Computational Methods for Building Physics and Construction Materials

CMBPCM Course 2024
April, 8 – 12

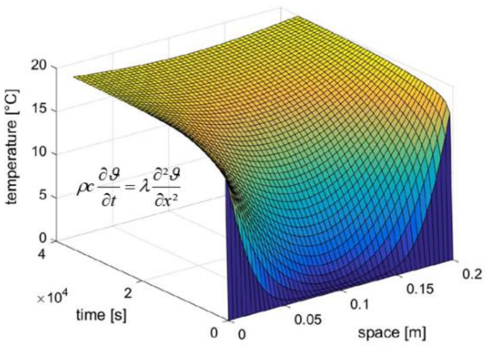
RILEM EAC Evaluation report

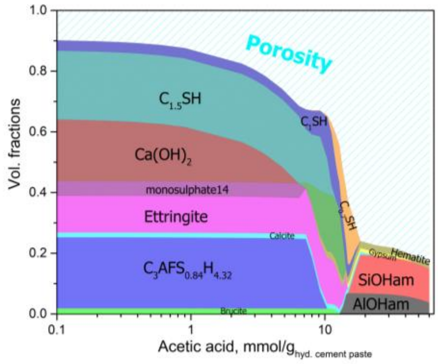
Main organizer:
Institute of Construction and Building Materials,
Technische Universität Darmstadt, Germany

Venue:
Hybrid course

Institut für Bauforschung und Lehrstuhl für Baustoffkunde

INSTITUT FÜR WERKSTOFFE IM BAUWESEN





Computational Methods for Building Physics and Construction Materials

TU Darmstadt
May 16, 2024

unite! University Network for Innovation, Technology and Engineering

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TECHNISCHE UNIVERSITÄT DARMSTADT

RWTH AACHEN UNIVERSITY

Subject: Evaluation report CMBPCM course 2024
Purpose: RILEM EAC feedback
Date report: 16-05-2024
Authors: Prof. E.A.B. Koenders / Dr. N. Ukrainczyk / M.Sc M. Löher / M.Sc M. Mayer / Prof. Th. Matschei (RWTH Aachen) / F. Georget (RWTH Aachen)

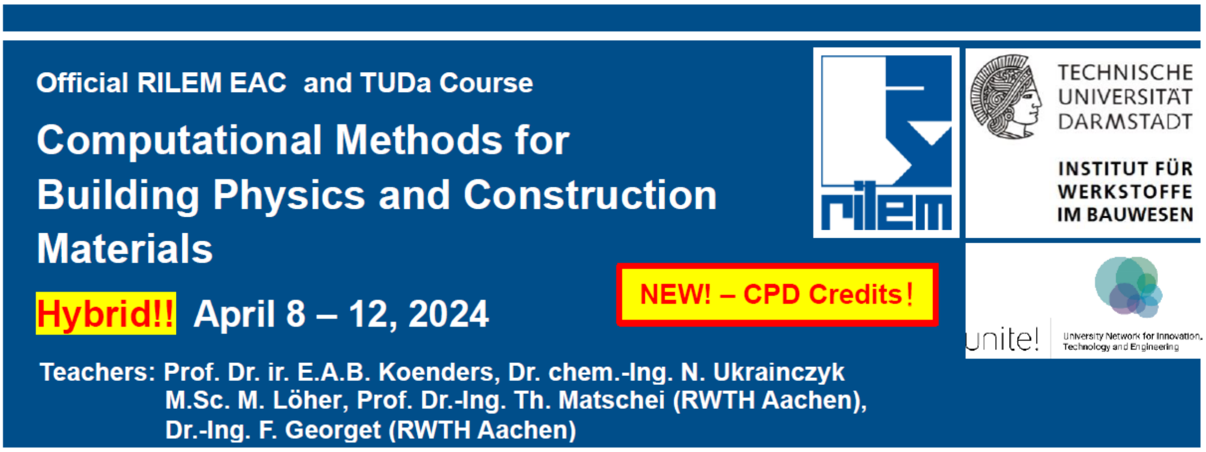


Figure 1: Hybrid course organized by the Institute of Construction and Building Materials of the TU Darmstadt in conjunction with the Institute of Building Materials of the RWTH Aachen.

