Education in Computational Thermodynamics, ICME and Materials Design – the KTH experience

John Ågren
Materials Science and Engineering
KTH
100 44 Stockholm, SWEDEN

ROYAL INSTITUTE OF TECHNOLOGY

Acknowledgement:
Bo Sundman, Lars Höglund, Greg Olson, Mikael Lindholm, Anders Engström, Paul Mason, Malin Selleby, Martin Walbrühl, Annika Borgenstam

hero-m

ROYAL INSTITUTE OF TECHNOLOGY

Contents

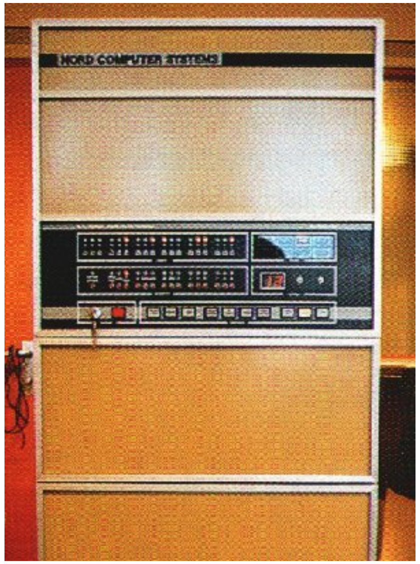
- How it started - late 1970's
  - Student exercises
- Early 1980's
  - New softwares
  - Industrial training
- First course in materials design 1995
- Materials design, Hero-m and quantum metallurgy
- Important issues and Warning

ROYAL INSTITUTE OF TECHNOLOGY

How it started - late 1970’s

1976 the MSE department at KTH procured a Nord-10 16-bit mini computer (the second computer at the KTH campus)

- Dramatic increase in computer capacity at MSE.
- Used in research; CALPHAD and software development
- Used in education; Sundman and Ågren developed the first computer exercises for undergraduate students.
  - Calculation of a binary phase diagram
  - Simulation of microsegregation during solidification of binary alloy



ROYAL INSTITUTE OF TECHNOLOGY

Some unexpected issues in the early days

- Most students disliked computers – thought computers were ridiculous!
- Although students had courses in programming they had never touched a key board prior to the exercise!
- Students could not do much coding themself – the teachers had to spend hours of debugging lousy codes.
- The students did not see the point of the exercises because they had no time to spend efforts on the actual modelling – all efforts were used in coding/debugging.
  - The physical models had to be extremely simple!
- All computer work were performed in time-sharing mode.
  - Response times approached minutes when 30 students were working on the same mini computer.

Attempts to solve the problems

- Students executed codes that were prepared in advance by the teachers.
- Now more complex problems could be handled and some written material about the underlying physics were handed out prior to the exercise.
- But…
  - The concept ”user interface” was hardly known and the students got a list of parameters to input (in the right order and format).
  - The computer exercise became rather meaningless – most of the time spent to make the correct input.
- Result…
  - The students were not likely to understand that computers could play a role in materials science.

Early 1980's

- The situation started to change.
  - Computers became more powerful - faster
  - The newly developed Thermo-Calc with its command interpreter (state of the art) allowed more flexible calculation set-up (possible to correct errors in input)
- But still difficult to use
  - At least several days of training needed to master the user interface
- Nevertheless…
  - It had become possible for the students to define ”their own” problems after learning the basics of the interface.
  - Students could now understand what they were doing!

ROYAL INSTITUTE OF TECHNOLOGY

Industrial training

- In the late 70’s industrial firms started to recognise the potential of the new technology.
- In the early 80’s they wanted to perform calculations ”in-house”.
- A demand for new type of courses grew
  - Practical hands-on with a minimum of theory – emphasis on what type of problems could be solved
  - Typically 1 week training was needed in order to learn how to
    - Calculate various type of phase diagrams
    - Handle calculational difficulties that frequently occured

ROYAL INSTITUTE OF TECHNOLOGY

Meanwhile back in the university…

- Minicomputers (still operating on time-share basis as main frames) became more powerful, less expensive and much more common.
- The university started to make investments in rooms for computer terminals, a common terminal network so one could connect any terminal and computer.
- Both students and teachers started to appreciate the new technology.
- In courses some laboratory practicals were replaced by ”computer practicals”.
  - Less expensive than traditional laboratory work
- The DICTRA code was developed and introduced in the education.

