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NUMERICAL INVESTIGATION OF STIRRING ENERGY FOR VARIOUS EQUIPMENT IN THE METALLURGICAL INDUSTRY

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The mixing phenomenon is very important for different equipment in the metallurgical industry. During the general metallurgical process route (e.g., arc furnace, ladle furnace, and continuous casting), subsequent operations are optimised to reach high productivity and premium product quality. Particularly important are nonmetallic inclusions in the molten steel that need to be removed during the processes to avoid detrimental effects on the final product properties. Also, homogeneous melt temperature is needed in most processing steps for better process control. Thus, these aspects are the basis for the extensive investigation on the role of the process parameters during the optimisation of the production operations.

Due to the difficulties in experimental observations of the features and phenomena such as nonmetallic inclusions or velocity and temperature distributions, the mathematical and numerical modelling approaches are more often used. During the mentioned processes, the most critical phenomena usually occur close to each equipment's walls and are related to turbulent metal flow. The dissipation rate of the turbulences in the melt volume is specified as stirring energy. The value of stirring energy is related to the flow and should be validated for each device in the metallurgical industry as a crucial parameter in the mixing process. The influence of the flow pattern, the value of the maximum and average velocities inside the melt and the geometrical shape of the furnace or tundish is significant on the power required to obtain the best mixing process and on the costs of the operations, which should be reduced. This is also important to further optimise and develop novel stirring devices to obtain the best cleanliness and homogenised properties.

Therefore, this paper presents an in-depth analysis of the turbulence dissipation rate occurring in the liquid metal in different metallurgical equipment based on the advanced numerical calculations from the Computational Fluid Dynamics (CFD) area. The stirring energy for each device is analysed and lined up in accordance with the range of its values. As a result, a better understanding of the mixing phenomenon in each stage of the metallurgical process route is possible, allowing improvement in the cleanliness of the molten steel or aluminium.

APPLICATION OF THE INTERVAL LATTICE BOLTZMANN METHOD IN TWO-DIMENSIONAL ADVECTION-DIFFUSION PROBLEM

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In the paper a two-dimensional lattice Boltzmann model is developed to analyze the advection-diffusion problem during the pressure-driven parabolic Poiseuille fluid flow in a pipe. The gravitational effects are neglected. The velocity profile is the same at any cross section of the pipe. The mathematical model of the problem analyzed is based on the interval version of lattice Boltzmann equations supplemented by the boundary-initial conditions. In the proposed model the standard two-dimensional 9-speed lattice (D2Q9) with wed-node approach is used. The main concept behind this work was to use the directed interval arithmetic to analyze the thermal processes with the use of the uncertainly defined parameters in the mathematical description. In the final part of the paper the numerical examples of two-dimensional heat transfer analysis with the use of the bounce-back boundary conditions are shown.

The approach presented, used to solve the advection-diffusion problems, is novel and in theory as well as in practice it is valuable to develop the interval lattice Boltzmann method. The generalization of LBM allows one to find the numerical solution in the interval form and such information may be important especially for the advection-diffusion problems with the use of the parameters estimated experimentally, for example diffusivity or viscosity coefficient. This type of numbers may also be helpful in interpreting a series of laboratory tests instead of statistical tools. The results of an experiment can be "locked" in a suitable range and calculations can be made for such a new interval parameter. The advantage of interval numbers over fuzzy numbers in such issues is simpler interpretation of results, which are given in the form of intervals.

The application of the interval numbers in numerical solving of differential equations gives the results comparable to sensitivity analysis, but is much less complicated during its implementation. Such analysis shows how the perturbation of input parameters can influence the final results.