1. Course objective:

This year, the RILEM EAC course “Computational Methods for Building Physics and Construction Materials” was organized again as a hybrid course and provided both online attendance and participation at the TU Darmstadt (Figure 1). The course was organized by the Institute of Construction and Building Materials of the Technical University of Darmstadt, in conjunction with the Institute of Building Materials of the RWTH Aachen, and was this year again supported by RILEM and the European university network on innovation, technology and engineering UNITE!. The main objective of the course is to teach PhD, MSc and/or post-doctoral students, the basic principles of computational methods that can be employed for solving differential equations that are common in building physics and construction materials. This year, for the second time the lectures on Friday were on thermodynamic modelling of cement in the morning, and high performance computing in the afternoon. For the whole course, emphasis was on numerical solution strategies with Excel and Octave as programming platform, explicit and implicit discretization for the finite difference method, method of lines, boundary conditions and implementation strategies of physical temperature and moisture processes, and kinetics and thermodynamics of cement hydration processes that frequently occur in construction materials and finally an introduction to high performance computing. Typical problems addressed in this course are transient heat transport and chloride diffusion problems, multi-layer systems, coupled moisture – heat systems, whereas also the particle structure kinetics and thermodynamics of cement hydration were addressed. In total, the course was structured as a 5 full day (intensive) program, by teaching every day a different

Figure 2: Lecture room at the TU Darmstadt.

aspect of computational modelling. In the morning sessions theoretical lessens were provided (Figure 2) and in the afternoon demonstration and exercise sessions (see Appendix 1).

The course teachers were Prof. Eddie Koenders, Dr. Neven Ukrainczyk, M.Sc Max Löher, M.Sc Maximilian Mayer, Prof. Thomas Matschei, and Dr. Fabien. Georget, where the first four are from the Technical University of Darmstadt and the last two of Institute of Building Materials of the RWTH Aachen. At the end of the course students were asked to fill out a course evaluation form of which the results are attached in Appendix 2. After the course, a RILEM certificate of attendance was sent to each student individually. As the course is also an officially registered TU Darmstadt Master course it has a value of 6 ECTS credit points. With this, all students who attended this CMBPCM course could also opt for these credit points, and use it e.g. for their graduate school program. However, for this they have to comply with the course requirements, meaning they have to pass the homework exercise and the exam organized by the TU Darmstadt.

2. Course program:

The course program (see appendix 1) was designed in such a way that the core lectures addressing theoretical backgrounds on computational modelling were scheduled in the morning, while the demonstrations and exercise sessions were scheduled in the afternoon. However, due to the extended lectures on Friday, this concept was adapted a bit, by having the demonstrations and exercises directly packaged (see appendix 1). In general, this concept was very successful and appreciated by the students.

The used software was Microsoft Excel, the freeware program called Octave, the Lite version of Hymostruc, the student edition of WuFi and the GEM-Selektor. Along with these software programs, specially prepared programming codes, made by the teachers, were provided as part of the lecture material. The basic idea of the course is that after successful attendance of the course, students learned how to use this software and understand the provided codes which they can employ for their personal research interests and/or future modelling developments.

