CMM-SolMech 2022 conference

S11 Particle-based methods in computational mechanics

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INVESTIGATION OF THE BEHAVIOR OF INTACT AND CRACKED STEEL PLATES UNDER STATIC AND DYNAMIC LOADING

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In this study, the behavior of intact and cracked steel plates under static and dynamic loading is investigated using the non-local method. The pre-existing cracks on the plates are considered five different orientations including center crack, inclined center crack, single edge crack, double edge crack, and inclined edge crack. Also, the energy released rate criterion is applied to accurately predict the crack growth. As a result, the impact of initial crack orientation, crack growth, loading conditions, and the length of horizon on the behavior of the plates are evaluated. The non-local relationships are applied to the equation of motion and the principle of virtual work is employed to solve the associated Lagrange's equation. Moreover, the mass of the material points is obtained and plugged into the developed Newton's equation, which subsequently extracts acceleration values at the material points. In the next step, the velocity and displacement of different material points are specified by integrating the equation of motion. It is also determined that the model accuracy would be further improved if the length of horizon function is closer to 0.0001 m. Besides, the proposed analysis confirms that by increasing the number of material points from 50 to 500, the accuracy of the crack branching was considerable improved. Furthermore, the present study shows that the lowest and highest load capacity are related to the plates with double edge crack and single edge crack, respectively. It is also proved that as the crack angle increases, the plate load carrying capacity under combined tensile and shear edge loading was improved. The results of the non-local method are compared with the closed formed analytical solutions, as well as the finite element method (FEM), and extended FEM (XFEM) showing the high accuracy and robustness of the developed non-local method for predicting the crack growth path, micro-cracks and branching of cracks.

Keywords: Static and Dynamic Loading, Micro-Mechanics, Non-local Method, Material Point.

NUMERICAL MODELLING OF THERMAL PROPERTIES OF PARTICULATE LIGHTWEIGHT COMPOSITES

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Reducing the thermal conductivity of the thermal insulation material is of considerable scientific and technological importance. To meet the demand for energy savings in industrial furnaces, particulate lightweight alumina-silicate-based composites have been used to reduce thermal conductivity. The limited understanding of the microstructure and heat transfer mechanisms in composites imposes restrictions on the design and fabrication of efficient thermal insulation materials. Both the composition and the topology of the microparticles of the composite play a significant role in the achieving of the required thermo-mechanical properties.

The numerical discrete-particle approach combined with the finite method is developed to evaluate the thermal conductivity, and it is applied to the simulation of the particulate lightweight alumina-silicate-based composites containing certain type of microparticles: mullite hollow microspheres (MHM). The proposed technique was adjusted by series of numerical tests and comparison with analytical and experimental data. A detailed numerical thermal analysis was performed to investigate the contribution of individual microparticles and the assembly of microparticles to thermal conductivity.

The thermal conductivity of the porous concrete binder was considered as a benchmark for further thermal analysis. Particular cases of selected samples were solved to discover the heat propagation mode. The modelling concept was demonstrated by particular samples with one, two and more MHM.

Sample No. 1 (S1) with one MHM embedded in a concrete binder included the analysis of Composite 1 (C1) and Composite 2 (C2). Sample No. 2 (S2) with two MHM embedded in a concrete binder included the analysis of Composite 3 (C3). Pore volume fraction (volume of air) of C1, C2, and C3 was 3.35 %, 26.81 %, and 15.08 %, respectively. The thermal conductivity of C1, C2, and C3 has been determined numerically. The numerical results have been compared with the theoretical predictions.

The preliminary results revealed a relationship between the pore volume fraction and the thermal conductivity: a higher pore volume fraction resulted in lower thermal conductivity of the composites. Therefore, the developed numerical tool may be suitable to evaluate the correlation between the microstructure of composites and thermal conductivity.

