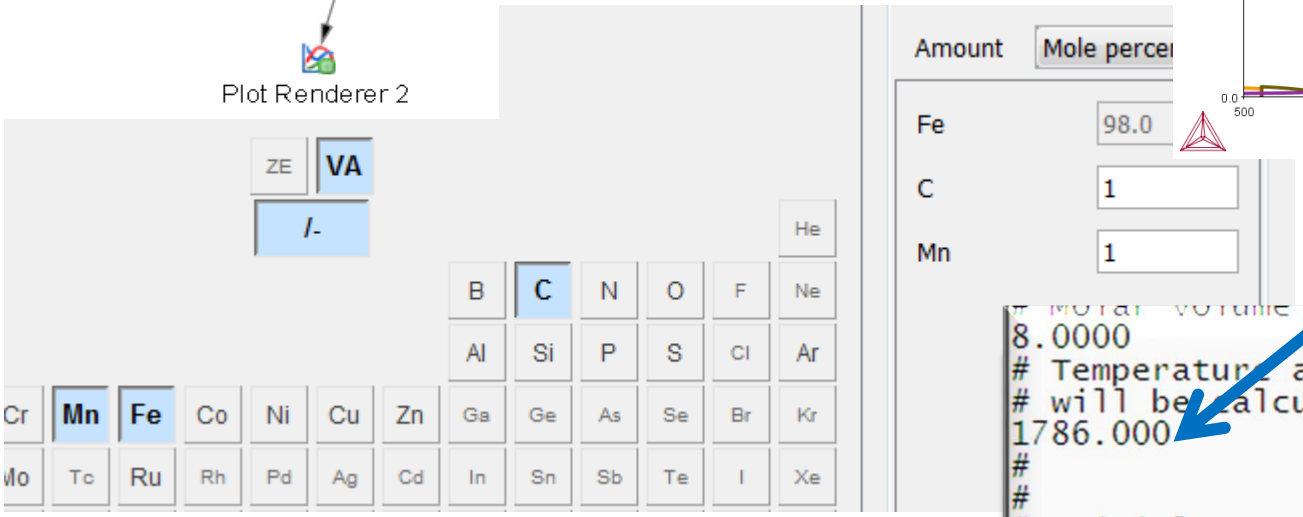
Get a feeling for what you are doing!

- What is a suitable domain size?
  - ➡ Might symmetries be exploited to minimize computational effort?
- What are the initial and boundary conditions?
- What is the alloy system of interest?
  - ➡ Which elements have to be considered?
  - ➡ May some elements be neglected?
- Which phases are to be expected?
  - ➡ during solidification?
  - ➡ during heat-treatment?
- Perform some thermodynamic calculations to learn more....

