

**Thermo-Calc
Software**

Recent developments in Software

Release of Thermo-Calc 2016a
Thermo-Calc Software AB

Thermo-Calc Software user group meeting 16 June 2016

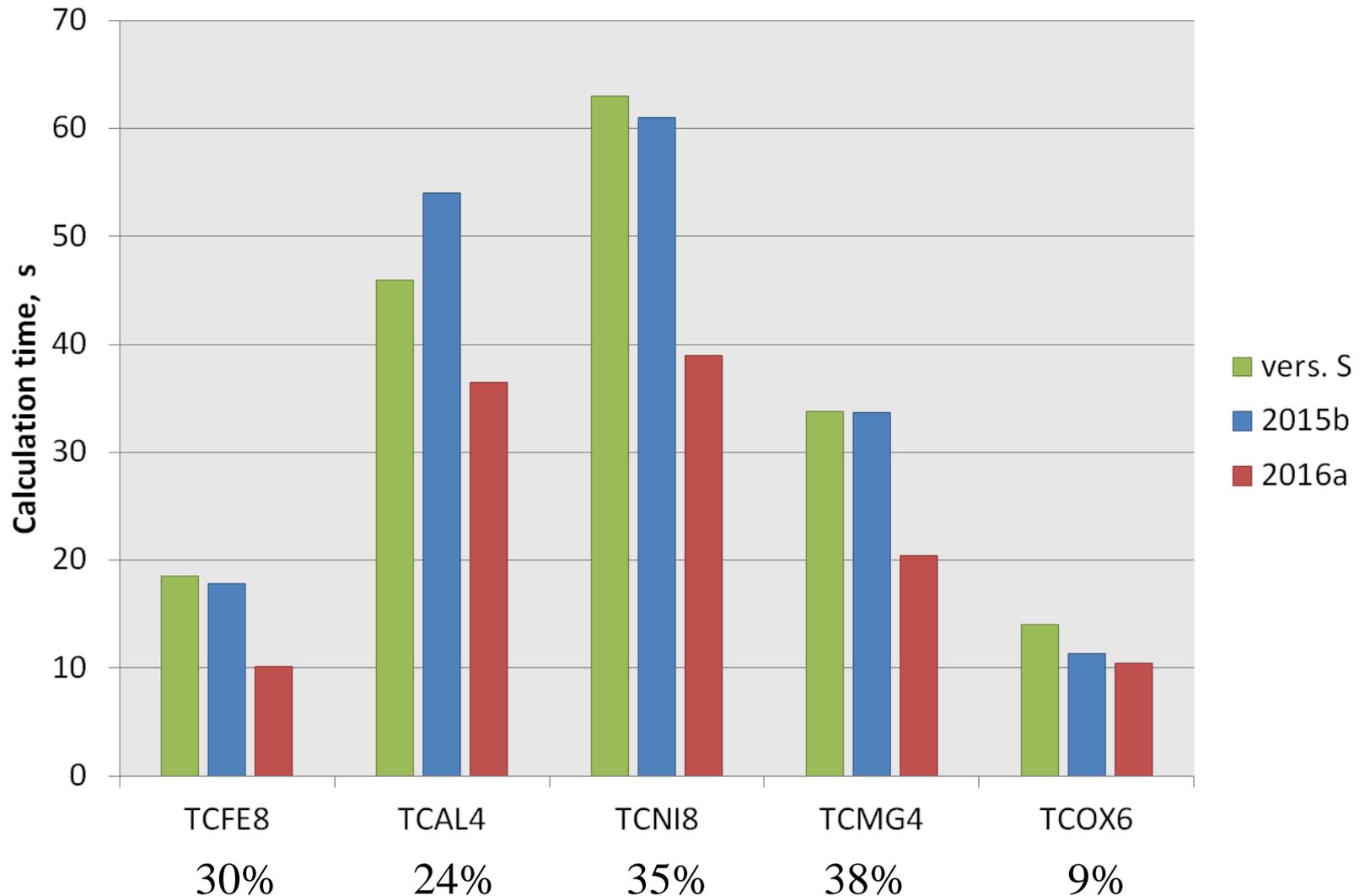
Thermo-Calc calculations considerably faster



- Global minimization optimized
 - Affects most calculations, e.g.
 - Single equilibrium
 - Property diagrams
 - Phase diagrams
 - Scheil
- Large databases optimized TCNI8, TCHEA1, (TCNI6, and TCNI7)
 - Loading of database faster
 - All calculations faster