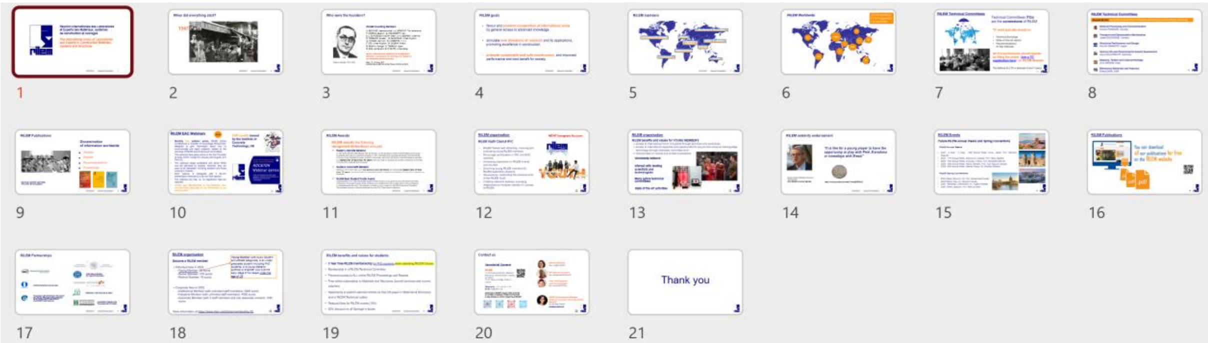


Figure 3: PPTs presented to introduce RILEM 2024.

The course started on Monday, early morning, by Prof Koenders, with an introduction of RILEM (Figure 3) followed by presentation of the university network UNITE! (Figure 4) and finally, a presentation of the course program and introducing the teachers. After that the official part of the course started. First, the basics of schematization and discretization were explained by Prof. Koenders, followed by the explicit discretization method for steady state problems and how to implement this in Excel. Main focus was on a cantilever and common bending beam with different types of loading, followed by an explicit schematization of a transient heat diffusion problem implemented in Excel as well. In the afternoon demonstrations were provided

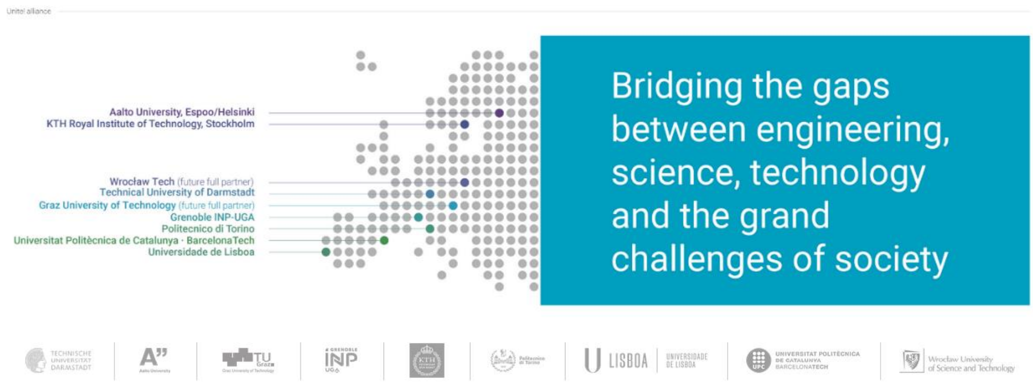


Figure 4: The European University UNITE!

starting with an introductory lecture on Octave followed by the explicit heat diffusion problem and implementation in Octave (Dr. Ukrainczyk). Finally, an exercise on chloride diffusion modelling was presented, schematized and implemented in Excel (M.Sc Löher).

On Tuesday morning, the course continued with the implicit method for solving system of (discretized) algebraic equations implemented in Octave by Dr. Ukrainczyk (Figure 5). First, the focus was on of Laplace's and Poisson's (steady-state) ordinary differential equations (ode), followed by the transient heat diffusion problem, implementing backward Euler and Crank-Nicolson discretization schemes in diagonal sparse matrix representations. After that the schematization and implementation of various boundary conditions, namely the Dirichlet, the Von Neumann and the Robin boundary conditions, and multi-layer systems in Octave was explained. In the afternoon, a demonstration on transient problems was lectured along with an example on the implementation of heat diffusion through a multi-layer system.