PERFORMANCE OF THE THERMAL DISCRETE ELEMENT METHOD IMPLEMENTED ON SHARED-MEMORY ARCHITECTURES

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Discrete element method (DEM) [1] can offer advanced models to represent microstructure and complex micromechanical behaviour of materials. Concept of the DEM presents numerical methodology, providing quantitative description of granular media by considering motion and deformation behaviour of individual particles in the frame of Newtonian mechanics. Nowadays DEM is acknowledged to be an effective procedure extended to cohesive powders, fracture and multi-physics. However, long computational time of DEM simulations limits the analysis of industrial-scale applications. Parallel computing has become an obvious option for increasing computational capabilities of the method. The emergence of general purpose GPU computing seems to offer the good possibility to simulate large-scale DEM applications [2].
The non-cohesive particle models for granular flows, the bonded particle model (BPM) for material fracture and the thermal discrete element model (TDEM) for thermal fields are often used to solve various applications. The considered DEM models are implemented in the OpenCL code for shared-memory GPU and CPU architectures to reduce computing time. The quantitative comparison of TDEM computational performance with that of various DEM models is presented for shared memory architectures. The performance measured on NVIDIA Tesla P100 GPU is compared with that attained by running the same OpenCL code on IntelXeon E5-2630 CPU with 20 cores. The performance analysis reveals that a relatively high CPU to GPU speedup ratio up to 7.4 has been achieved. The DEM models, performing the operations and storing the results in the data arrays of the bonds or contacts between the neighbouring particles, require a large amount of memory and long computing time. The presented implementation of the TDEM increases the used memory and the computing time of the BPM model up to 33.8% and 30.6% of the memory and the execution time of the simplest GN model, respectively, which is an acceptable increase in the computational resources required for modelling the additional coupled field.

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MODELLING OF FLUID FLOW IN POROUS MATERIALS USING A DEM-BASED NOVEL COUPLED THERMO-HYDRO-MECHANICAL MESOSCOPIC APPROACH

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Most of the physical phenomena in engineering problems occur under non-isothermal conditions. Moreover, even if the physical system is initially in a state of thermodynamic equilibrium, the physical phenomena or chemical reactions that occur may lead to local temperature changes and consequently to heat transfer. Therefore, understanding heat transfer in particulate systems is of great importance to many engineering applications such as environmental science, chemical and food processing, powder metallurgy, energy management, geomechanics and geological engineering. The need to consider the effect of heat transfer becomes critical in analyses of many multi-field problems in porous and fractured materials. The heat transfer may occur e.g. by diffusion, advection and radiation. Complex coupled thermal-hydraulic-mechanical (THM) processes, including heat transfer, fluid flow and material deformation simultaneously occur and are affected by many non-linear processes.

A novel DEM-based pore-scale thermo-hydro-mechanical model of two-phase fluid flow ([1] and [2]) combined with heat transfer in non-saturated porous materials of very low porosity for fracture propagation is presented. Numerical calculations were carried out for bonded granular specimens with a 3D DEM fully coupled with 2D CFD (based on a fluid flow network) and 2D heat transfer that linked discrete mechanics with fluid mechanics and heat transfer at the meso-scale. The heat transfer was related to both the fluid (diffusion and advection) and bonded particles (conduction). The coupled thermal-hydraulic-mechanical (THM) model was validated by comparing the numerical results with the analytical solution of the classic 1D heat transfer problem. Bonded particle assemblies with two different grain distributions were considered. Perfect accordance was obtained between numerical and analytical outcomes. In addition, the effects of advection on the cooling of a bonded particle assembly were numerically shown. Finally, the relevance of the THM model was shown in a thermal contraction test wherein fracture was taken into account in a bonded particle assembly.

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DEM SIMULATION OF THIN ELASTIC MEMBRANES FOR GRANULAR JAMMING APPLICATIONS

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In this work we present a simulation model for the interaction of a granulate and thin elastic membranes. A common approach to solve this coupled problem is to map the dynamics of the membrane to a mass spring system. This enables a purely particle based description and the dynamics of both, the granular particles as well as the membrane can be resolved by means of the discrete element method (DEM). However, this approach entails two significant problems: The amount of the particles which is needed to model the membrane, as well as the size and relative distances of these particles strongly depend on the interacting granulate. Furthermore, the particle representation leads to artificial roughness of the membrane. We resolve these limitations by introducing polygonal wall elements to detect the contacts between the membrane and the granulate. This allows to choose the number of nodes in the mass spring system purely based on the desired membrane characteristics while still providing a closed surface. Additionally the wall elements avoid artificial roughness of the membrane. Our model therefore enables more realistic simulations. Application examples for such systems include the granular gripper and granular jamming beams.