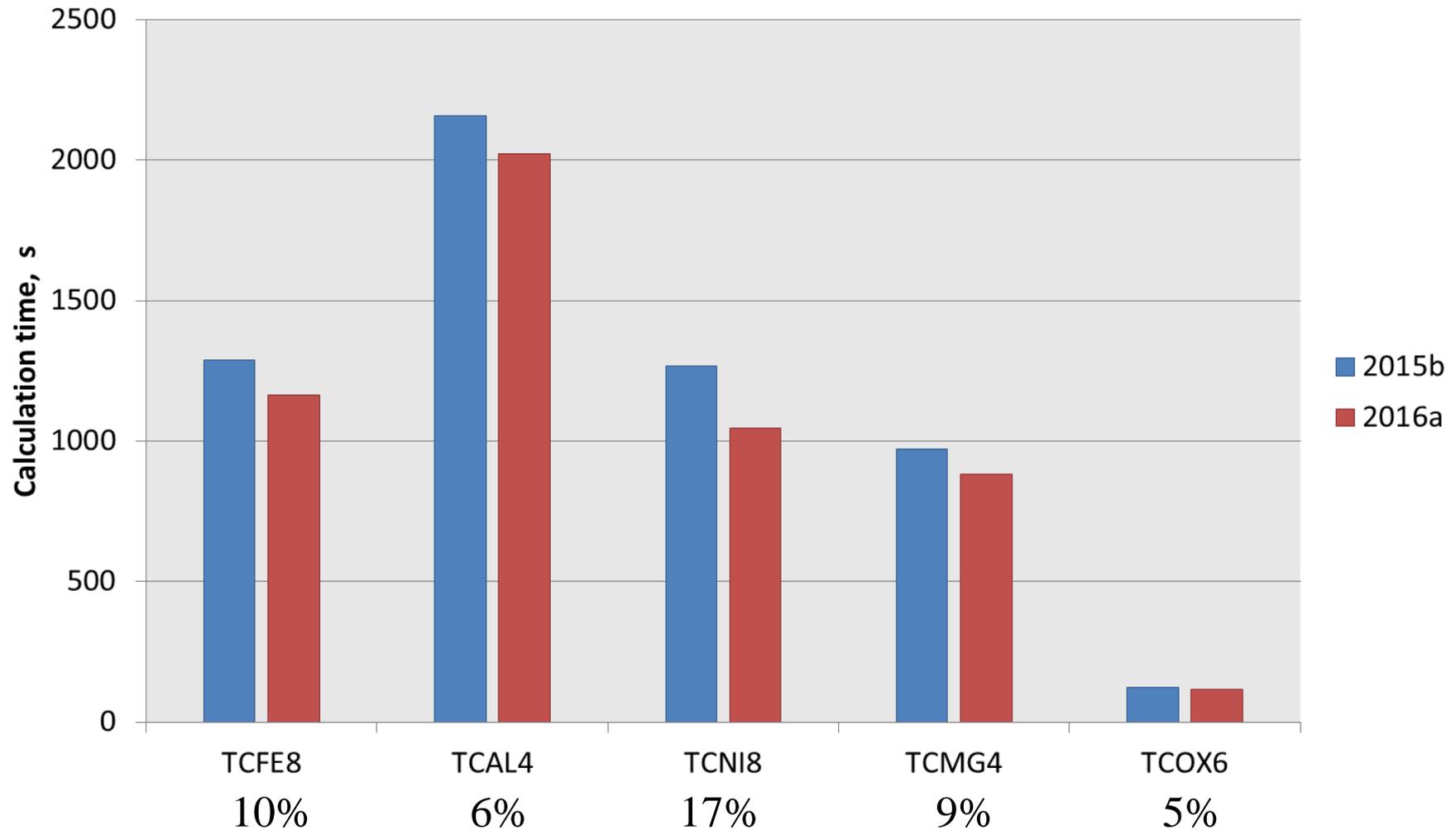
Property diagrams: Phase vs T

5-8 component alloys. 9-38% faster



Phase diagrams