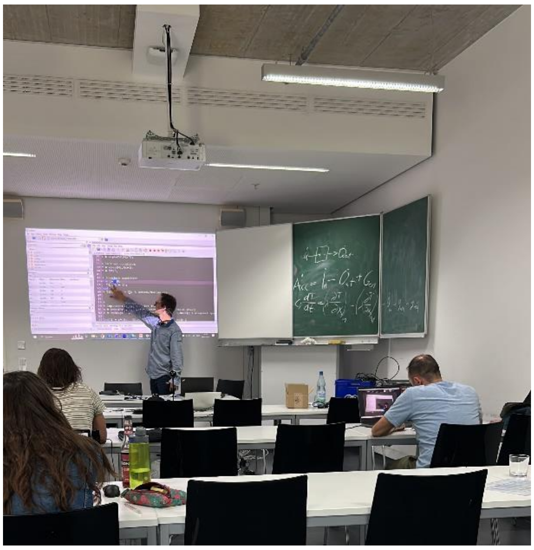


Figure 5: Dr. Ukrainczyk lecturing the course (Photo 2023).

On Wednesday morning the course continued with lectures by Dr. Ukrainczyk. First, the theory behind higher order (e.g. Runge-Kutta) discretization was presented, followed by strategies on how to deal with non-linear ordinary and partial differential equations (*ode* and *pde*). Advanced time integrators were presented for various types of time-based solution methods for stiff *ode* and *pde*. Method of Lines (MoL) was provided as well, demonstrating the powerful and easy to use time integrator tools readily available in the Octave toolbox. The theoretical part also considered a critical overview of all different methods learnt, systematically comparing their pros and cons, and concluding with a clear recommendation on which method one could use best, depending on the modeling case and its specific characteristics, such as: discretization size, desired accuracy, flexibility to adapt the code, computational cost/speed and ease of implementation. After that, an introduction to coupled *pde-ode* and *pde-pde* systems was lectured. The coupled system, which requires a predictor-corrector solution strategy, was explained in detail, along with two example implementations on heat-chemical reaction and heat-moisture demonstrated in Octave in the afternoon. The afternoon was also used to demonstrate implementation of advanced time integrators and Method of Lines examples in

Octave. The last lecture of the day was an exercise of a coupled heat-moisture problem conducted with the commercial software WuFi. The software was explained and a typical heat-moisture problem was demonstrated by M.Sc Mayer.

On Thursday morning the course continued with hydration modelling by Prof. Koenders, starting with a lecture on particle structure generation for cement/binder based systems. The lecture is on providing the students insights on how to setup a basic particle structure that complies with the particle grading and water/binder ratio of binder systems and forms the starting point for hydration kinetics modelling, which was the next lecture, provided by Dr. Ukrainczyk. This lecture was on how to model the volume changes and rate of hydration driven by the chemical cement reactions. Main hydration rate mechanisms are introduced for single particle dissolution, nucleation and diffusion, followed by theory on integrated multi-particle (Hymostruc) approach. In the afternoon, Dr. Ukrainczyk (Figure 6) demonstrated how this theory can be implemented in Octave and showed a few examples on the developed basic cement hydration model as well as on how to generate and visualize 3D particle structure. The last lecture was on an example and demonstration with the software Hymostruc Lite, provided by Prof. Koenders (Figure 6). During this demonstration lecture the model possibilities and simulation options were explained and the graphical output and 3D visualizations demonstrated, while also the output possibilities of the model were shown.

Figure 6: Prof. Koenders and Dr. Ukrainczyk lecturing the course (Photos 2022/2023).