Get a feeling for relevant temperatues

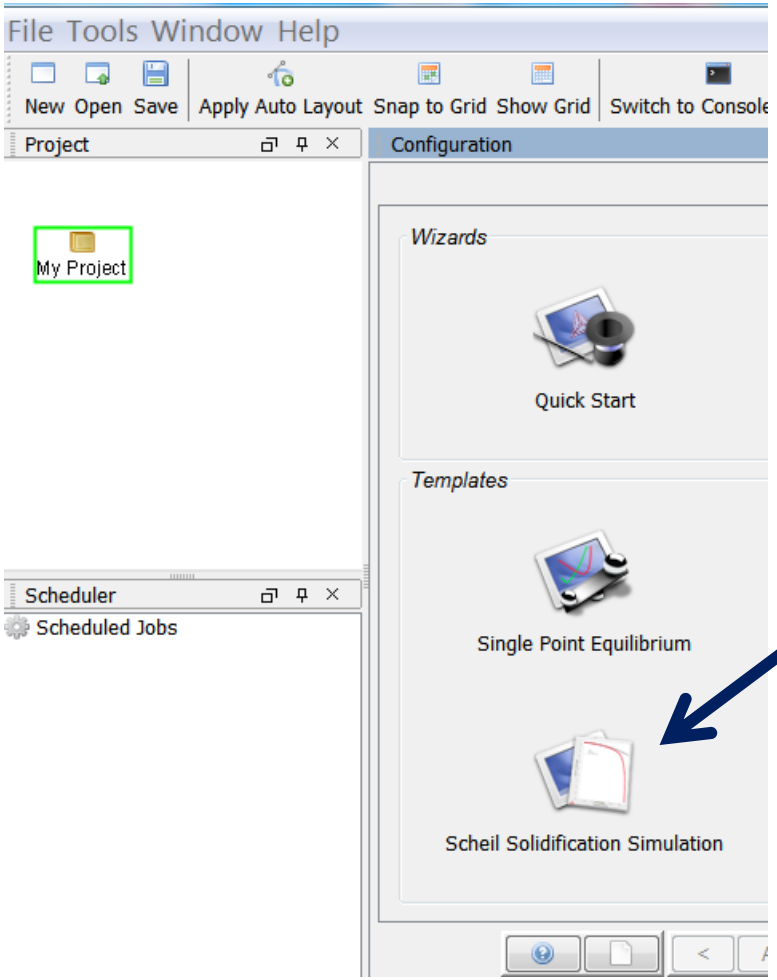






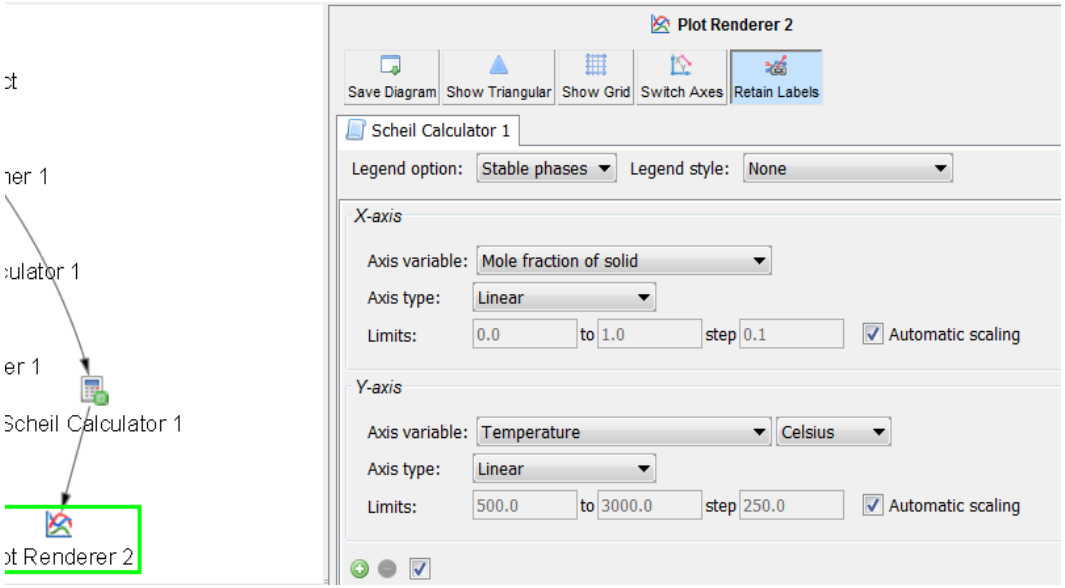

```
8.0000
# Temperature at which the initial equilibrium
# will be calculated? [K]
1786.000
#
#
# Initial concentrations
# ======================
# How shall initial concentrations be set?
```