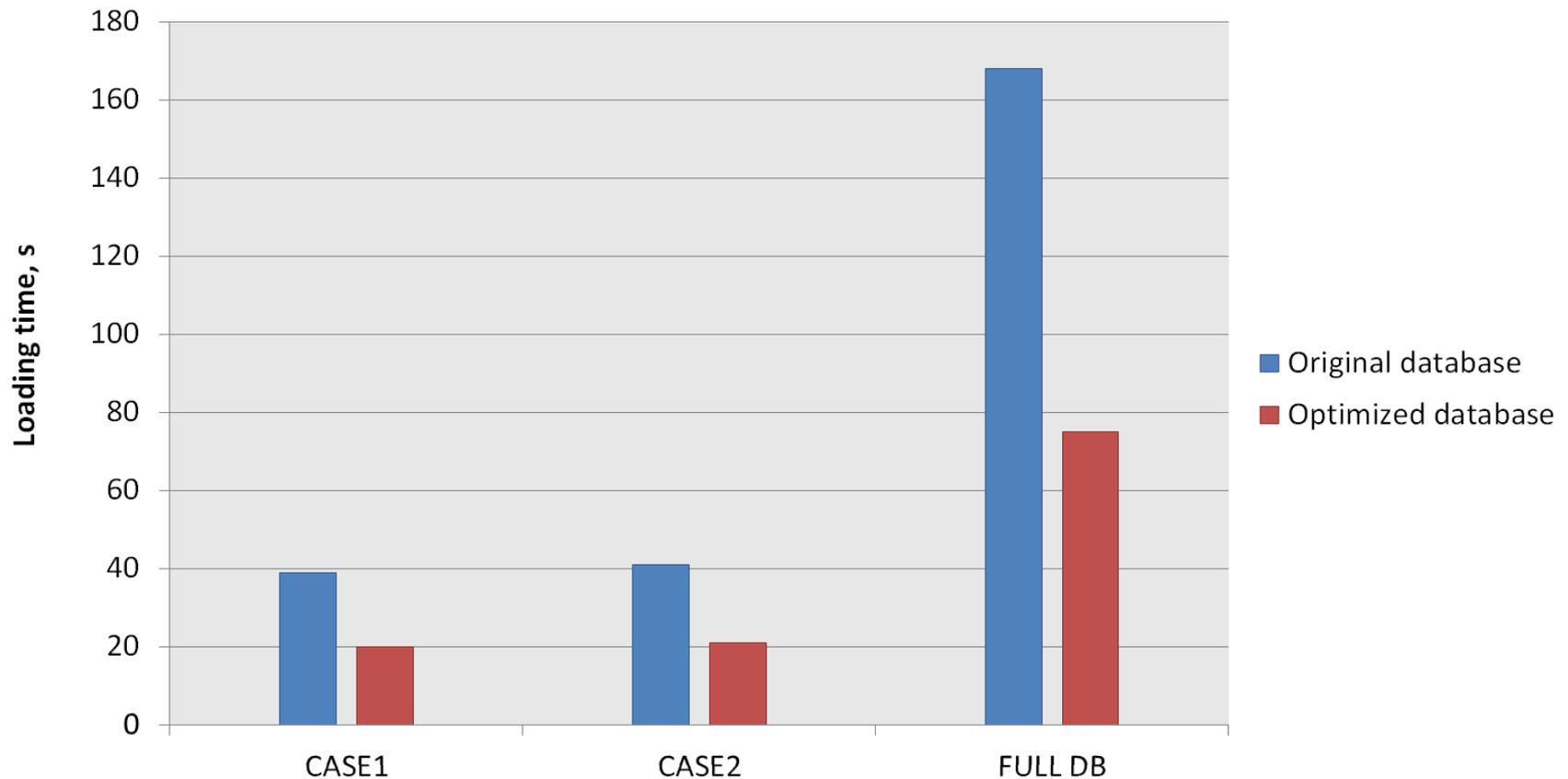
5-12 component alloys. 5-17% faster



Optimized databases

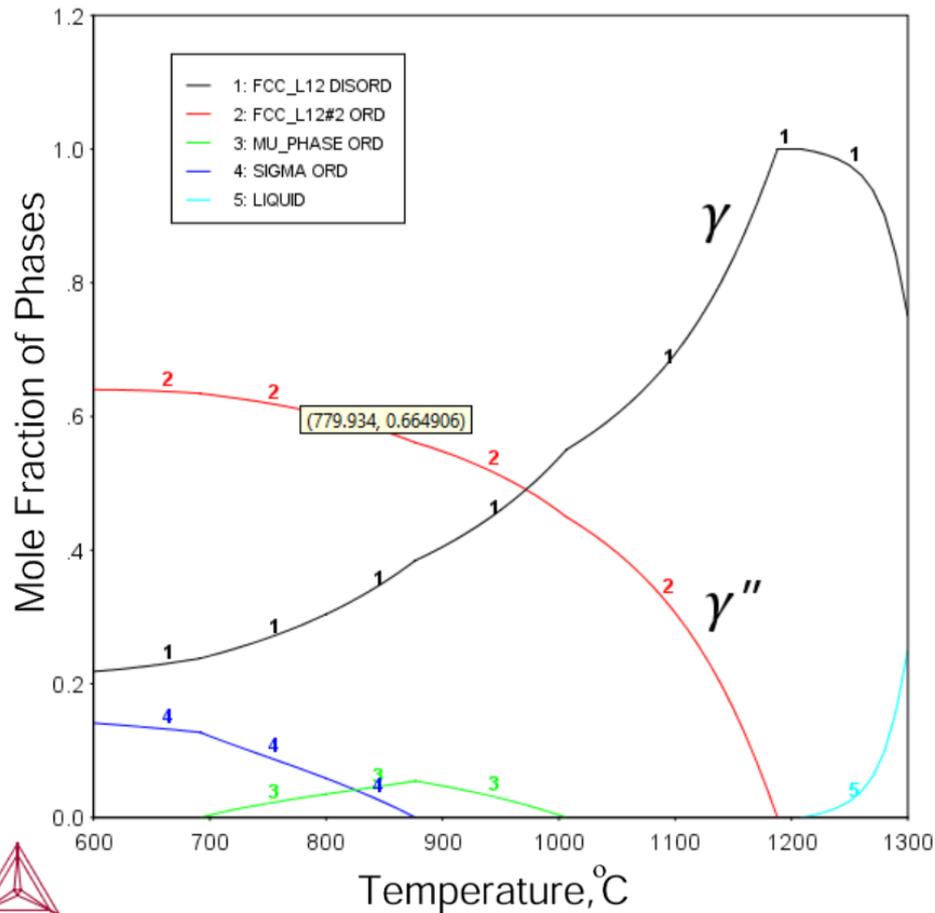