Also this year, the lectures on Friday were the renewed lecture + demonstration on thermodynamic modelling in the morning and a lecture on high performance computing + demonstration in the afternoon. The lecture on thermodynamic modelling of cement-based systems was provided by Prof. Matschei, followed by a demonstration lecture on the implementation of this theory using the GEM-Selektor by Dr. Georget (Figure 7). Both these lectures are considered a logical and more in-depth continuation of the lectures provided on

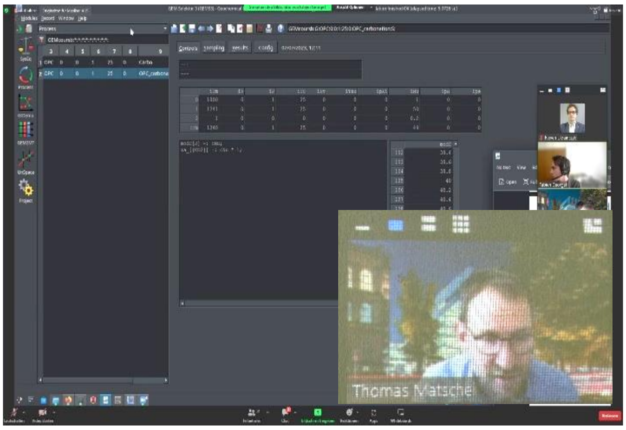


Figure 7: Left: GEM-Selektor demonstrated by Prof. Matschei (insert) and Dr. Georget. Right: M.Sc Löher lecturing High Performance Computing.

Thursday (Koenders/Ukrainczyk). In the afternoon the last lectures of the course were on high performance computing (HPC) provided by M.Sc Löher. The lecture was on the theory of high-performance computing systems and how they can be employed for solving large numerical problems. After that, M.Sc Löher provided a demonstration lecture on the possible accelerations of various CPU cores and GPU usage for a HPC compared with regular computer systems like desktop and laptop. A benchmark was demonstrated and discussed.

3. Number of persons:

The official number of registered participants for the full online CMBPCM course was 33 (excluding teachers), 32 full week students and 1 for two days. From these students were 8 PhD student, and 16 were from the UNITE! University network.

4. Target group:

The target group was as expected, i.e. Master students predominantly from TU Darmstadt and UNITE! partner universities, as well as mostly PhD students, a few Postdocs, and one Professor. The course structure enables all educational levels to learn from the provided content.

5. Country of participants:

The attendees of the CMBPCM course were from 12 different countries. From these, Finland 8x, UK 1x, South Korea 2x, France 2x, Germany 10x, Dubai 1x, Singapore 1x, Brazil 1x, Morocco 1x, Switzerland 1x, Norway 2x, Denmark 1x. The students who registered via the TU Darmstadt system were from various countries and enrolled in international student programs.

6. Teachers:

The teachers of the course were: Prof. Dr. Eddie Koenders (TU Darmstadt, course responsible), Dr. Neven Ukrainczyk (TU Darmstadt, senior lead scientist), M.Sc Max Löher (TU Darmstadt, junior scientist) and M.Sc Max Mayer (TU Darmstadt, junior scientist), Prof. Dr. Thomas Matschei, (RWTH Aachen, Institute Director) and Dr. Fabien Georget (RWTH Aachen, senior scientist). All teachers showed professional skills and provided inspiring lectures to the students during the theoretical morning sessions as well as during the practical demonstration and exercise sessions in the afternoon. The different backgrounds of the teachers, i.e. Building Engineer, Chemical Engineer, Mechanical Engineer and a wide research and educational experiences of all teachers provided a wide and comprehensive program of lectures, demonstrations and exercises, and presented a broad vision on the various aspects of computational modelling and implementation to the students.

7. Frequency and co-organization:

The CMBPCM course is an annual EAC supported RILEM Educational Course and an official TU Darmstadt course, which was this year organized for the eighth consecutive time, and was for the second time successfully organized as a hybrid course. Next year the CMBPCM course will be organized again by the Institute of Construction and Building Materials.

8. Date:

The course will be organized every year in the spring. The date for the next year CMBPCM course will be in or around the second week of April 2025. The next course will again be organized as a hybrid course. For this, an updated teaching schedule is expected.

