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

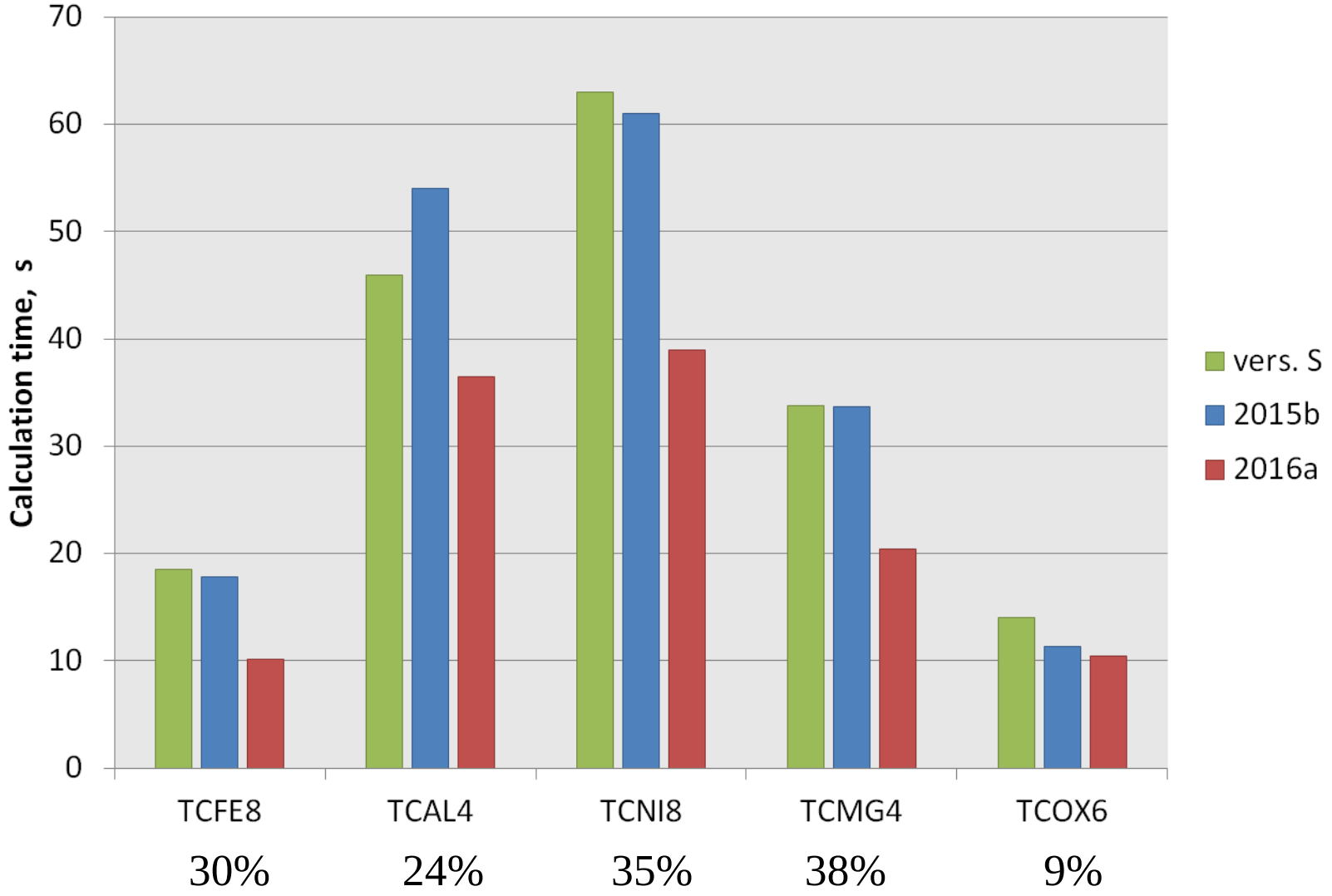
Thermo-Calc calculations considerably faster

