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May 30th – June 2nd, 2023
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**Book of Abstracts**

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## Neural network based coupling of CALPHAD and the FEM in thermo-chemo-mechanical calculations

**Roth, Stephan** *(TU Bergakademie Freiberg, Germany)* 16:40
**Zienert, Tilo** *(TU Bergakademie Freiberg, Germany)*
**Kiefer, Bjoern** *(TU Bergakademie Freiberg, Germany)*

Modeling thermo-chemo-mechanical coupling is of increasing interest in the investigation of processes such as stress corrosion cracking, hydrogen embrittlement, etc. Phase-field models that capture, e.g., diffusion, degradation, and phase-transformations, require the formulation of the chemical energy as a contribution to a total potential to be minimized in a variational framework [1]. The chemical energy, as a function of composition and temperature, can be incorporated using the CALPHAD method, either by direct implementation of the CALPHAD model with known parameters from databases or by calling an external CALPHAD software such as Thermo-Calc. In finite element (FE) simulations, the latter approach neccessitates a coupling of FE software to CALPHAD software, since the state potential has to be calculated in each integration point of the model, for each solution increment. In order to avoid sequential calls of external CALPHAD-software, which would drastically increase the overall computation time, here a numerical approach based on neural networks (NN) is proposed. The idea is to train the neural network with CALPHAD data such that the NN represents the chemical energy in relatively wide ranges of composition and temperature. The trained NN can then be included as a Fortran code to the computational framework and provides the chemical energy as well as its derivatives without any external software. The latter is only required for providing the training and validation data needed to calibrate the NN. Here, we specifically make use of the free Python library ffnet [2]. The procedure is demonstrated and verified by the example of a simple Ag-Au-diffusion couple with well defined chemical energies. The comparison between a direct and the NN-based implementation is drawn, demonstrating the quality of the proposed approach. Finally, the applicability to more complex multi-component, multi-phase problems, see [3], is addressed.

[1] B. Svendsen, P. Shanthraj, and D. Raabe. Finite-deformation phase-field chemomechanics for multiphase, multicomponent solids. JMPS, 112:619-636, 2018.
[2] M. Wojciechowski. ffnet 0.8.3, `https://ffnet.sourceforge.net/`.
[3] A. Seupel, S. Roth, and B. Kiefer. Phase-field modeling of chemically reactive multicomponent/multi-phase systems. PAMM, 10.1002/pamm.202200154, 2022.

## A FEM-PD coupling based on an Arlequin approach to impose boundary conditions in Peridynamics

**Pernatii, Anna** *(Otto-von-Guericke Universität Magdeburg, Germany)* 17:00
**Gabbert, Ulrich** *(Otto-von-Guericke Universität Magdeburg, Germany)*
**Willberg, Christian** *(German Aerospace Centre (DLR) Braunschweig, Germany)*
**Hesse, Jan-Timo** *(German Aerospace Centre (DLR) Braunschweig, Germany)*

The peridynamic approach (PD) is a continuous theory that is well suited for solving damage problems. Because of the non-local formulation, PD can predict the response of a material and fracture patterns with high probability in high dynamic processes. In PD, some parameters differ from the continuum formulation and have some deviation in discretized PD systems, such as a horizon. A material constant becomes a parameter dependent on the mesh

size.
A sticking point, which has to be considered, is that an incomplete horizon at the boundaries results in an unphysical variation of the material's stiffness in these regions. Material points at the boundaries do not have an entire non-local neighborhood, meaning the points have fewer bonds and are softer than points within the domain. This leads to the so-called surface effect. The difficulties in applying the classical local initial and boundary conditions happen because of the non-local character of the PD. To overcome this problem, several correction techniques have been developed. Nevertheless, a standard method to describe them is not available yet.
An alternative approach is the application of the earlier proposed FEM-PD coupling, which can be seen as a local-nonlocal coupling method. The damage-free zones are analyzed by the FEM as classical local theory, while the domain where the fracture is expected is modeled with the PD as a non-local theory. Consequently, the reduction of the computational effort as well as the imposing of the conventional local boundary conditions, is achieved. The coupling method is based on the Arlequin method - an energy-based procedure where the energy of a system is found as a weighted average of both systems. The mechanical compatibility in the overlapping zone of both domains is reached by implementing constraints with the help of the penalty method. In the paper at hand, the focus is on imposing BCs. The proposed method is applied to both static and dynamic applications. The accuracy and convergence behavior is evaluated by analyzing test examples.

## Adaptive time integration for dynamic problems in the Theory of Porous Media using an EVI-formulation

**Sunten, Julia Nicolina** *(University of Duisburg-Essen, Germany)* 17:20
**Schwarz, Alexander** *(University of Duisburg-Essen, Germany)*
**Bluhm, Joachim** *(University of Duisburg-Essen, Germany)*
**Schröder, Jörg** *(University of Duisburg-Essen, Germany)*

In classical binary (Solid and Liquid) dynamic Theory of Porous Media (TPM) formulations, two dependent factors influence the numerical efficiency: The number of unknown quantities and the choice of the time integration scheme. Following the approach of Diebels and Ehlers in [1], the disadvantage of ten scalar unknowns ($U_{DE} = \{u_S, v_S, w_{LS}, P\}$, Solid displacement, Solid velocity, difference velocity, pore pressure) is compensated by the full range of possible time integration schemes as the relations $u'_S = v_S$ and $u''_S = v'_S$ can be treated by any implicit time integration method. On the other hand, the approach of Breuer in [2] only requires seven scalar unknown quantities ($U_B = \{u_S, w_{LS}, P\}$), but depends on the existence of a time integration method which is able to determine the second material time derivative of the Solid displacement. To overcome this dependency drawback Chen et al, see [3], presented the idea of an EVI-formulation (Embedded Velocity Integration), where the unknowns are $U_{EVI} = \{v_S, w_{LS}, P\}$. The Solid displacement is now determined as the temporal integration and the acceleration as the temporal derivative of the Solid velocity. This contribution presents the idea of [3] and combines it with an adaptive explicit singly diagonally implicit Runge-Kutta scheme, see [4], which was already used for TPM problems in [5]. Thereby a maximum of numerical