TCNI8(TCNI7, TCNI6), TCHEA1

- Half the loading time



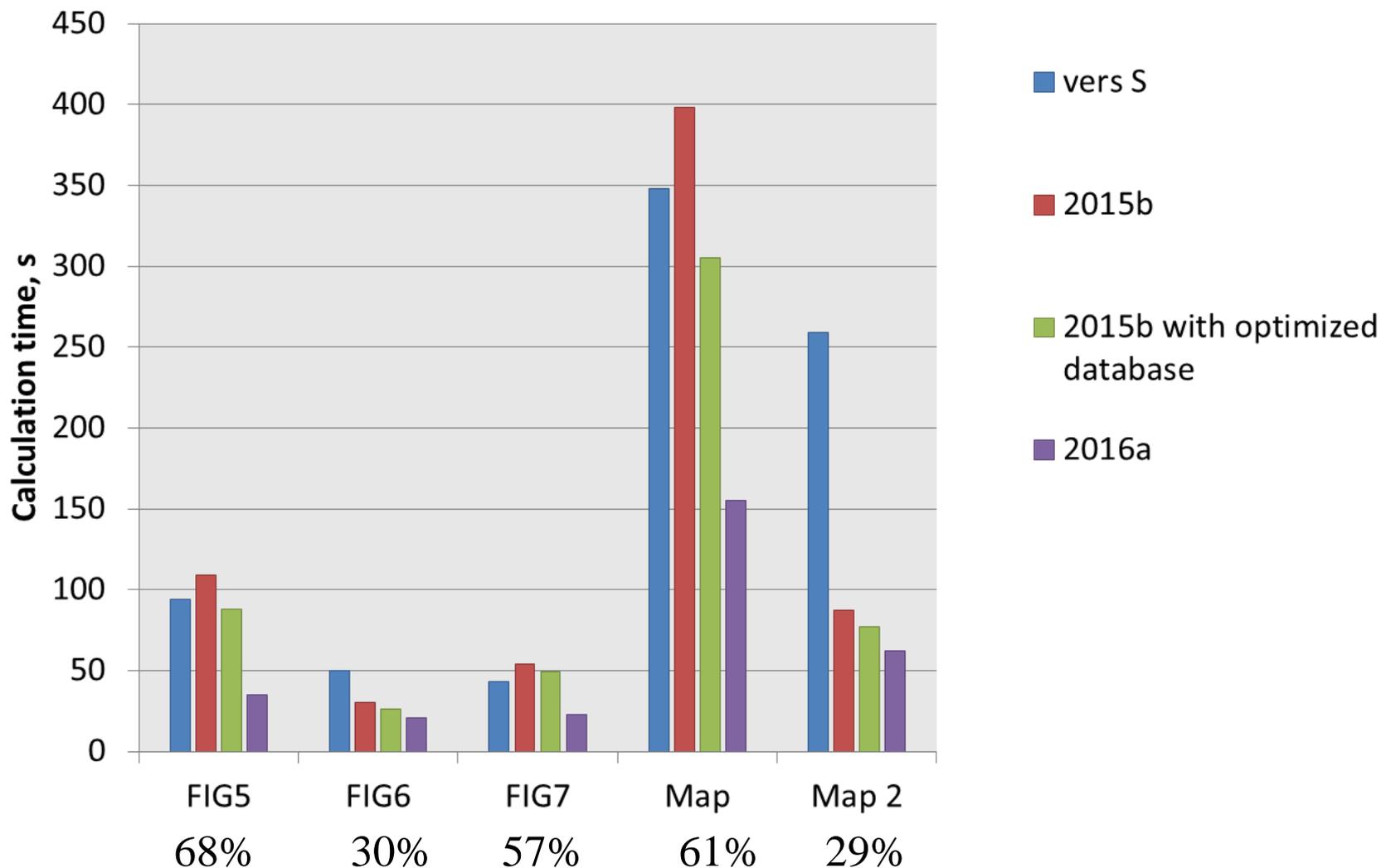
Benchmark TCNI: Extended database information