- 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

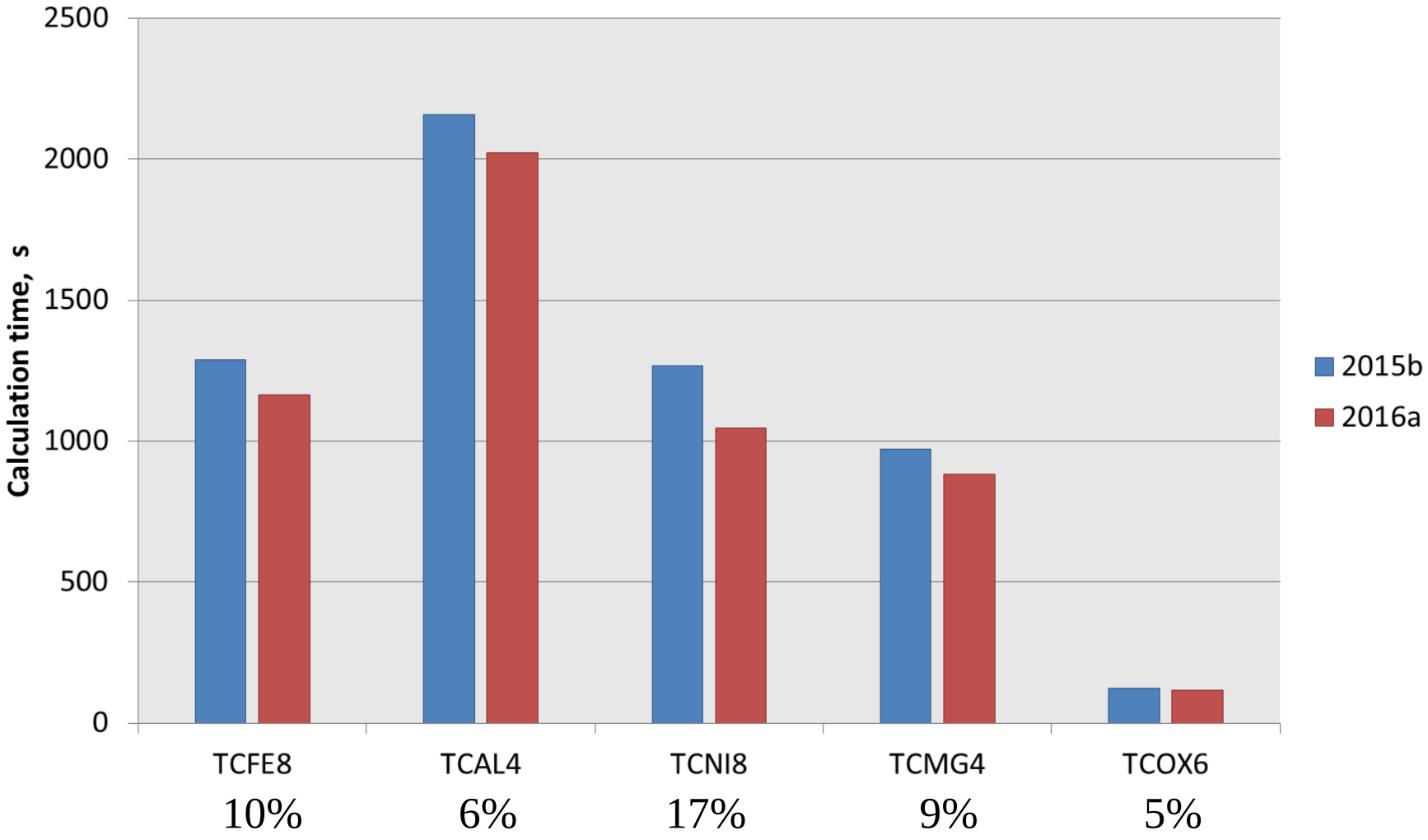
Thermo-Calc Software

5-8 component alloys. 9-38% faster



Phase diagrams