NUMERICAL STUDY OF HEAT CONDUCTION OF SPARK PLASMA SINTERED MATERIALS

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Presented work proposes the comprehensive analysis of heat transfer and thermal conductivity of porous materials manufactured by spark plasma sintering (SPS). Intermetallic nickel aluminide (NiAl) was selected as the representative material. Due to the complexity of the studied matter, the following investigation was based on experimental, theoretical and numerical approaches. The samples were manufactured in different combinations of SPS process parameters - sintering temperature, time and external pressure and next tested by laser flash method to determine the effective thermal conductivity of porous samples. Moreover, the extensive microstructural characterization was performed using scanning electron microscopy (SEM) and micro computed tomography (micro CT) with a special focus on the structure of cohesive bonds (necks) formed during the SPS process. The experimental results of thermal conductivity were compared with various theoretical models results (parallel, Maxwell-Eucken, Landauer) and numerical one. Here, a finite element framework based on micro CT was employed to analyze the macroscopic (ETC, geometrical and thermal tortuosity) and microscopic parameters (heat fluxes magnitude with angle deviation, local tortuosity) for samples with various porosity. The comparison of different approaches of ETC evaluation revealed the necessity of consideration of additional thermal resistance related to sintered necks and located on powder particle contacts. Since the micro CT analysis cannot determine the grain (particle) boundaries, a special methodology/algorithm was implemented to identify the corresponding spots in the volume of FE samples. Such specified finite elements were treated as the resistance phase with lowered thermal conductivity. The algorithm has been verified by simple benchmarks showing a desirable efficiency. To calibrate the new FE approach with experimental results, multiple simulations with various content of resistance phase elements and different values of thermal conductivity of the resistance phase have been performed for each sample. Finally, the Landauer relation has been modified to take into account the thermal barrier of necks and their thermal conductivity depending on sample densification. Modified theoretical and FE models brought updated ETC results, which after comparing with the experimental one reveals satisfied agreement.

DETERMINATION OF THERMAL CONDUCTIVITY OF POROUS MATERIALS MANUFACTURED BY FAST/SPS BY DEM SIMULATION

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Numerical modelling of heat conduction using the discrete element method (DEM) will be presented. Numerical simulations have been performed to determine the effective thermal conductivity of porous materials manufactured by FAST/SPS. Sintered porous media can be considered as sphere particles connected by necks, which are created during the sintering process. Therefore the discrete element method employing bonded spherical particles is a suitable tool to model thermal problems of such systems.

The model discrete element method for heat conduction analysis developed is based on the thermal pipe-network approach. It employs lumped capacitances concentrated at the centres of the particles which are connected by heat-conducting bars (thermal pipes). The governing equations are based on the balance of the rate of heat-storing in the lumped capacitances and rate of heat flow through the pipes, and any other contributions of heat transfer. The effective thermal conductance of the pipe has been determined using the analytical approximation.

The DEM is applied to the simulation of transient heat flow in cylindrical samples built from spherical particles representing NiAl powder particles at a different stage of sintering. The steady-state temperature field is used to determine the effective thermal conductivity from the Fourier law of heat conduction. Numerical results have been validated using own experimental results. Quite a good agreement between numerical and experimental results has been found.

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MERCURYDPM: FAST, FLEXIBLE, PARTICLE SIMULATIONS

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We introduce the open-source package MercuryDPM, a code for discrete particle simulations, that we are developing [1]. It simulates the motion of particles, by applying forces and torques that stem either from external body forces, (e.g. gravity, magnetic fields, etc.) or from particle interaction laws. For granular particles, these are typically contact forces (elastic, plastic, viscous, frictional).