- Fig 7 Alloy:
Ni-11.5Cr-15.5Co-6.5Mo-4.3Al-4.3Ti-0.5Hf



Benchmark TCNI8

29-68% faster compared to 2015b



High DPI monitors

- 2015b: Not following Windows display settings

Thermo-Calc 5.1-SNAPSHOT

File Tools Window Help

New Open Save Switch to Console Mode

Project Configuration System Definer 1 Results Plot Renderer 1

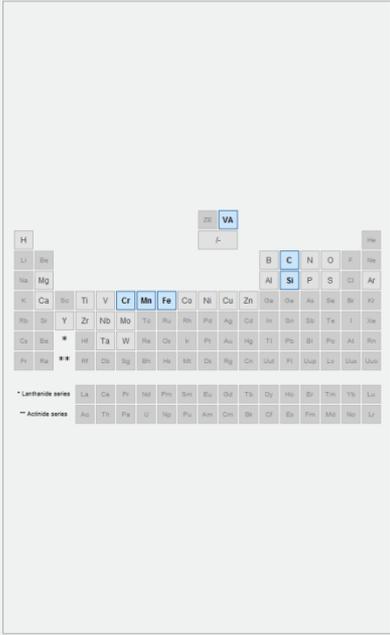
My Project
System Definer 1
ultrium Calculator 1
Plot Renderer 1

Scheduler
Scheduled Jobs

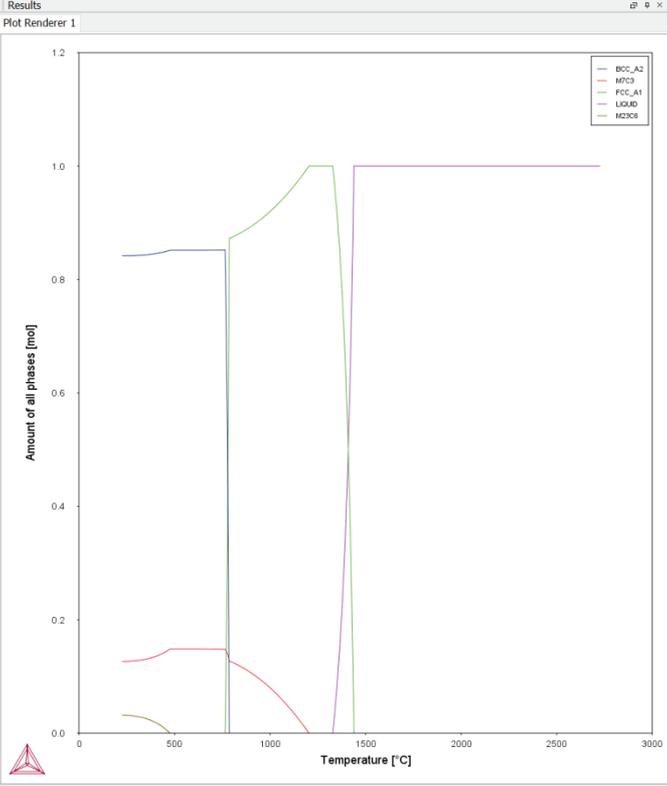
Select database: TCFEB Open user database

Elements Species Phases and Phase Constitution Components Data Sources Description

Periodic Table Alphabetic List Material



Amount of all phases [mol]



Temperature [°C]

Event Log

```

08:40:04,438 INFO Global test at 8.20000E+02
08:40:05,056 INFO Global check of adding phase at 7.49408E+02
08:40:05,499 INFO Calculated 20 equilibria
08:40:05,499 INFO Phase Region from 749.405
08:40:05,501 INFO BCC_A2#1 M23C6#1 M7C3#1
08:40:05,534 INFO Global test at 6.70000E+02
08:40:06,079 INFO Global test at 6.70000E+02
08:40:06,534 INFO Terminating at 600.000
08:40:06,556 INFO *** Buffer saved on file: C:\Users\ROBANO~1\AppData\Local\Temp\TNSD06-1\STATE_1.POL
08:40:06,475 INFO The subprocess completed normally
  