DEVELOPMENT OF EFFICIENT ALGORITHMIC SOLUTIONS DEDICATED TO RANDOM CELLULAR AUTOMATA MODELS

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Digital microstructure of material morphology is more often required by complex, multi-scale, full-field numerical models. Generation of such digital material shadow for further use in multi-scale modelling is time-consuming and requires dedicated algorithmic solutions to provide expected results in an acceptable time. Therefore, the developed random cellular automata (RCA) grain growth model is being evaluated within the paper to identify possible algorithmic improvements allowing for faster generation of digital representation of material microstructures. The first analysis indicated that the most time-consuming part of the RCA approach is the neighbour-searching algorithm. Thus, several neighbour-searching algorithms were implemented in the current research and then compared with each other to identify the most effective solution. Particular focus was put on the methods of sorting by dimension, quadtrees, and fixed grids. The time measurements were used first to evaluate the effectiveness of each investigated method. Finally, analysis based on the hardware counters was performed and allowed to gather detailed information on implemented algorithms and revealed potential bottlenecks for further improvements.

NUMERICAL MODELLING OF SINGLE POINT INCREMENTAL FORMING BASED ON 3D PRINTED DIES

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Single point incremental forming (SPIF) is one of the sheet forming processes that, due to its flexibility, is gaining much attention in customized production. In general, in this process, a thin metallic sheet can be shaped by a stylus without the use of any dedicated lower die. However, such an approach limits the range of possible shapes of final products. Therefore, the authors are investigating the variation of the SPIF process with a lower polymer die obtained by 3D printing. The use of 3D printed lower die offers the possibility of developing a method for rapid prototyping of sheet metal parts, which allows obtaining highly complex shapes of the final product quickly and efficiently. Nevertheless, due to the complexity of the forming operation, the computer-aided technology design approach is used in the current study to evaluate both sheet and die behaviour under deformation.

The developed numerical models are based on the explicit finite element formulation, J2 plasticity and Johnson-Cook hardening model. The computational domain is discretized with the shell elements to speed up the computations. Particular attention during the study is put on the interaction between the unprocessed 3D printed die surface and a metallic sheet during forming operation. The work highlights examples of obtained results presenting capabilities of the proposed approaches, additionally supported by experimentally conducted SPIF tests.

MICROSTRUCTURE EVOLUTION ANALYSIS UNDER THERMAL LOADING BASED ON DISCRETE MODELLING METHOD

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Numerical models of welding processes allow to increase productivity and quality of welded joints and minimise the number of experimental trials. Such analysis can be helpful to understand how particular process parameters affect the final microstructure and eventually in-use properties. However, welding is a very complex problem to solve from the numerical point of view as a series of phenomena occurring during the process, such as melting and solidification, weld pool evolution, or generation of the heat-affected zone, have to be taken into account. Therefore, the subject of this paper is a comprehensive simulation of welding operation from macro- and microscale points of view. First, the macroscale temperature profiles regarding the weld pool evolution under TIG welding are investigated with the use of the finite element method. Then, the collected information in each time step is transferred to the three-dimensional space of the Monte Carlo (MC) method using the developed data exchange mechanism based on an interpolation method. This approach allows applying the MC method to investigate microstructure evolution explicitly during the welding process. The basic model assumptions and implementation details are presented within the work. Finally, examples of results regarding changes at the microstructure level due to the macroscopic welding parameters are discussed.

MODELING THE DEFORMATION AND DAMAGE BEHAVIOR OF TRIP STEEL AND ZIRCONIA PARTICLE COMPOSITES

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The TRIP Steel matrix-based zirconia particle composites have been shown to depict significantly higher strength and ductility due to strain-based phase transformation during deformation. The composites' macroscopic deformation depends on the microscopic behavior of each phase. Given an applied loading history, the local elastic and plastic anisotropy of differently oriented phases within the polycrystal leads to a variation in the micromechanical lattice response. The local mismatch between phases during plastic deformation leads to the accumulation of intragranular residual stresses, which considerably affects the deformation, formability, and damage evolution. Therefore, understanding the local micro-scale variation between different phases or lattices plays an important role in assessing and improving the performance of such materials for industrial applications.
In this work, a physics-based TRIP-TWIP crystal plasticity-based material model incorporated in the DAMASK framework is adopted with a simple ductile damage criterion to understand multi-scale material deformation behavior. The fitting parameters of the model are calibrated by comparing with experimental results of stress-strain, phase transformation, and damage initiation. Due to significant property differences, Zirconia particles are assigned elastic attributes with simple critical strain energy-based brittle damage criterion. Virtual and real RVEs are considered for running full phase numerical simulations using the fast Fourier spectral solver technique. In-situ tensile tests are carried out inside the electron microscope chamber on a deformation stage to obtain local experimental strain maps. The local strain distribution and damage initiation points predicted by the simulations are compared with experimentally obtained results, and a good correlation is found. The numerical simulation results are further processed to obtain local stress, transformation, and damage propagation. The outcomes of the study help in understanding the effect of microstructural attributes on the local deformation and damage evolution. This model can be adapted to engineer microstructural attributes for targeted applications with less experimental support.