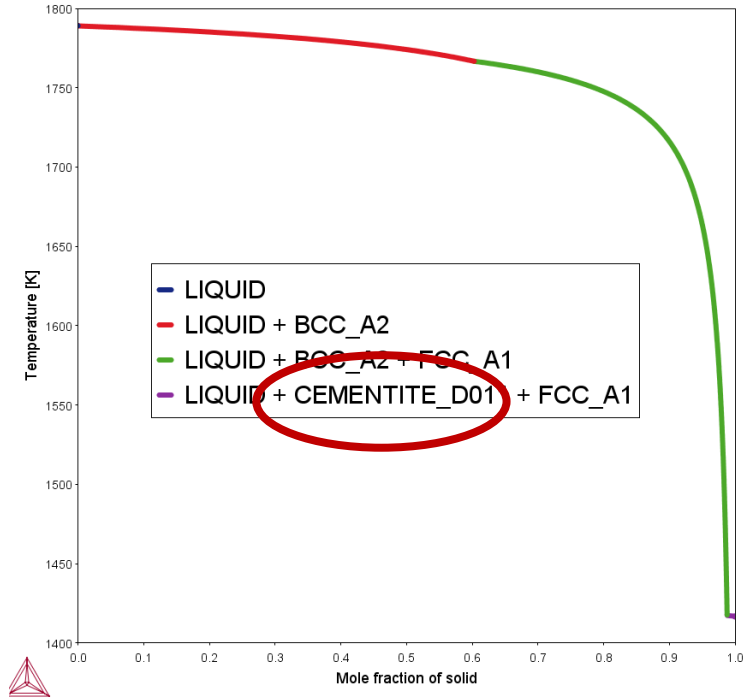
Perform a Scheil Calculation



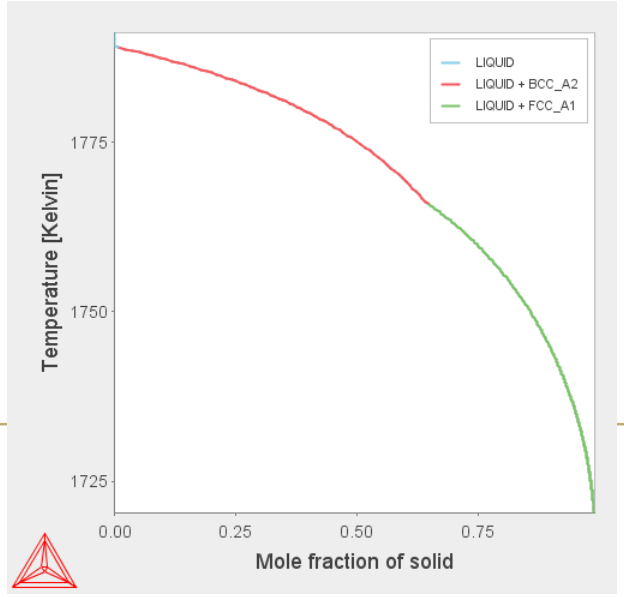
ShortCut to Scheil Module

A Scheil Calculation Result





TCFe10



TCFe6

Coupling to Thermodynamic (& Mobility) Data

```
# Phase diagram - input data
# ========================
# Is a thermodynamic database to be used?
 # Options: database   no_database
 database
#
 # Name of Thermo-Calc *.GES5 file without extension?
 #
GES_Files/Steel
 #
```

switch on-off TC coupling

name of GES5-file

GES files are needed for TQ coupled simulations

```
 # Frequency for complete relinearization [s] =
 1.
 #
 # A description of each pairwise thermodynamic
 # interaction has to be specified.
 #
 # Input of the phase diagram of phase 0  and phase 1:
 # ----------------------------------------------------
 # Which phase diagram is to be used?
 # Options: database  linear
 database
 # Maximal allowed local temperature deviation [K]
 -1.
```

complete relinearisation period

switch between TC coupling and linearized phase diagram for each phase interaction

maximum effective temperature deviation (-1: off)

Allocating the phases in the database to the phases in MICRESS

```
# The database contains the following components:
# 1: C
# 2: FE
# 3: MN
# Specify relation between component indices Micress -> TC!
# The main component has in MICRESS the index 0
# Thermo-Calc index of (MICRESS) component 0?
2
# Thermo-Calc index of (MICRESS) component 1?
1
# Thermo-Calc index of (MICRESS) component 2?
3
# 0 -> FE
# 1 -> C
# 2 -> MN
# The database contains 4 phases:
# 1: LIQUID
# 2: BCC_A2
# 3: CEMENTITE
# 4: FCC_A1
# Specify relation between phase indices Micress -> TC!
# The matrix phase has in MICRESS the index 0
# Thermo-Calc index of the (MICRESS) phase 0?
1
# Thermo-Calc index of the (MICRESS) phase 1?
2
# Thermo-Calc index of the (MICRESS) phase 2?
4
# 0 -> LIQUID
# 1 -> BCC_A2
# 2 -> FCC_A1
```