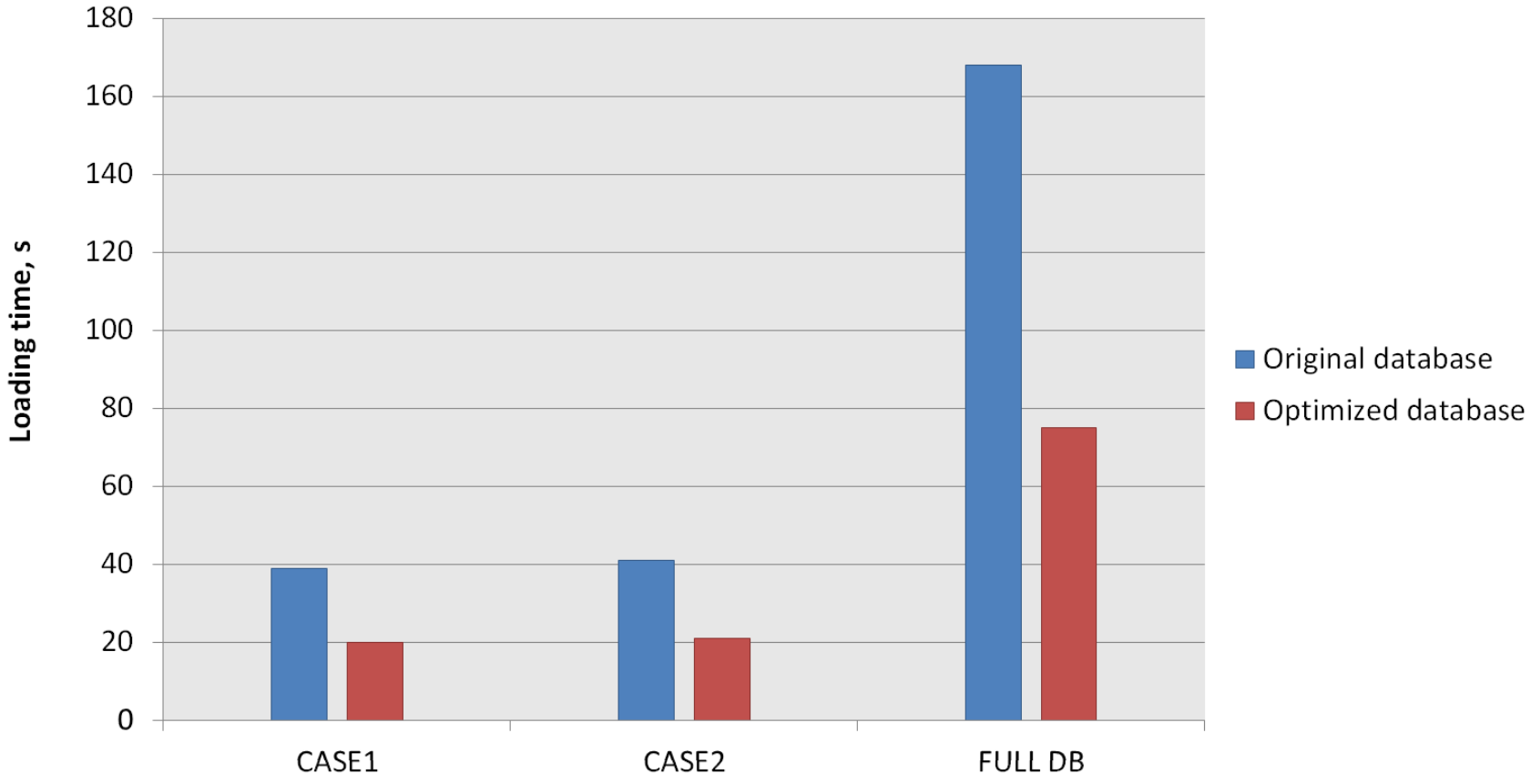
5-12 component alloys. 5-17% faster



Optimized databases

TCNI8(TCNI7, TCNI6), TCHEA1

- Half the loading time

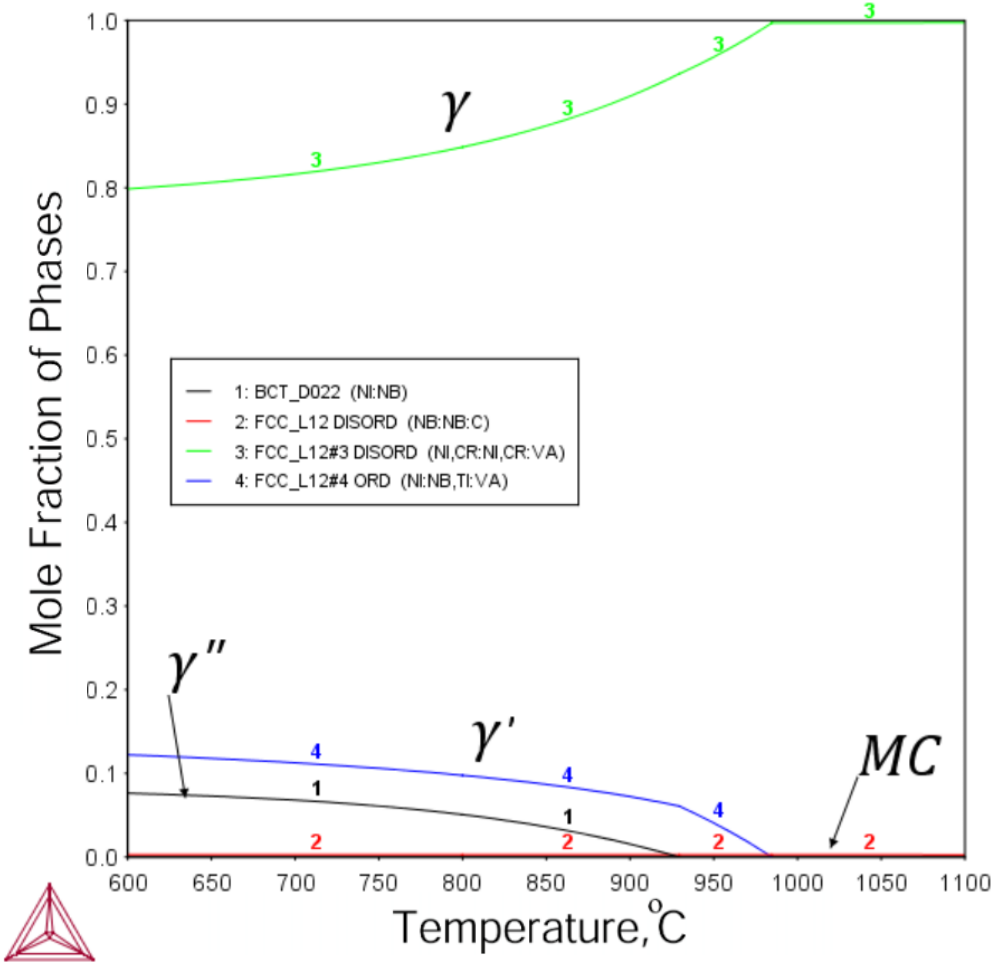