USING DIFFERENT SOLVERS FOR FFT-BASED MICROSTRUCTURE SIMULATIONS WITH A REDUCED SET OF FOURIER MODES

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Considering the simulation of the mechanical behavior of a heterogeneous microstructure, an algorithm using the Fourier representation of the Lippmann-Schwinger equation was introduced in [1]. The efficiency of this algorithm can be improved by using a model order reduction technique based on a reduced set of Fourier modes [2]. For the accuracy of this model order reduction technique, not only the number, but also the choice of Fourier modes is important [3]. Thus, in the context of complex microstrucutres, it is appropriate to use a strain-based sampling pattern [4]. Besides such a model order reduction technique, there are also more efficient solvers, such as the fast gradient method [5], to reduce the computational effort of the FFT-based microstructure simulation. In this talk, we will present the results of combining both, the model order reduction technique based on a reduced set of Fourier modes with efficient solvers, such as the fast gradient method.

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DEVELOPMENT OF THE GRAIN GROWTH MODEL BASED ON THE RANDOM CELLULAR AUTOMATA METHOD

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Numerical simulations can help in predictions of metals morphology and its evolution. Cellular Automata (CA) is one of methods that are commonly used for modelling of microstructure for all types of metallic alloys. The main goal of this paper is development of grain growth simulation based on random cellular automata method (RCA). Such solution is dedicated to preparation of digital microstructure morphologies that can be further used for many different type of multi-scale simulations, like dynamic and static recrystallization or phase transformations. In the RCA approach, computations are realized in a mesh-free environment within the cloud of CA cells. Therefore, each simulation requires an initial distribution of cells across the computational domain. Flexibility of this approach gives new opportunities to create more sophisticated models, but it is also a source of challenging problems because predictions of such algorithms can be significantly affected by the setup parameters (e.g., the density of CA cells, type of neighbourhood, neighbourhood radius etc.). In this work particular attention was put on development of cell distribution algorithms and selection of the proper initial simulation parameters. This work contains a comparison of three distribution algorithms based on the regular, hexagonal, and random cells' alignment and analysis of their influence for model predictions. The impact of initial parameters for propriety of generated microstructure was also investigated. Finally, an application of the proposed solution was presented and discussed to highlight capabilities of the developed solution.

INVESTIGATION OF INFLUENCE OF TI64 LATTICE DEFECTS ON MECHANICAL PROPERTIES USING IMAGE-BASED FEA

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This work presents the results of the numerical investigation of the influence of defects in Ti-6Al-4V lattice structures on mechanical properties using image-based FE modeling. The numerical modeling using the finite element method of the deformation process of diamond structures of the Ti-6Al-4V titanium alloy with various relative densities (18.5%, 27%, 50% and 66%) obtained by the additive method such as laser power bed fusion (LPBF). In numerical calculations, geometric models reconstructing the real shape of the investigated structures were used. These three-dimensional models were created on the basis of images obtained by means of x-ray computed tomography (CT) and x-ray computed microtomography (micro-CT). In order to take into account the shape of structures with their defects, in numerical calculations, on two levels of accuracy of mapping the shape details two tomographic techniques were used [1]. In the work was studied the influence of the accuracy of the structure geometry mapping, in particular the imperfections occurring in the structures, on their mechanical properties, deformation process and stress and strain fields. The comparison of the deformation process of the Ti-6Al-4V lattice structures resulting from the different relative density of the material were also described. The effect of the material's relative density on the location of the stress concentration in deformed structures was determined. The stress and strain distributions in the studied mesostructures at the moment of macroscopic fracture initiation in the material were also analyzed.