ROYAL INSTITUTE OF TECHNOLOGY

Some lessons learned

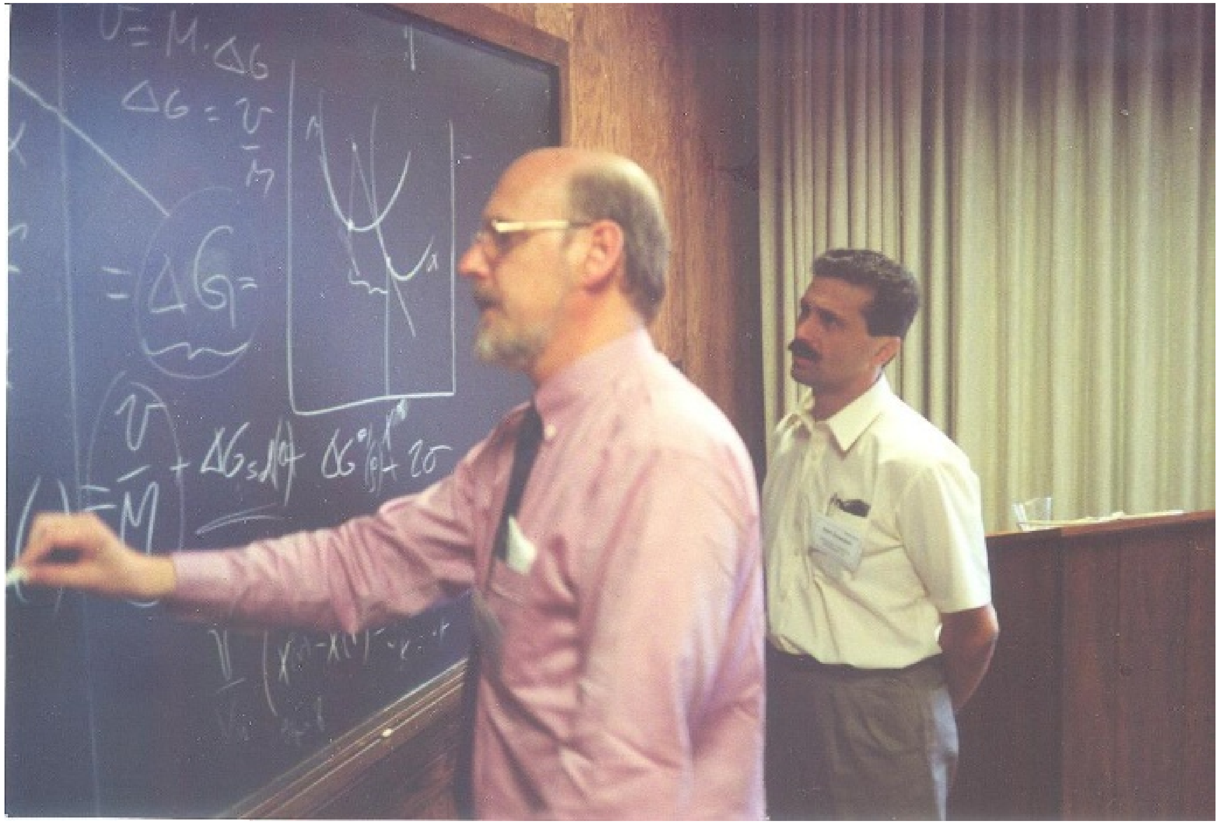
- Traditionally education in thermodynamics and kinetics was given to the students during the first and second year.
- The teachers had no experience of the new CALPHAD technology nor had they experience of modelling and calculations.
  - Such education was of no value for the students
  - It could not serve as a basis for the emerging field of computational thermodynamics
  - In fact it did more harm than good!
- The whole education in thermodynamics needed revision!

However…

- Even though there was a great support for revision of the materials education at KTH there was no common vision of how.
  - Outside the materials field it usually meant to get rid of metallurgy and physical metallurgy and replace it with more chemistry and physics.
  - Unfortunately it was the education in chemistry and physics (responsible for the basic education in thermodynamics and diffusion) that were old fashioned and needed revision.
- The materials education was then revised many times.

ROYAL INSTITUTE OF TECHNOLOGY

- In connection with the CALPHAD conference in Madison 1994 a course in Thermo-Calc and DICTRA was held at Northwestern University.