Benchmark TCNI8:

Extended database information

- Fig 5. 718 Alloy:

Ni-18Cr-18Fe-3Mo-0.5Al-1Ti-5.3Nb-0.02C-0.005B

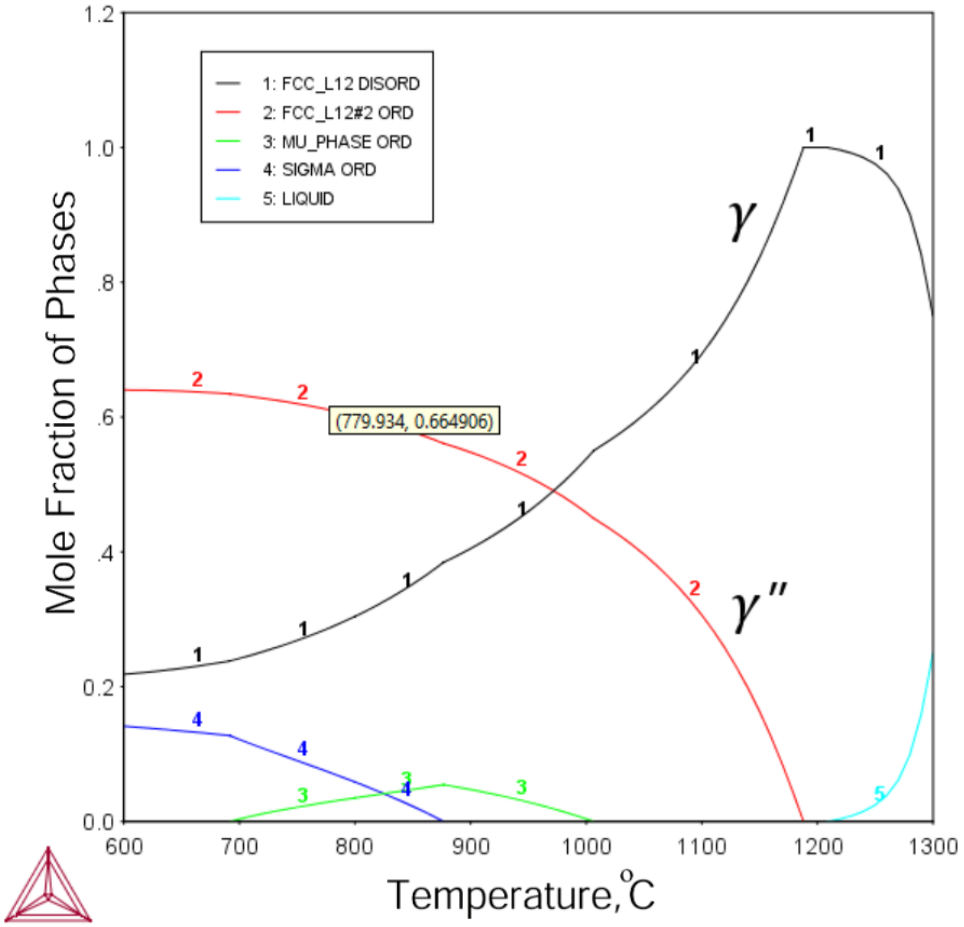


Benchmark TCNI:

