Notes on New Physical & Hybrid Modelling Trends for Material Process Simulations

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Abstract. The more innovative production techniques for faster, cheaper and better-quality parts have encouraged more ambitious research works on numerical simulation of material & processes designs. A brief description of such ambitious work has been presented in this paper where some explanations of scientific and technical basis for some of latest physical & hybrid trends in material process simulations are concisely discussed. The topics of combining numerical, analytical and data-driven schemes along with evolving & dynamic mesh methods for simulation of dynamic material processes like casting, extrusion, Additive Manufacturing (AM) are also briskly described. Other trends like multi-scale and multi-resolution schemes for solidification (multi-phasing) and cooling applications are addressed, and fresh ideas of hybrid physical-data driven models (using Genetically Algorithm Symbolic Regression, GASR) and their applications are tersely presented. The effects of increasing computational power on hybrid multi-scale modelling and its implications for future of material modellings are also presented shortly. For the short paper herein, it has not been intended to publish the detailed results of new simulation technologies, rather it is focused on describing some new physical & hybrid trends for future of material process simulations.

1. Introduction
To establish new and innovative hybrid techniques, which help to improve industrial manufacturing process chains, more sophisticated & upgraded analytical and numerical simulations are required. The centre stone of such an idea is to combine the various existing capability of numerical techniques while in the same time, start to look over the hedge on emerging technologies on other branches of physical science and technology. The key here is to integrate sound physical & analytical techniques with emerging numerical simulation technologies and supplement the integration process with benefits of hybrid modelling scheme. The increasing computational power during last couple of decades has greatly affect the way the traditional material process simulations were conducted and more advanced schemes like multi-scaling and coupled multi-physical material modelling have quickly emerged [1,2]. Furthermore, the pace of design for more energy-efficient and quality-oriented industrial processes has significantly picked up in the last two decades where more innovative and smart virtual tools are utilized. One of the basic steps for promotion of such ground breaking numerical simulation technology would be to develop a platform where advanced coupled numerical techniques can basically be utilized within an Artificial Intelligent (AI) controlling arena.
The innovative potential of such an adapted technology is significant in which new material & process design concepts can be quickly interrogated by validating series of virtual-scenarios using reliable & verified numerical tools. In the research work herein, brief descriptions of ongoing research work on new numerical concepts (e.g., dynamic zoning, multi-resolution/grid…), hybrid physical data driven modelling and integration of AI-computational framework (e.g., using GASR…) have been introduced
to address long-standing problems of speed, accuracy and reliability of numerical tools for material processes. The hybrid numerical solution proposed herein is based on new computational concepts which institutes the sound physical/mathematical models and does not only rely on improved software solutions for the material & process simulations. Hence, some fundamental numerical aspects of the new simulation technique are shortly described. In addition, some outcomes of simple case studies which have been utilized using the proposed hybrid framework have been shown where the aspects of hybrid physical-data driven modelling are interrogated using the developed GASR tool. One of the main contributions of this paper is to briefly show how new computational technologies combined with hybrid modelling and suitable AI scheme can transform the traditional material and process simulation techniques.

2. New Dynamic & Evolving Approaches

The traditional time-spatial discretization & meshing schemes for numerical domains representing real-world physical domains have extensively been utilised in the past to define simpler subspaces (elements) with approximate/exact functions (e.g., shape functions). Different so-called meshing/gridding algorithm with continuous or discrete natures have been introduced which fragments the single numerical space into smaller elements/cells/particles. Although, today's meshing technology has become very efficient even for complex and multi-body geometries and also bodies with large deformations during simulations (e.g., adaptive re-meshing), the issue of dynamic change of domain during simulation and its appending discretisation scheme has systematically not been addressed. For the dynamic processes like continuous casting process, the traditional numerical discretisation was based on discretising the whole cast-billet domain where transient casting simulation would be performed using piece-wise activation of billet at small time steps.

