

- **Lectures and Practical Training**

Mark Asta, Berkeley Univ, USA

Jean-Claude Crivello, ICMPE-CMTR, CNRS, France

Nathalie Dupin, Calcul Thermodynamique, Orcet, France

Suzana G. Fries, ICAMS, Ruhr Univ Bochum, Germany

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Christine Guéneau, CEA Saclay, France

Jean-Marc Joubert, ICMPE-CMTR, CNRS, France

Lina Kjellqvist, Thermo-Calc Software AB, Sweden

Rudy Konings, ITU, Karlsruhe, Germany

Malin Selleby, MSE, KTH Sweden.

Bo Sundman, KTH Sweden, & INSTN - CEA, France

Caroline Toffolon, CEA Saclay, France

This school is a sequel to the very successful schools on the “**Fundamentals of Thermodynamic modelling**” organized for three successive years at INSTN, CEA Saclay. In 2014, it will be more dedicated to thermodynamic assessments using the Calphad method.

**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 but some teachers have experience

- **ORGANISERS**

Bo SUNDMAN

KTH, Sweden & INSTN - CEA, Saclay, France

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- **INFORMATION**

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- **On line REGISTRATION**

[www.mse-chair.org](http://www.mse-chair.org)



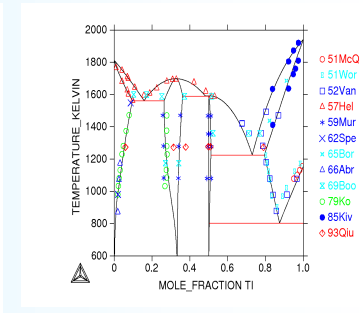
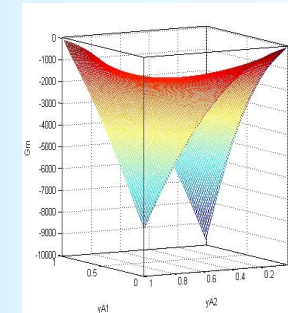
<http://www.centre-port-royal.com>

(30 km from 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) reproducing experimental

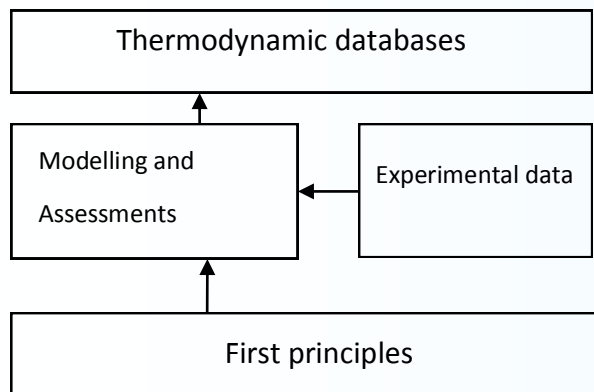
The aim of the school is to provide an advanced course on thermodynamic modelling using the Calphad method. A central part of the school will be the practical assessment of model parameters of multi-component systems for the development of thermodynamic databases. Such databases are a fundamental part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

June 23-27, 2014

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**
- Setting up model 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, **Suzana G Fries**
- **Software session 6:** Assessment practice
- Documentation and reporting, **Bo Sundman**

### Friday: Integration and feedback

- **Presentation of results** by students
- Integration of assessments in multi-component data bases and software, **Lina Kjellqvist**
- **Evaluation and feedback to teachers and software developers** by all.

### Highlights:

More than half of time at the school is devoted to practical assessment of real systems by the students with assistance by experts. The Fe-Ti-X system has been selected as a case study as it has many important modelling features: magnetism, chemical ordering, metal-nonmetal system, vacancies and other defects etc. 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: March 31, 2014.**

Language: English

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

Price : 1700 €

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](mailto:constantin.meis@cea.fr))**

**Deadline for grants applications February 14<sup>th</sup>, 2014**