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STABILITY AND ACCURACY IN DYNAMIC-TRANSIENT MULTISCALE SCHEMES FOR WAVE PROPAGATION

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Dynamic multiscale schemes - dynamically coupling domains of different spatial scales - may offer tremendous improvement in computational efficiency. However, this advantage comes at the cost of accuracy and potential constraints on stability of the model. The dynamic coupling of different spatial scales makes multiscale models susceptible to the introduction of spurious reflections at the interface of the two domains. The artificial reflections are a characteristic of numerical errors that significantly affect the accuracy of results. Specifically, these spurious wave modes may be detected and misinterpreted as acoustic emission sources or reflections from structural discontinuities.

In this paper, we analyze convergence properties of a dynamic-transient multiscale scheme for wave propagation. We first outline the stability conditions for a numerical scheme involving two spatial scales and determine parameters that influence the stability space. Next, we study artificial reflections and distortions of waves transmitted across the scales' interface in a dynamic multiscale model coupling two different (local) elastic wave propagation modeling techniques. As example models we use one based on finite differences, namely the local interaction simulation approach (LISA), and second employing cellular automata for elastodynamics (CAFE).

The analysis is based on the concept of numerical impedance, whose mismatch between the domains is a measure of reflection. Numerical impedance contrasts with traditional impedance in continuous media, as the former is affected by spatial discretization parameters in addition to elastic constants and density. In this paper we derive analytical formulas for determining the individual numerical impedances of the domains. Then, the individual numerical impedances are used to develop methods capable of predicting the coefficients of artificial reflections and transmission in the multiscale model of any configuration. It is shown that numerical impedance mismatch - owing to varying spatial gird sizes in the domains being coupled - causes spurious reflections at the interface while also affecting the quality of transmissions across the interface. All the derived analytical formulas are validated against numerical simulations' results.

To minimize artificial reflections and develop a smooth and convergent multiscale model, compensation schemes that can minimize numerical errors are proposed. Three different compensation schemes - based on different strategies involving model parameter tuning and development of a transition zone at the interface - are proposed. The results from the compensation schemes are validated with numerical simulations' results.

A NUMERICAL SIMULATION OF SINGLE AND TWO-PHASE FLOW IN POROUS MEDIA

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Image-based modelling can be used to analyze mass transfer phenomena through porous media, with particular applications to porous metallic filters. The aim of these analyses is to improve our understanding and characterization of the way fluids move through variable pore-scales. This work presents numerical simulation of single and two-phase flow conducted in the COMSOL Multiphysics software. The X-ray microtomography images of porous sintered metallic filter were used to generate geometric model. The created geometric models allowed to calculate basic parameters such as porosity permeability. X-ray microtomography images were converted to DXF files to obtain geometric model for 2D and 3D flow computations. Following, multiphase flow models have been utilized focusing on the capturing of the liquid-gas interface motion. For a simulation of fluid distribution inside pores the models based on incompressible Navier-Stokes equations and their extension to diffuse interface (Cahn-Hilliard) model are used.

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CURRENT ADVANCEMENTS AND CHALLENGES IN MULTISCALE DOMAIN-DECOMPOSITION SIMULATIONS OF POLYMERS