MercuryDPM is an object-oriented C++ algorithm with an easy-to-use user interface and a flexible core, allowing developers to quickly add new features. It is parallelised using both MPI and OpenMP and released open-source under the BSD 3-clause licence. Its developers' community has developed many features, including moving (wearable) curved walls (polygons, cone sections, helices, screw threads, level-sets, nurbs, triangulated, etc.); state-of-the-art granular contact models (wet, charged, sintered, melting, cohesive, etc.); specialised classes for common geometries (inclined planes/chutes, hoppers, etc); non-spherical particles (multisphere, superquadric, bonded particles, deformable clusters); general interfaces (particles/walls/boundaries can all be changed with the same set of commands); liquid droplet/spray models; STL readers for industrial geometries; restarting; visualisation (xBalls and Paraview); a large self-test suite; extensive Doxygen documentation; and numerous tutorials/demos.

For efficiency, it uses an advanced contact detection method, the hierarchical grid. This algorithm has a lower complexity than the traditional linked list algorithm for polydispersed flows, which allows large simulations with wide size distributions.

It also contains a coarse-graining tool: MercuryCG, which is both integrated and usable as a stand-alone tool. Coarse-graining is a novel way to extract continuum fields from discrete particle systems. It ensures by definition that the resulting continuum fields conserve mass, momentum and energy, a crucial requirement for accurate coupling with continuum models. The approach is flexible and the latest version can be applied to both bulk and mixtures; boundaries and interfaces; time-dependent, steady and static situations; and, even experimental data. It is available in MercuryDPM either as a post-processing tool, or it can be run in real-time, e.g. to define pressure-controlled walls.

Finally, MercuryDPM is coupled with the open-source FEM solver oomph-lib via the integrated coarse-graining tool. There are many uses of this coupling (in development), including interaction with elastic bodies, both fully and unresolved fluids, and heterogeneous multiscale coupling.

We will demonstrate the features of the code via several examples including: (wet) highly-polydisperse mixing in a rotating drum, wear on vibrating sieves, and sack filling.

Visit https://mercurydpm.org for more information about MercuryDPM. Training and consultancy is available via our spin-off company MercuryLab (https://mercurylab.org).

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THE PARTICLE FINITE ELEMENT METHOD IN SOLID MECHANICS - ASPECTS ON CONTACT MECHANICS AND PLASTICITY

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The Particle Finite Element Method (PFEM) consists of a standard FEM combined with a repeated remeshing and shape-detection of a cloud of points [1]. It is therefore well suited for the modeling of large material deformations in solid mechanics including material separation, [2], which occur in manufacturing processes. A crucial component in the modeling of such processes is a robust contact model. The remeshing and shape detection schemes developed in the PFEM can be used as contact search and contact meshing techniques. Contact constraints are enforced within contact patch/ contact domain elements. This straightforward and robust discretisation technique does not restrict the use of different enforcement methods, e.g. Penalty, Lagrange Multipliers or an extended approach adding a Nitsche-type contribution [3]. For the use of inelastic material laws, several challenges arise, e.g. the proper treatment of history variables [2]. Within this contribution, PFEM and its application in solid mechanics is presented along with aspects on contact mechanics and plasticity.

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SIMULATION OF ELASTIC WAVE PROPAGATION IN CONCRETE USING DISCRETE ELEMENT METHOD

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Ultrasonic waves are widely used in non-destructive testing (NDT). They are mostly applied to detect and localize damage or determine elastic properties. Concrete elements are extensively used in engineering structures. It is important to check their condition, detect existing damage and prevent its future growth. NDT methods allow condition monitoring and detection of potential threats related to developing defects. For a comprehensive interpretation of results, experimental investigations can be enhanced with simulations of wave propagation using numerical models. The calculations are typically performed in software implementing the finite element method (FEM). Since the discrete element method (DEM) is more suitable for concrete, the consideration of wave simulation in DEM software is justified. Although, there are few works dealing with the issue of simulation of elastic wave propagation in DEM software. The DEM allows computing the motion of a large number of elements. Its main advantage is the high level of detail of the behaviour of each particle (at the aggregate level), without losing macro behaviours (specimen level). The current work is aimed at giving theoretical feedback of the wave problem in Yade software. Moreover, the proposed method is verified by experimental investigation. Research is carried out on laboratory models of concrete plates. Ultrasonic tested specimens are compared with their numerical models to confirm the appropriateness of the application of DEM for modelling elastic wave propagation in concrete.