Although the technique can successfully be applied to some industrial casting applications, the size of the numerical matrices and system of equations are large for the duration of the analysis (deactivation of elements at start of process would not remove their matrices from the equation solver). To mitigate this problem, there have been some attempts to introduce innovative discretization techniques [3-6] for dynamic systems including mixed & merge/splitting element and cell division techniques. In these techniques the numerical domain can be divided into Lagrangian, Eulerian and Arbitrary Lagrangian-Eulerian (ALE) zones. For the casting and extrusion (and also additive manufacturing) applications, the transient extension of the part during the simulation can numerically be modelled using splitting element layers at interfaces. Although the approach can alleviate the existence of large system of equation from start of simulation, it has limitations in terms of interface geometries & boundaries for more complex dynamical systems.

The new concept of dynamic & evolving domain (internal & external) and its discretization techniques have been developed recently [7-11] to overcome numerical problems related to continuous generation of the numerical domains. It would treat the changing & mutated parts of the domain as a dynamic zone which can move\evolve in predefined or calculated manner and ultimately be attached to the main domain through mapping-boundary concept. As the newly generated zones (or meshes) are attached to the main domain, a mapping procedure would be performed to handle the new material\energy input. For the continuous casting & extrusion simulations, a directional boundary evolution scheme can analytically be implemented where transient extension of the part is modelled using predefined directional vector. The technique can be summarized in the following steps; firstly, the initial starting geometry, its discretization and boundary conditions are modelled and initial system matrices are assembled. Secondly, the initial time steps/iterations are solved (using a multi-physical solver) and based on the generation speed, the coordinates are updated. Thirdly, the geometry and discretized grids are modified and adapted by adding a single\multiple layer mesh-zone based on the evolution of the domain. In the fourth step, the system matrices are modified\appended and the input energy is distributed amongst the newly generated sub-domain. For the fifth step, the time history results (from previous time steps) are mapped to the newly generated sub-domain till the energy balance is achieved (e.g., through the energy sink\source concept). Finally, the previous converged solution is used as a first step for a newly updated domain while the simulation scheme continues with the new geometry\mesh till the next
evolution step is triggered. More comprehensive discussion about the dynamic & evolving domain technique can be found in [7-11].

Case Study: In this case study, an industrial contact-less vertical casting process with rectangular cross-section has been modelled using the dynamic & evolving domain technique [8]. To avoid complicated mould-filling & fluid-thermal-mechanical interaction simulation, a simple filling simulation has been performed and initial state of billet is assumed (after 50mm casting) along with initial thermal conditions. A preliminary structured mesh has been generated with thermal and displacement degrees of freedom. The convection and radiation of the melt (at the top) and billet surface (after solidification) are taken into account using results of Computational Fluid Dynamics (CFD) simulations. A series of appropriate temperature-dependent Heat Transfer Coefficient (HTC) curves, based on experimental data and empirical calculations were also defined for the top free-surface air convection\radiation, water jet impingement and bottom free-convection zones. Figure 1 shows the CFD cooling simulation, empirical and experimental HTC curves for casting simulation along with the results of dynamic mesh and evolving method for a real-size industrial application (double symmetric quarter-model) at different time steps.

Figure 1. a) Schematic workflow for evolving domain framework; b) dynamic mesh generation for rectangular cast billet at different time steps; c) CFD cooling simulation for casting mold; d) water convective HTC curves
Despite of significant progress in developing dynamic generative systems and their numerical solvers, many of the existing software tools for industrial processes are still based on fixed-domain FE activation method. The typical practices to handle the process simulations are based on predefined geometry & mesh which are solved using FE mesh at discrete time steps by step-wise activation scheme. To compare the CPU performance of these techniques, a pilot study has been carried out for the vertical continuous casting application to compare the computational time using parallel processing technology. The research work has been split into two parallel activities, namely; the experimental/analytical work to calculate the Heat Transfer Coefficient (HTC) during casting process and numerical simulations of two different approaches using the same size billet (and mesh). The experimental work has been carried out to measure the transient temperature-time curves across the billet cross section, while the secondary analytical works have also been performed to calculate the HTC and cooling rates [12].