```

Search the web and Windows

SWE 08:41
SV 2016-06-15

High DPI monitors

- 2016a

Thermo-Calc 6.0-SNAPSHOT

File Tools Window Help

New Open Save Switch to Console Mode

Project Configuration Results

My PProject

System Definer 1

System Definer 1

Databases

TCFE9: Steels/Fe-Alloys v9.0 SNAPSHOT Package: Steels and Fe-alloys (TCFE9, MOBFE3)

MOBFE3: Steels/Fe-Alloys Mobility v3.0

Elements Species Phases and Phase Constitution Components Data Sources Description

Periodic Table Alphabetic List

Material

Material name:

Amount Mass percent

Fe	66.05
C	0.68
Cr	20.89
Mn	1.61
Ni	10.28
Si	0.49

Load material... Save material as...

Scheduler

Scheduled Jobs

Event Log

13:36:31,443 INFO Time = 1.4496E+02 Temp = 7.7315E+02 P[1] <>= 2.7263E-09 vf = 7.9275E-04 Nv = 9.3393E+21 dG = -1.3026E+04 Jv = 0.0000E+00 tau = 0.0000E+00 Jc = 0.0000E+00 bin# = 46

13:36:31,450 INFO Time = 1.4467E+02 Temp = 7.7315E+02 P[1] <>= 2.7491E-09 vf = 8.1275E-04 Nv = 9.3390E+21 dG = -1.3026E+04 Jv = 0.0000E+00 tau = 0.0000E+00 Jc = 0.0000E+00 bin# = 46

13:36:31,461 INFO Time = 1.4841E+02 Temp = 7.7315E+02 P[1] <>= 2.7721E-09 vf = 8.3333E-04 Nv = 9.3390E+21 dG = -1.3026E+04 Jv = 0.0000E+00 tau = 0.0000E+00 Jc = 0.0000E+00 bin# = 46

13:36:31,473 INFO Time = 1.5019E+02 Temp = 7.7315E+02 P[1] <>= 2.7954E-09 vf = 8.5449E-04 Nv = 9.3390E+21 dG = -1.3026E+04 Jv = 0.0000E+00 tau = 0.0000E+00 Jc = 0.0000E+00 bin# = 45

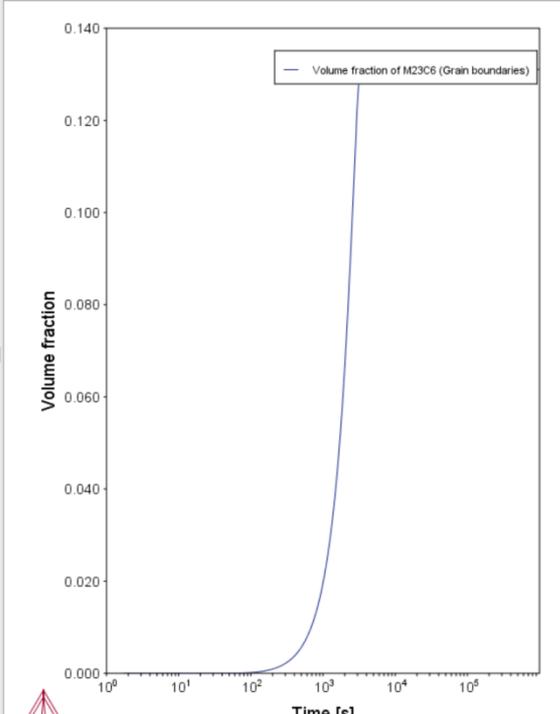
13:36:31,485 INFO Time = 1.5188E+02 Temp = 7.7315E+02 P[1] <>= 2.8188E-09 vf = 8.7626E-04 Nv = 9.3381E+21 dG = -1.3026E+04 Jv = 0.0000E+00 tau = 0.0000E+00 Jc = 0.0000E+00 bin# = 45

Plot Renderer 1 Plot Renderer 2

Volume fraction of M23C6 (Grain boundaries)

Volume fraction

Time [s]