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Scale-bridging simulations for polymers, which range from atomistic resolution to length and time scales relevant in engineering, are still challenging due to the amorphous nature of the material. In contrast to crystalline materials with established multiscale approaches, polymers require a specific treatment that takes into account the chain-like structure of the macromolecules with possible entanglements or crosslinks. In the present contribution, we summarize the theoretical background of multiscale domain-decomposition techniques together with the challenges in the context of polymer modelling. In a second part, we introduce the Capriccio method, which has been enhanced and further extended in our recent work to capture the highly inelastic nature of polymers. In particular, the Capriccio method combines a Finite Element (FE) treatment with Molecular Dynamics (MD) simulations, which are confined only to distinguished regions requiring detailed knowledge about processes taking place at the atomistic scale. With such a hybrid concept, the numerical cost, which is the limiting factor of MD simulations, can be significantly reduced and system sizes relevant for engineering purposes come into reach of simulation techniques with atomistic or molecular resolution. Recently, we have shown that the Capriccio method is appropriate for multiscale simulations of polymer nanocomposites to obtain mechanical property profiles of the matrix-particle interphase that evolves in the immediate vicinity of the filler particles. These regions, however, are not accessible by mechanical testing, such that the constitutive relations follow from the atomistic and molecular interactions. Furthermore, we employ the Capriccio method to simulate fracture processes of polymers under consideration of molecular effects. There, the MD region is confined to the proximity of the crack tip, whereas the remaining parts are simulated by FE. With this set-up, the MD region can be subjected to boundary conditions that are not feasible within the classical MD framework.

CONCENTRATION AND INFLUENCE TENSOR FIELDS IN MICROMECHANICAL SYSTEMS, DERIVED FROM GREEN'S FUNCTIONS

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Composite material mechanics typically rests on a few micro-to-macro transition rules: strain and stress average rules, macro-to-micro stress and strain concentration relations in elastic systems, as well as influence relations linking eigenstrains (eigenstresses) to total strains (stresses) in systems with elastic and inelastic strains. While these rules are normally given on the basis of different ad hoc arguments, which are not necessarily mutually consistent, we here derive them from two fundamental theoretical concepts in mechanics and mathematics: (i) the principle of virtual power, formulated for microheterogeneous continuum material systems subjected to macroscopic kinematic boundary conditions, delivers stress, strain, and volume force average rules; (ii) the Green's function theory for elasticity provides series-type integral expressions for the concentration and influence tensor fields. These tensors exhibit key average and symmetry characteristics, which are used to derive, on the basis of eigenstressed matrix inhomogeneity problems of the Eshelby-Laws type, phase-specific estimates for concentration and influence tensors. The latter estimates fulfill the elastic reciprocal theorem and guarantee the symmetry of the homogenized elasticity tensor for different phase shapes and orientations, hence overcoming an important limitation of the classical Mori-Tanaka-Benveniste scheme. The benefits of the developed scheme are illustrated with a non-trivial benchmark example.

A MICROMECHANICALLY MOTIVATED MULTISCALE APPROACH TO MODEL LASER POWDER BED FUSION PROCESSES

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For an extensive industrial application of metal additive fabricated parts, especially made by laser powder bed fusion processes, an increased understanding and better prediction of the material and structural response for example in terms of eigenstresses and warpage is necessary. Complex physical interactions arise during the production, in particular concerning metallurgical and thermal processes. Thus, appropriate models related to the process itself and the underlying material behaviour need to be established in order to facilitate time efficient simulations. This motivates the multi-scale approach proposed in this contribution, where the aim is to extract a micromechanically and physically justified inherent strain. The inherent strain method was first introduced for welding simulations, where a purely mechanical simulation can be used to predict the final deformation and stresses of the part. This method is now also established for additive manufacturing simulations. The model at hand is based on three different levels of finite element simulations and material models, i.e. the laser scan model, the laser hatch model and the part model, cf. [1]. On the smallest scale, respective the laser scan model, a phase transformation approach is incorporated in a thermomechanically coupled model, explicitly modelling the three states of the material, namely the powder, molten and re-solidified phase, cf. [2,3]. The detailed model is used to calibrate the heat source of the next level, i.e. the layer hatch model. The layer hatch model is employed to extract and define the inherent strain used as input for the part model. With this strain it is now possible to simulate whole parts using a purely mechanical simulation. The simulations of the laser scan model and layer hatch model do not have to be repeated for a constant set of material and laser parameters. The modelling and simulation of a twin cantilever beam is used to show the capabilities and very good match with experimental data of the presented framework. It is concluded that the applied multi-scale approach incorporating the inherent strain method allows the implementation of physically well motivated micromechanical material models in large scale simulations of additive manufactured parts.

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