For the computational efficiency analyses, two identical geometric setups with a same mesh resolution are defined and the thermal boundaries are generated using thermal-mechanical contact elements. For the traditional activation method, the entire domain including the starting head and full-length billet are meshed. However, the whole billet elements (except the first mesh block) are computationally deactivated to resemble the real dynamic casting process. These deactivated mesh blocks are then activated stepwise during the transient simulation based on the casting speed. While for the dynamic mesh approach only the starting head and the first billet mesh block (50mm long mesh block) are generated at the start of simulation and the rest of the meshed billet are gradually appended to the domain at transient time steps (i.e., at solver restarts). Three different billet lengths, namely; 0.5m, 1.0m and 1.4m have been simulated using parallel processing scheme with 16 cores [13]. Figure 2 (b) shows the measured temperatures/comparison of CPU time for both techniques using three different size models. As it appears from the results, as the length of the billet is increasing the dynamic mesh technique is increasingly outperforming the traditional activation method using the same number of cores.
3. Hybrid Modelling & Smart Process Technologies

The use of hybrid physical-data driven modelling and its application in material science and engineering have increasingly been promoted over the recent years and the implementation of Machine Learning (ML) and AI technologies within alloy designs and processes have gradually been utilized accordingly. These emerging techniques have a tremendous potential for future of material engineering, industrial manufacturing and their processes where it has already been demonstrated that their potential to generate values in various process applications and material modelling domains are significant [14,15]. For the industrial manufacturing chain, ML & AI mean algorithm-based and data-driven schemes which enable better problem-solving capabilities with superior digital capabilities like; more accurate predictions, better decision reasoning, continuous learning & improvement and for some cases even un-supervised autonomous decision making. The hybrid models are categorically grouped into different classes, namely: auxiliary, augmented, full and dynamic hybrid models where different applications can be handled using an appropriate type of a hybrid model. The description of these models can briefly be presented as;

- For auxiliary hybrid models, parameters in the physical/empirical models are function-fitted using ML & AI tools
- In augmented hybrid models, physical models are augmented with terms/parts derived by function-fitting features of ML & AI tools
- Fully hybrid models where data trends from ML & AI are used along with physical laws to derive the hybrid model.
- Trained (or dynamic) hybrid models where the existing hybrid model is a subject of ML & AI tools for improvement

As these techniques are becoming ostensible for many material & process modelling applications including dynamic casting and forming applications, the need for greater understanding of technology utilization has raised within material & process simulation communities. The modelling capabilities of these techniques share the same fundamental intentions, namely; faster and more accurate modelling and the ability to dynamically change the rules & functions using new emerging data. Different smart data-driven approaches have recently been developed for physical applications where different classes of hybrid models including dynamic models can easily be handled. GASR is one of the interesting data processing technique where measured and/or calculated data can be fitted by suitable mathematical formula (from different family of functions…) using genetic and/or evolutionary algorithms. The technique has gradually been developed for computer implementation in recent years and some computer tools are already available based on GASR technologies. HeuristicLab [16] is one of open/source academic software tools which have been developed to deal with variety of data-driven modelling problems. It is prominently useful for problems where computational simulations are combined with optimization and design features within science & engineering research activities.

Case Study: Although many analytical approaches for cooling systems during material processes have been developed using sound physical-mathematical techniques, the number of parameters and their fitting into real-world processes have always been a challenge. The phenomena such as multi-phase fluid evolution (e.g., boiling regime), its flow dynamics and contact between the coolant and the hot surfaces have been estimated using parameter-fitting in these formulations. As stated earlier, the combination of physical & smart data-driven methods can fundamentally be used to find an optimised multi-parameter solution for the analytical formulation of bubble dynamics during cooling. The GASR technique has willingly been used herein to form a multi-dimensional search space developed for parameter fitting. The calculation of bubble drag forces during the impingement cooling on the billet hot surface has been calculated using insertion of scenario-based micro CFD simulation results into smart GASR tool. Figure 3 shows the schematic bubble dynamics on hot surface for horizontal & vertical plate [10] along with micro-CFD simulations of bubbles with varying diameter for calculation of drag forces on bubbles. It also illustrates the graphical presentation of tree-diagram for GSAR
function fitting and its error estimation curves along with resulting function for bubble drag force with varying water velocities and bubble diameters.