First course in materials design 1995

- Inspired by Olson's activities at Northwestern University the first course in materials design was launched at KTH 1995 by Mikael Lindholm.
- The format was simple
  - A couple of lectures, mainly about Thermo-Calc and DICTRA
  - A project defined by industry
  - The project performed as team work with a project leader and as final examination; a report as well as an oral presentation.
- The Materials design course became quickly the most popular course in the materials education! It was a modern course using
  - Modern tools
  - Project-based education
  - Industrial collaboration

ROYAL INSTITUTE OF TECHNOLOGY

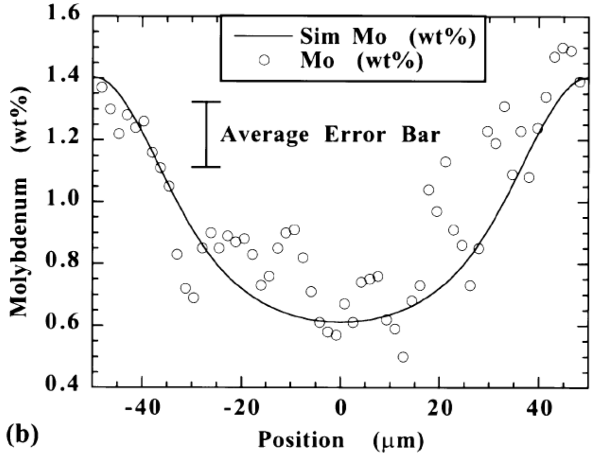
International collaboration: Materials design classes at Northwestern and KTH published in Met Trans 1998

Microsegregation Behavior during Solidification and Homogenization of AerMet100 Steel

H.E. LIPPARD, C.E. CAMPBELL, T. BJÖRKLIND, U. BORGGREN, P. KELLGREN, V.P. DRAVID, and G.B. OLSON

H.E. LIPPARD, C.E. CAMPBELL, Graduate Students, V.P. DRAVID, and G.B. OLSON, Professors, are with the Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208. T. BJÖRKLIND, U. BORGGREN, and P. KELLGREN, Students, are with the Division of Computational Thermodynamics, Royal Institute of Technology, Stockholm, Sweden S-100 44.

Manuscript submitted January 22, 1997.



(b)

Further in history…

The first separate course in DICTRA was given at the NKK Steel company in Japan 1995. Teachers: Anders Engström, Lars Höglund and John Ågren.

KTH VETENSKAP OCH KONST
ROYAL INSTITUTE OF TECHNOLOGY

- PCs came, terminals disappeared.
- 1997 Thermo-Calc was founded as a commercial company
- The education directed towards professionals in industry as well as PhD students was taken over by Thermo-Calc.
- Now the training courses are offered in Sweden and worldwide.

ROYAL INSTITUTE OF TECHNOLOGY

An important development

- The first industrial course in Thermo-Calc was for a whole week.
- The course offered now is also 1 week but includes Thermo-Calc (2 days), DICTRA (2 days) and PRISMA (1 day).
- Using the graphical interface in Thermo-Calc students have been able to perform advanced thermodynamic and diffusion simulations with no prior experience of the softwares and less than 1h of introduction
  - 2017 ”EIT Raw Materials” financed through Horizon 2020
  - 2019 At Northwestern university

ROYAL INSTITUTE OF TECHNOLOGY

Materials design, Hero-m and quantum metallurgy

- As a result of another reorganization KTH changed the name of its education in Materials to “Materials Design” 2003.
- Around 2000 the MSE department at KTH started to build up competence in DFT and Ab-initio calculations when Börje Johansson was appointed guest professor at KTH.
- Initially there were a competion between DFT and CALPHAD but it was soon realized that both sides need each other.
  - If CALPHAD had not been invented it had to be invented now!
- The Hero-m center was launched in 2007
- The initial aims were to develop the tools for materials design based on ICME.

ROYAL INSTITUTE OF TECHNOLOGY

- A course in DFT for metallurgists was developed: ”Quantum Metallurgy”.
- DFT is now an important part of the Materials design course.
- But DFT is taught as an engineering tool rather than as quantum mechanics.

Important issues

- Softwares are now so easy to use that students may concentrate on the true engineering or scientific issues.
- Important that students learn to master many tools:
  - CALPHAD including diffusion
  - High level calculations of heat flow and mechanical behaviour by means of FEM
  - DFT and Ab-initio MD
- They should also learn how the tools are connected.
- But... they have to master them as tools, i.e. they should understand what type of engineering problems each tool is good for without knowing all subtle scientific details.

ROYAL INSTITUTE OF TECHNOLOGY

Warning

- The dramatic sucess of computations has killed a lot of experimental activities
  - Computations are easier
  - They can be performed on office hours
  - They are inexpensive
- But experiments are important and
  - In the best of worlds computations guide us to do the most precise experiments.
  - In the worst case calculations replace experimental work.
- We thus have to emphasize for the students that computations can never replace experimental work.
  - They are just another tool to support materials engineering.
- A Myth: A more primitive user interface gives the students a deeper understanding. Not true!
  - The deepest understanding is obtained using a slide ruler!?

ROYAL INSTITUTE OF TECHNOLOGY

Thermo-Calc Educational material available (free) for download at https://www.thermocalc.com/academia/teachers/educational-package-for-teaching/