

- **Lectures and Practical Training**

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This school was first arranged in June 2014 by INSTN, CEA Saclay. It is dedicated to thermodynamic assessments using the Calphad method explaining all steps from collecting experimental and theoretical data, selecting models, using the PARROT module of Thermo-Calc and verifying the result in a successful assessment

Important note:

All students have to bring a laptop for use during the school with their preferred software installed. During the school it will be possible to install the free version of Thermo-Calc. All teaching will use the Thermo-Calc software.

- **ORGANIZERS**

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- **INFORMATION**

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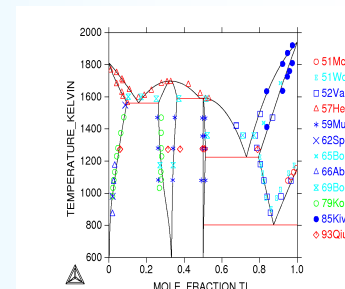
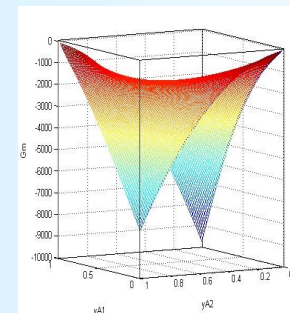


<http://www.centre-port-royal.com>
(20 Kms South-West of Paris)



“School for Advanced Thermodynamic Assessments”

Summer school



Develop models for the Gibbs energy of individual phases (left) in order to calculate phase diagrams (right) representing experimental data.

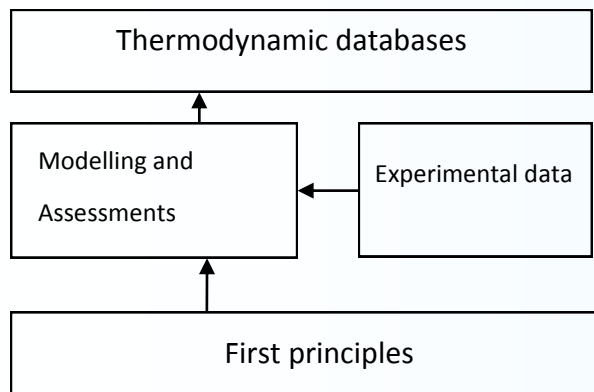
The aim of the school is to provide an advanced course on thermodynamic modelling using the Calphad method. A central part of the school will be the practical assessment of model parameters of multi-component systems for the development of thermodynamic databases. Such databases are a fundamental part of the materials genome initiative and for the Integration of Computational Materials

July 6 — 10, 2015

Centre Port-Royal, France

• Scope

The central theme of the teaching is computational thermodynamics and the school will teach practical assessment of multi-component systems using thermodynamic models. The importance and use of different kinds of theoretical and experimental data will be explained and how theoretical calculations can be combined with experimental data by thermodynamic models and integrated in multi-component databases applicable to modern materials.



• Who should participate ?

PhD students, post-docs and scientists,

- working with assessment of thermodynamic systems and interested to gain a better understanding of modelling and how to handle the assessment software,
- wishing to enhance their comprehension as to how atomistic simulations can be applied for establishing multi-components phase equilibria and diagrams,,
- interested in learning how to model defects, interstitial solutions, chemical and magnetic ordering,
- wishing to become familiar with the coupling between thermodynamics, phase diagrams and microstructures,
- interested in integrating thermodynamic databases in simulations of phase transformations.

Monday : Calphad and experimental data

- Welcome and presentations of teachers and students
- Calphad basic techniques and models, **Bo Sundman**
- Experimental techniques, calorimetry, **Rudy Konings**
- Experimental techniques, phase diagram, **Jean-Marc Joubert**
- **Software Session 1:** Basic examples on individual laptops

Tuesday: Calphad and theoretical data

- Models for ordering, **Nathalie Dupin**
- Experimental techniques, activity meas., **Christine Guéneau**
- First Principles methods 1, **Mark Asta**
- Creating setup and experimental data files, **Caroline Toffolon**
- **Software Session 2:** Assessment practice

Wednesday: Thermodynamic assessments

- First principles methods 2: **Jean-Claude Crivello**
- Special modelling for ionic systems, **Malin Selleby**
- **Software Session 3:** Assessment practice
- General questions and answers, **All**
- **Software session 4:** Assessment practice

Thursday: Validation of assessment

- **Presentation of results** by the students
- **Software session 5:** Assessment practice
- Stable and metastable extrapolations, **Bo Sundman**
- **Software session 6:** Assessment practice
- Documentation and reporting, **Nathalie Dupin**

Friday: Integration and feedback

- **Presentation of results** by students
- Integration of assessments in multi-component databases and software, **Bo Sundman**
- **Evaluation and feedback to teachers and software developers** by all.

Summary:

More than half of time at the school is devoted to practical assessment of real systems by the students themselves with assistance from the teachers. The Cu-Mg system has been selected as a case study as it is wellknown and has many important modelling features. However, the students are encouraged to bring the systems they are currently working on for discussions.

A week is too short to perform a complete assessment of any system but the students will have a chance to understand how the available software tools can be used in particular cases.

Registration deadline: April 30, 2015.

Language: English

The school is held in France, close to INSTN. CEA-Saclay (20 km South of Paris).

Registration Fee : 1800 €

Includes: Hotel accommodation, meals, local transport, proceedings.

A limited number of grants is available from the INSTN and the STT (contact constantin.meis@cea.fr)

Deadline for grants applications January 31, 2015.