Extended database information

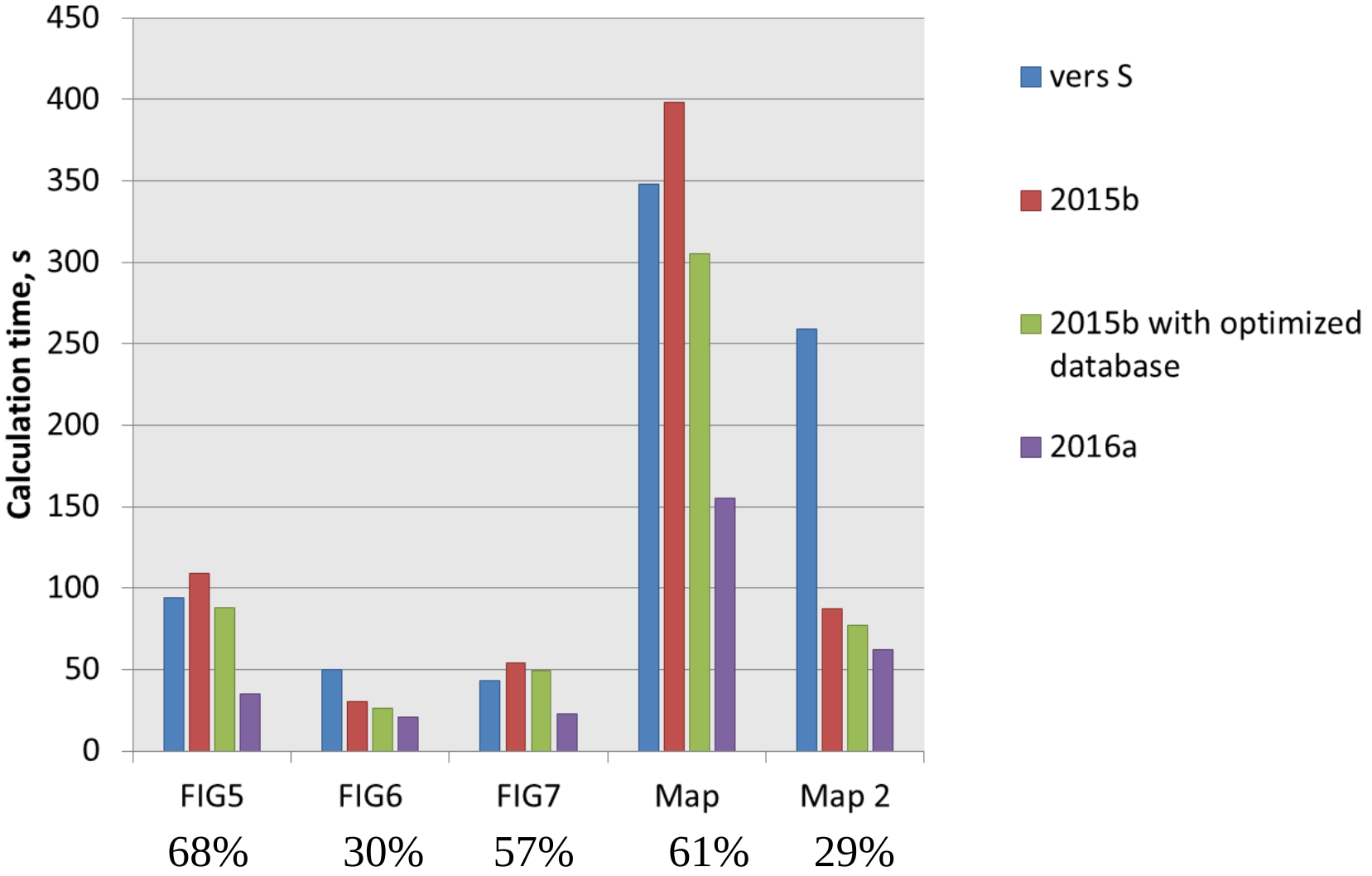
- Fig 7 Alloy:

Ni-11.5Cr-15.5Co-6.5Mo-4.3Al-4.3Ti-0.5Hf



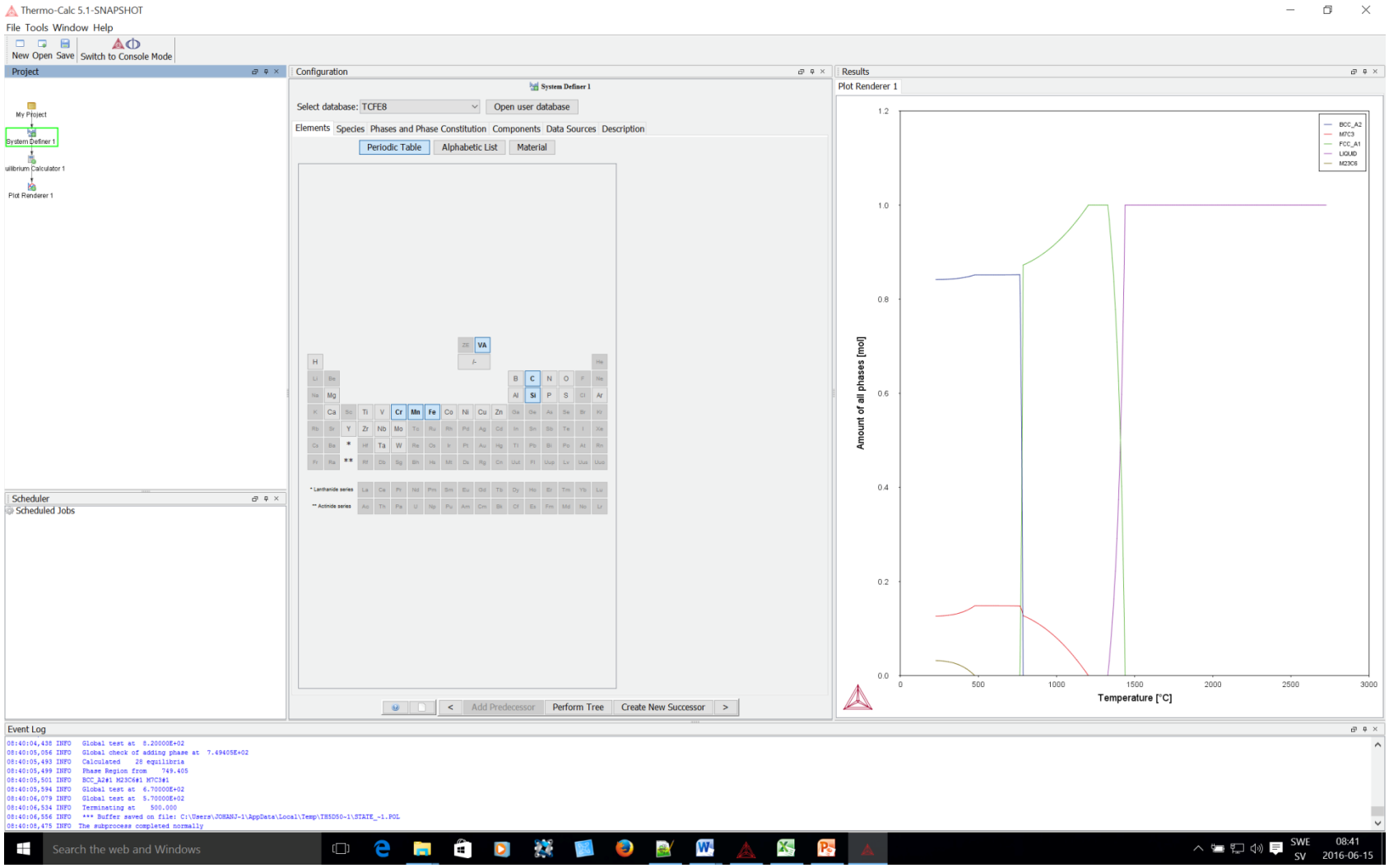
Benchmark TCNI8

29-68% faster compared to 2015b



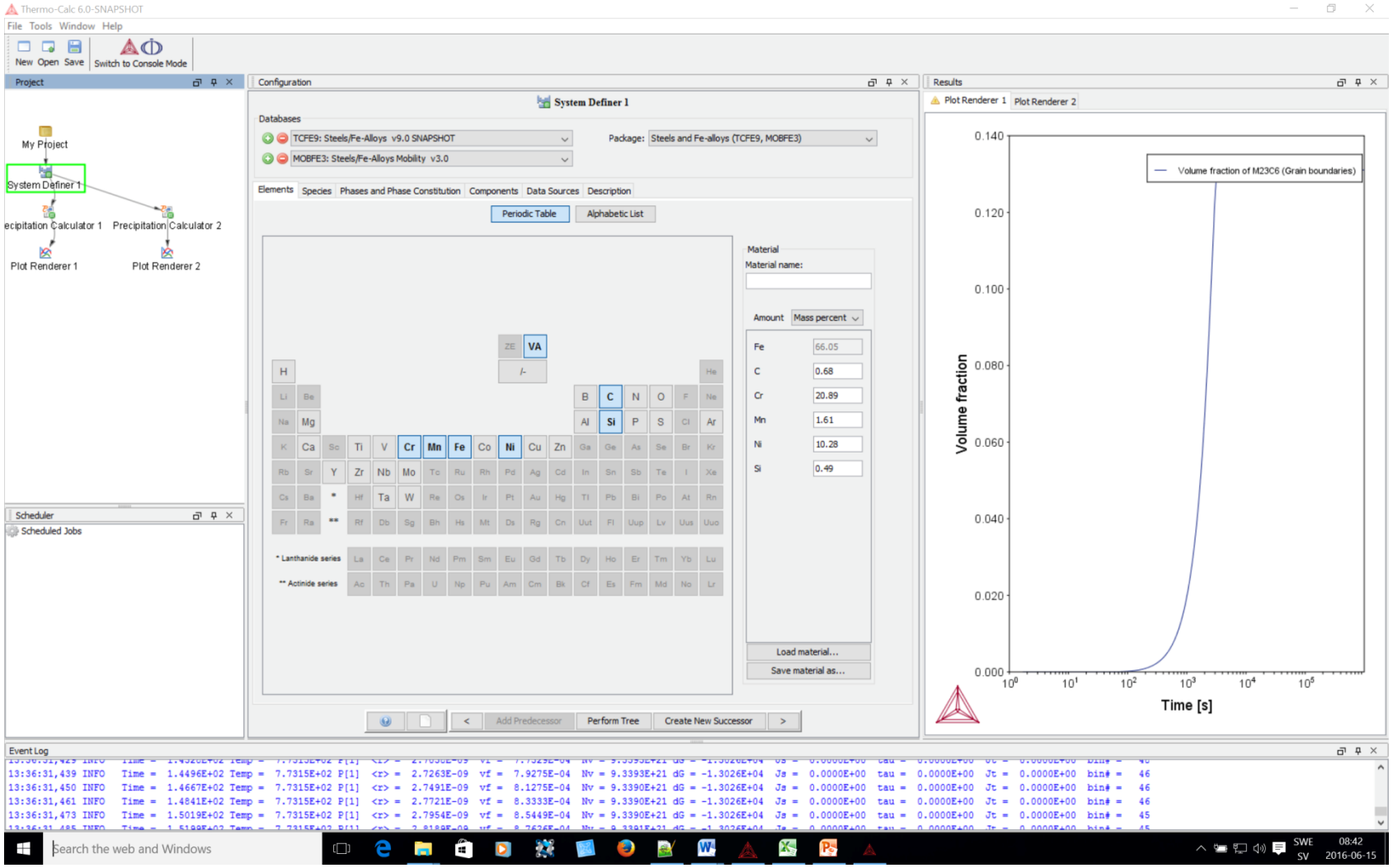
High DPI monitors

- 2015b:Not following Windows display settings



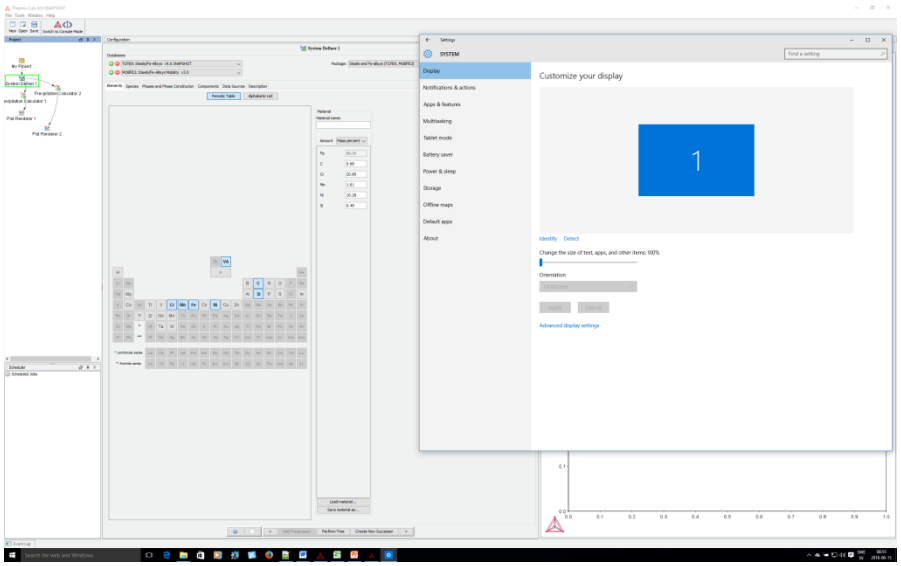
High DPI monitors

- 2016a

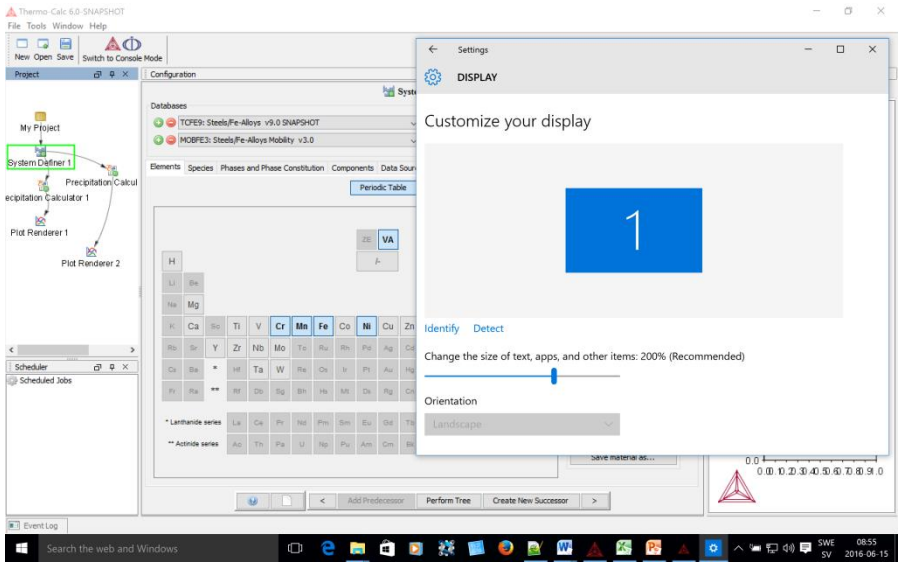


High DPI monitors

- 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.

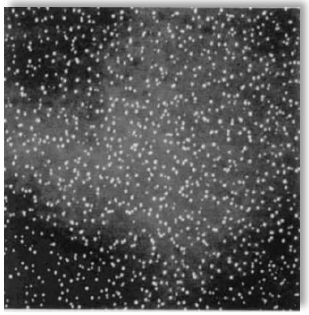
- The ENTER_MOBILITY_ESTIMATE
  - Previously constant values, but now functions of temperature, for example Arrhenius expressions.
  - The estimate is entered for a specific element in a specific phase

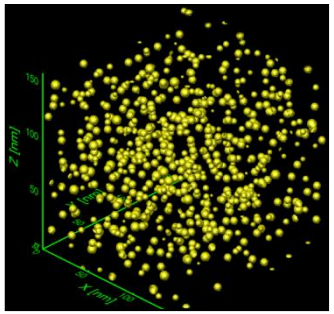
TQ – Fortran API

- 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.





Input

- Alloy composition
- Temperature - Time
- Simulation time
- Thermodynamic data
- Kinetic data
- Property data (Interfacial energy, volume, etc.)
- Nucleation sites and related microstructure information

Precipitation module

Output

- Particle Size Distribution
- Volume Fraction
- Number Density
- Average Particle Radius
- Critical radius
- Matrix composition
- Driving force
- Nucleation rate
- TTT

Precipitation module(TC-PRISMA)

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- 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

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Now demo...