element 1,2,3 in database

component numbers

phases1, 2, 3, 4 in database

phase numbers

Need for another ges5 file

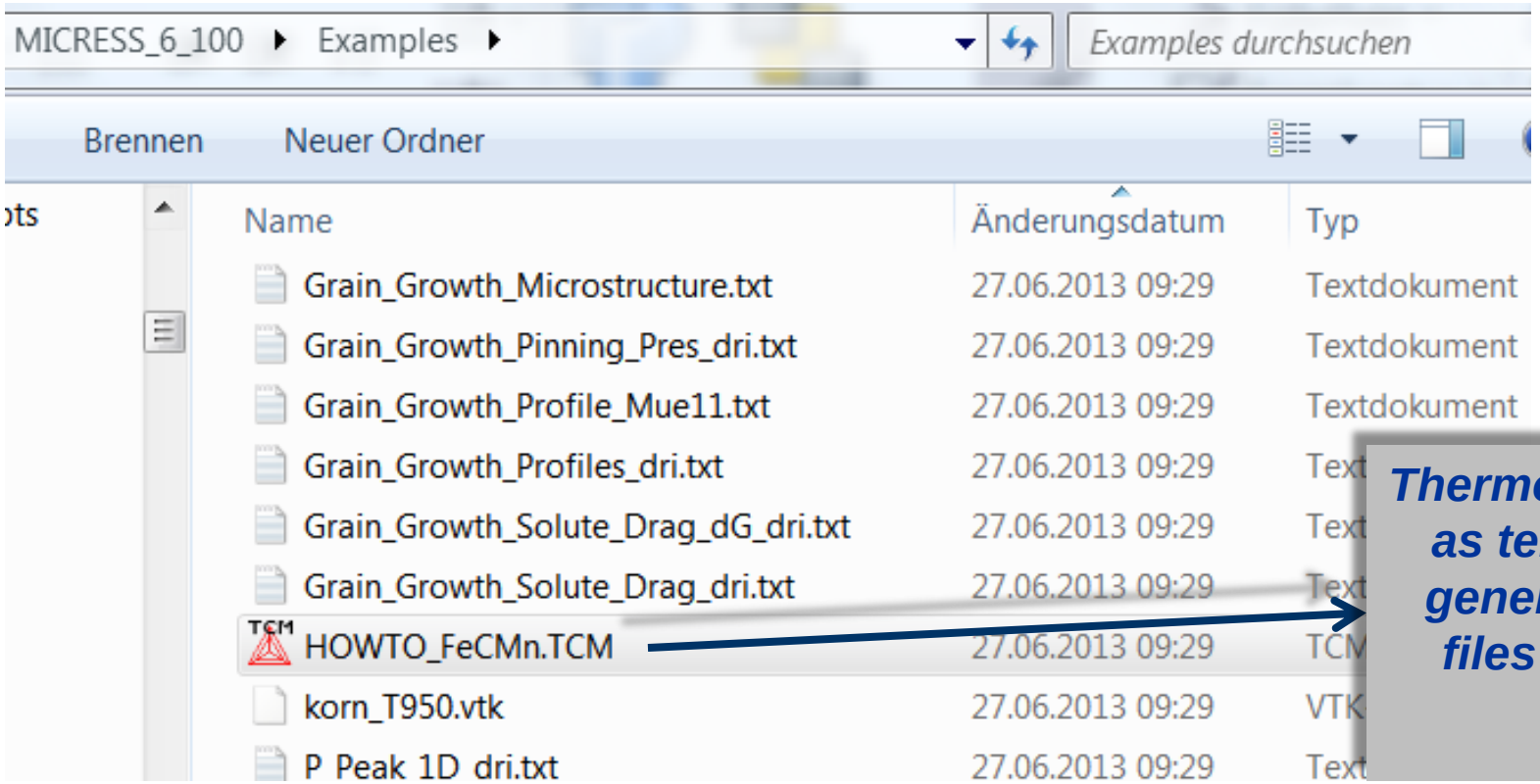
- The number of phases in MICRESS
  may be less or equal the number of phases in the ges5 file

- The number of chemical elements in MICRESS
  must be equal the number of elements in the ges5 file

A new ges file thus is needed if

- a desired element is not contained in the actual ges5 file
- an element in teh actual ges file shall not be considered
- a desired phase is not listed in the actual ges5 file

Use Template for ges file creation

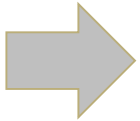


ThermoCalc Macro file as template for the generation of .ges5 files for MICRESS

detailed description of the „HowToFeCMn_ges_file“ Macro template

```
@@ lets see what we are doing:
set-echo
@@select thermodynamic database
go dat
@@for example TCFe6 iron and steel database
sw TCFe6
@@define elements in alloy systems
d-sys fe c mn
@@list the system
l-sy CONSTITUENT
l-sy phases
@@define phases of interest
@@first reject all phases
rej phases *
@@then restore phases of interest
@@e.g. fcc liquid and bcc
rest phases liq fcc bcc
@@get defined system into Ges Workspace
get
@@append mobilty database
app mob2
```

```
@@define elements in alloy systems (same as above!!)
d-sys fe c mn
@@list the system
l-sy CONSTITUENT
l-sy phases
@@define phases of interest
@@first reject all phases
rej phases *
@@then restore phases of interest for diffusion
@@(and modelled in database!)e.g. fcc and bcc:
rest phases fcc bcc
@@get defined/appended system into Ges Workspace
get
@@ goto Gibbs Workspace
go gibbs
@@ save Gibbs Workspace to file (here: FeCMn.ges)
save FeCMn
```



on-line demo

Next : Hands-on

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Create your first simple ges5 file

- Copy „HowToFeCMn“ macro to „MyGESFile“
- Edit MyGesFile
- Switch to TCFe database
- Switch to mobFe database
- Add element Chromium Cr
- leave phases unchanged
- Name output FeCMnCr
- Run MyGESFile macro using ThermoCalc
- Copy created ges file to ges file directory
- Run the modified DeltaGamma Example