9. RILEM support:

RILEM guidelines are complied with and a presentation about RILEM was provided during the introduction session of the course, which was given by Prof. Koenders. Students are informed about the RILEM activities and also about the three-year free membership for PhD students.

10. Flyer:

A flyer has been made in paper and PDF form and was distributed actively among potential participants as well as via the RILEM website, the TU Darmstadt website and other online platforms (Appendix 3).

11. Evaluation:

After the course, students were asked to fill in an evaluation form. The results of this evaluation will be used to improve the course for the forthcoming year. An overview of the results is shown in Appendix 2.

APPENDIX 1

Course program 2024

Program of the CMBPCM 2024 course

CMBPCM	Time	08. Apr 24 Monday	09. Apr 24 Tuesday	10. Apr 24 Wednesday	11. Apr 24 Thursday	12. Apr 24 Friday
	8.45 - 9.00	**Welcome - introduction RILEM and UNITE!**				
Lectures	9.00 - 10.15	**V1** Introduction schematization and discretization	**V5** Transient implicit implementation in Octave	**V9** Advanced time integrators and coupled systems	**V13** Particle structure schematization for cement microstructures	**V17** Thermodynamic (TD) modelling of cement hydration
Lectures	10.15 - 10.45	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
Lectures	10.45 - 12.30	**V2** Transient discretization problem, explicit method in Excel	**V6** Implementation of boundary conditions and multi-layer systems in Octave	**V10** Transient heat-moisture systems, implementation in Octave	**V14** Cement hydration kinetics theory	**V18** Demo + Exercise: GEM-Selektor for TD hydration modelling
	12.30 - 13.30	Lunch break	Lunch break	Lunch break	Lunch break	Lunch break
Demos	13.30 - 15.30	**V3** Demo on Octave and explicit transient implementations	**V7** Demo on implicit transient implementations	**V11** Demo on coupled heat moisture systems Octave/WUFI	**V15** Demo hydration in Octave and Hymostruc	**V19** High Performance Computing
	15.30 - 16.00	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
Exercise	16.00 - 17.30	**V4** Exercise: Chloride diffusion explicit excel/Octave	**V8** Exercise: Heat diffusion in a multi-layer wall in Octave	**V12** Exercise: Heat-moisture problem in Octave/WUFI	**V16** Exercise: Cement hydration in Octave/Hymostruc	**V20** Demo + Exercise: High Performance Computing

Teachers	
(dark blue)	Prof. Koenders
(light grey-blue)	Dr. Ukrainczyk
(yellow)	Dr. Ukrainczyk/Dr. Mankel
(light teal)	Prof. Matchei/Georget
(bright blue)	MSc. Löher

APPENDIX 2

Evaluation results CMBPCM 2024

Online Evaluation Questions and Results CMBPCM 2024

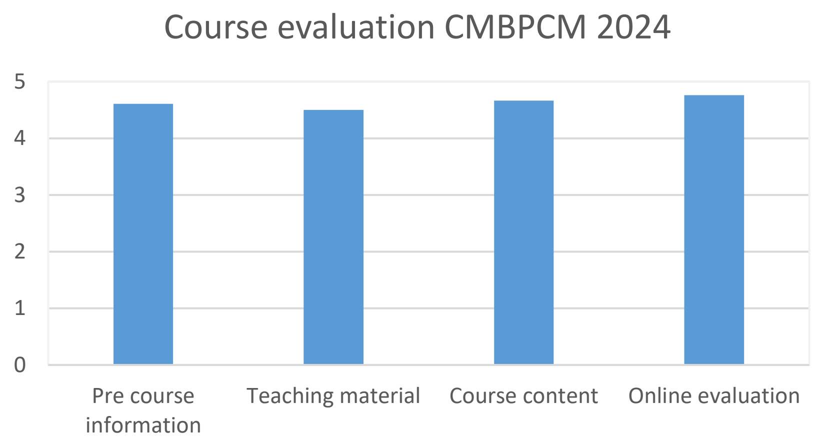
Questions asked:

Pre-course information:
Was the pre-announcement (flyer) of the course clear enough?
Was the E-mail contact appropriate?
Was the registration form appropriate?
Was the (RILEM) Website information appropriate?