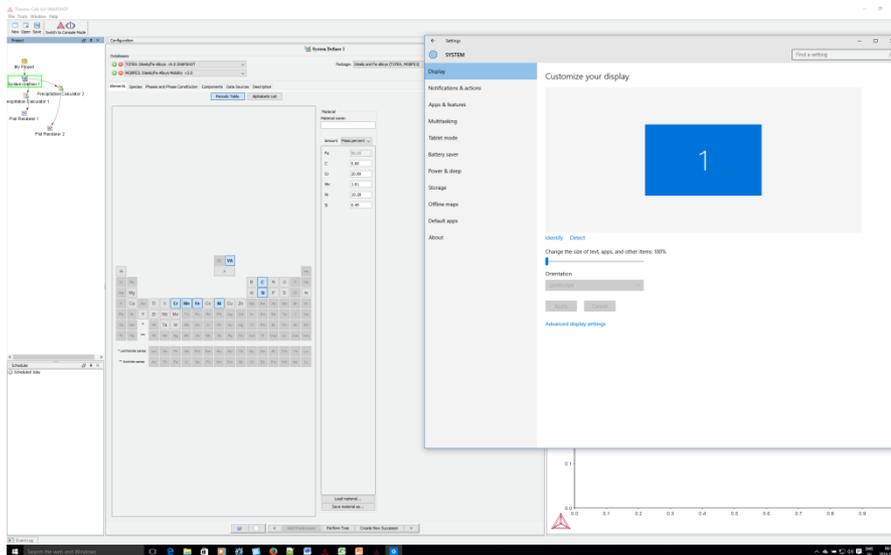


Search the web and Windows

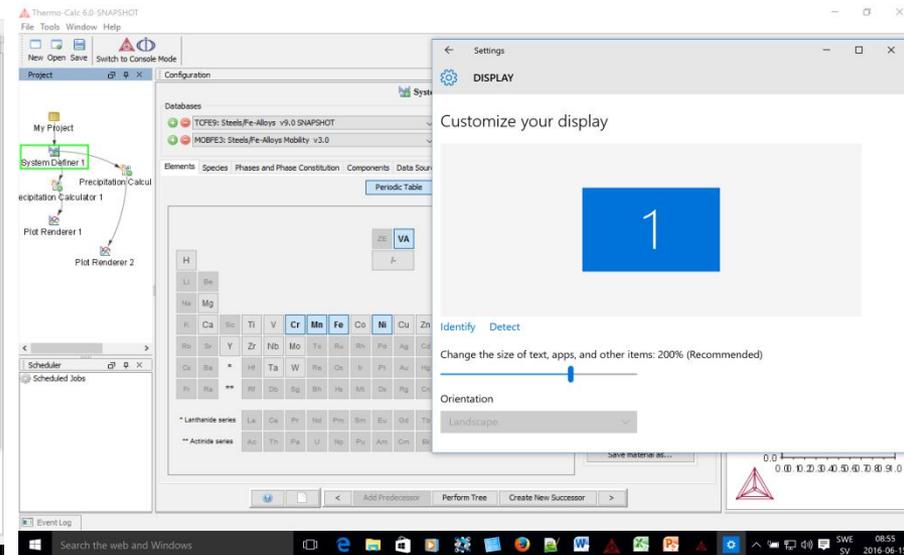
Windows Taskbar: Search, Start, File Explorer, Edge, Mail, Photos, Music, Settings, Task View, Cortana, Thermo-Calc, Word, PowerPoint, System Tray: Network, Volume, SWE, 08:42, 2016-06-15

High DPI monitors

- 2016a – Now scales with Windows display settings



100% Size



200% Size

Diffusion module(DICTRA)