Teaching material:
Providing PDFs of the lecture notes was sufficient?
Quality of the lecture notes?
Quality of the exercises?
Quality of the demonstrations?

Course content:
What is your opinion about the quality of the lectures in general?
What is your impression about the quality of the whole course?
Was the teaching level appropriate?

Online evaluation:
Was the quality of the online platform sufficient?
The possibility for asking questions was enough?
Were the questions satisfactory answered?
Would you be interested in an advanced course?
Offering streaming of the recordings for one week after the course is a good idea?



(Average results of 10 students, with 5 = the highest grade)

APPENDIX 3

Flyer 2024

Official RILEM EAC and TUDa Course

Computational Methods for Building Physics and Construction Materials

Hybrid!! **April 8 – 12, 2024**

NEW! – CPD Credits!

TECHNISCHE UNIVERSITÄT DARMSTADT

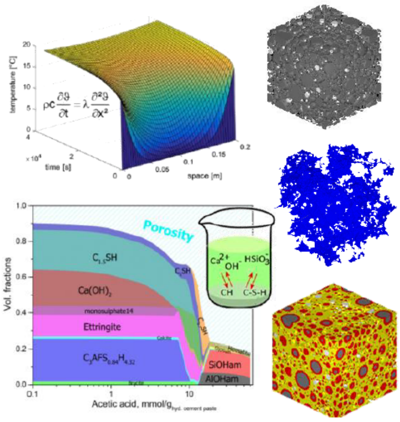
INSTITUT FÜR WERKSTOFFE IM BAUWESEN

unite! University Network for Innovation, Technology and Engineering

Teachers: Prof. Dr. ir. E.A.B. Koenders, Dr. chem.-Ing. N. Ukrainczyk
M.Sc. M. Löher, Prof. Dr.-Ing. Th. Matschei (RWTH Aachen),
Dr.-Ing. F. Georget (RWTH Aachen)

Course description:

The course contains detailed lecturing on computational methods covering differential equations, numerical solution strategies, explicit and implicit discretization, Method of Lines, boundary conditions and implementation of physical processes that frequently occur in construction materials. Emphasis will be on the Finite Difference Method applied to transport processes in porous construction materials, such as concrete and insulation materials, and on hydration modelling. Typical problems that will be addressed are thermal, moisture and reactive transport modelling, multi-layer systems, coupled moisture - heat systems, cement particle structure, hydration kinetics and thermodynamic modelling, and the first steps towards high performance computing. The course provides a full solution strategy, starting from a physical problem, to schematization and discretization, to boundary conditions evaluation, implementation and to a computational solution.



Key topics:

- Steady state problems – discretization and implementation in Excel
- Transient problems – explicit & implicit heat and moisture flow – implementation in Octave
- Coupled and multi-layer systems for heat and moisture flow, discretization and implementation in Octave
- Particle structure formation and hydration kinetics of cementitious systems
- Thermodynamic modelling of cement hydration with GEM-Selektor
- High Performance Computing for large multi-core systems
- Demonstrations and exercises with examples for all topics

Course program:

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	15.30 - 16.00	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
Exercise	16.00 - 17.30	V4 Exercise: Chloride diffusion explicit excel/Octave	V8 Exercise: Heat diffusion in a multi-layer wall in Octave	V12 Exercise: Heat-moisture problem in Octave/WUFI	V16 Exercise: Cement hydration in Octave/Hymostruc	V20 Demo + Exercise: High Performance Computing