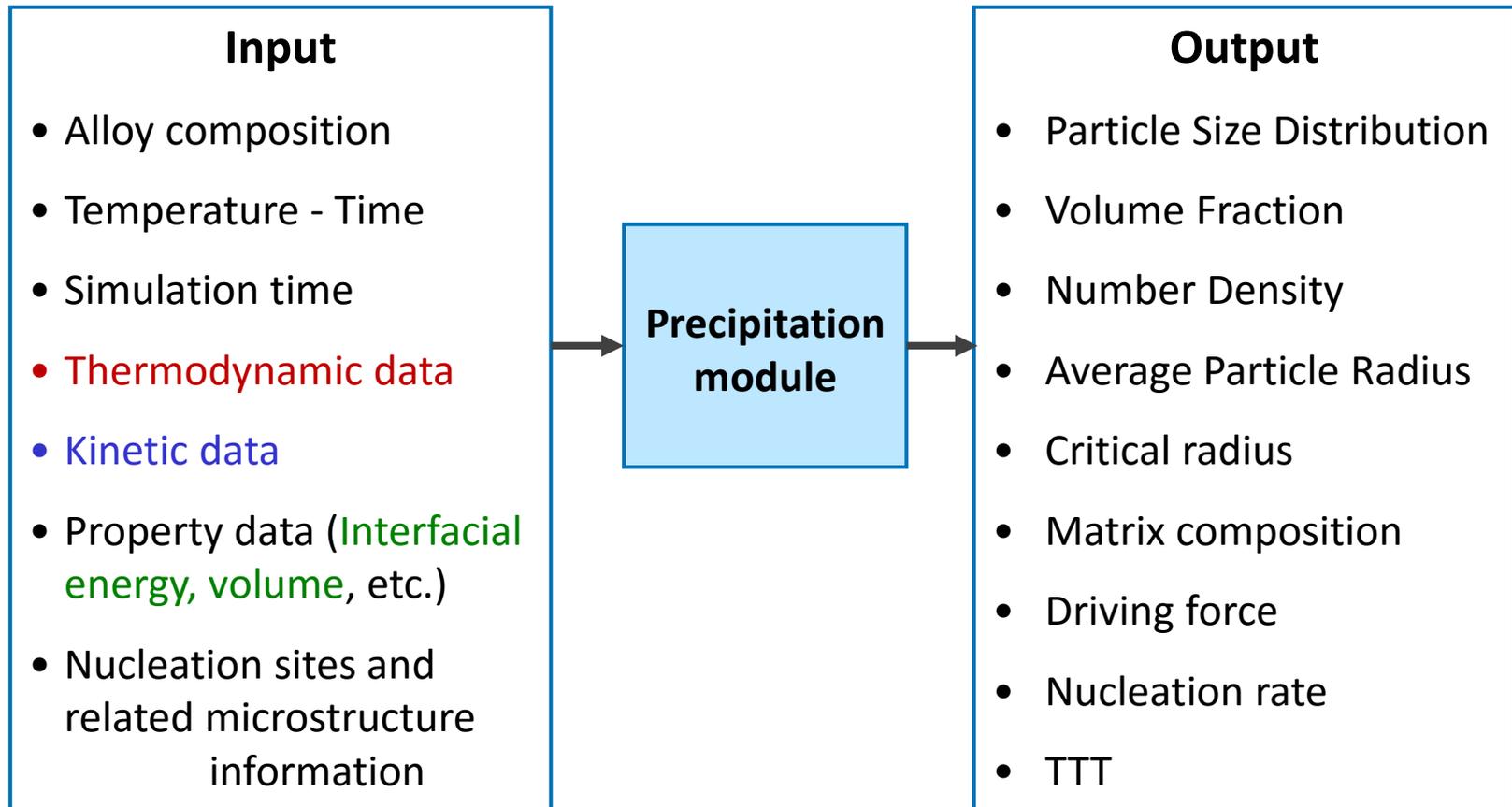
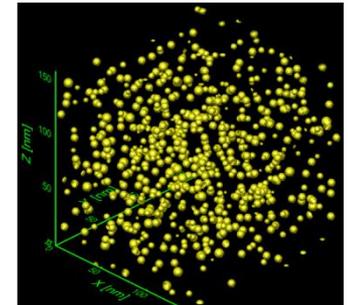
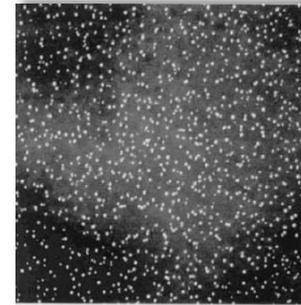
- **Automatic Switching Between Classic and Homogenization Model**
 - There are two models available for solving moving phase boundary problems, the classic model and the homogenization model.
 - The automatic switch is enabled by default, but can be turned off.
- **The ENTER_MOBILITY_ESTIMATE**
 - Previously constant values, but now functions of temperature, for example Arrhenius expressions.
 - The estimate is entered for a specific element in a specific phase

TQ – Fortran API

- Chemical diffusivities are now cached,
 - As long as the site fractions, temperature and pressure remain unchanged they are not re-evaluated when requested; they are just read from the cache.

Precipitation module(TC-Prisma)

- Simulate concurrent nucleation, growth and coarsening of second phases in multicomponent systems.



Precipitation module(TC-PRISMA)

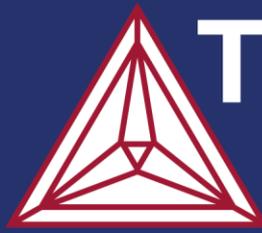


- Benefits with integration:
 - Better control of system, e.g. adding composition sets of phases
 - Improved plotting and tabulation
 - Easier to add new features
- Additional new functionality
 - Multiple nucleation sites of same phase, e.g. $M_{23}C_6$ nucleated at dislocations and grain corners.
 - Improved handling of precipitation of phases within miscibility gaps, e.g. M-CN FCC_A1 & FCC_A1#2
 - Wetting angles considered in heterogeneous nucleation
 - Multiple phases in TTT simulations
 - Added TTT stop criteria: % of equilibrium fraction

Precipitation module(TC-PRISMA)



- All Thermo-Calc 2016a users can test drive Precipitation module in demo mode
 - Limited to two components
 - Demo database-packages
 - Steels, Nickel- and Al-based alloys
 - Included examples uses these demo packages



Thermo-Calc Software

Now demo...



Thermo-Calc 2016a

©2016 Thermo-Calc Software AB. All rights reserved