Figure 3. a) Schematic bubble dynamics on hot surface horizontal plate; b) micro-CFD simulations of drag forces on bubbles; c) graphical tree-diagram for GSAR function fitting of drag force and; d) resulting function for bubble drag force with water velocity $v$ and bubble diameter $d$

4. Smart Multi-Scale/Resolution Technologies

The multi-scale and scale-bridging computational techniques has continuously been promoted in last two decades to deal with material evolutions during industrial processes. The extent and limitation of conventional isolated macro & also lower-scale material models and their lack of accurate data bridging & failure to accurately predict the inherent material evolutions during processes have encouraged the development of multi-scale and multi-resolution models. These models take advantage of available faster & cheaper computational power & resources. Generic scale transition & bridging technologies have already been developed to convert physical & experimental data of the materials characteristics
(e.g., atomistic, microstructure…) into numerical discrete & continuum models suited for predictive tools at the engineering scale [17,18]. These bridging technologies are basically developed to enhance the existing trend towards digitization and virtualization of material processes. Although many researchers have attempted to develop a general framework for multi-scaling and bridging technique, the fact that length/time scales may vary over 12 orders of magnitude has restricted the computational implementations. The “Computational Material Engineering” concept have also been introduced based on more systematic approach for conventional and new material designs/processes (e.g., additive manufacturing…) and many interdisciplinary researches have been conducted to reduce the time & resources for development of products from concept-stage to end products.

To ease the computational overburden for multi-scale modelling, the concept of multi-resolutions and overlapping techniques have also found its way into numerical simulation of material processes where multi-grid/domain & co/parallel-solver computational technologies have been developed [19,20]. The secondary partitioning and zoning technique have been carried out where zones of interest can be flagged out and detailed lower-scale numerical discretisation (e.g., overlapping grid) can be setup for phenomena-based simulation using superior resolution. The following steps can be taken to carry out representative multi-resolution simulation for material processes;

- Identification and characterization of the numerical domain & its material evolution phenomena for overlapping multi-grid modelling. The detailed zones of interest can be connected to the main macro-scale domain through direct mapping, discrete integration point or statistical mapping schemes.
- Evaluation and implementation of possible discretisation scheme (e.g., continuous, discrete) and solver technologies for both macro-scale domain and its overlapping lower-scale zones.
- Identifying data flow (e.g., inputs-outputs) and appropriate post-processing scheme for both main domain and its high-resolution zones.

The combination of multi-scale/resolution and ML technology would hugely enhance the prediction & optimisation power of the material & process simulations. The use of appropriate ML technology (e.g., genetically-algorithm schemes) for improving material models and their parameters and also the discretisation properties of the numerical domain would boost the efficiency of the existing multi-scale simulation tools.

**Case Study:** In the final case study herein both features of new evolving domain technology and smart multi-scale/resolution can be combined for material continuous casting applications. The industrial process simulations for production chain which conventionally starts with the casting simulation and incorporates thermal evolution, mechanical stress/strain calculations and cracking & damage during casting process, has generally been carried out at macro scale. However, multi-scale/resolution simulation of casting process has recently gain momentum due to challenges and barriers which have to be overcome to capture the underlying physical/chemical phenomena (e.g., during solidification process). In particular, multi-resolution and multi-grid approaches have been developed to deal with evolution of microstructure during solidification phenomena [19].

The combination of these overlapping multi-resolution techniques with evolving and dynamic domain schemes (presented earlier in the text) would enable the seamless simulation of continuous casting and even processes like extrusion and AM [21]. Further improvement can also be achieved by incorporating hybrid modelling and ML techniques into the simulation framework to improve the predictability of material models at different length/time scales (e.g., microstructure…). Figure 4 shows the application of the technique for semi-continuous casting process (undergoing development). The combination of evolving domain technique, multi-resolution scheme and hybrid & ML approach (using combination of Neper [22]–Heuristic Lab [16] software) can be utilized for the industrial application.

The more detailed description of undergoing evolving method and overlapping multi-resolution technique for casting applications which involves Lattice Boltzmann–Cellular Automata method can be found in [19,20]. The analysis of detailed microstructure zone at micro-scale length were carried out using Neper and Gmsh [22] open-source tools and the Ansys® commercial solver has been used for
finite element analyses of grain structure. Finally, the GASR has been employed (using Heuristic Lab...
Figure 4. a) Simulation of casting process using evolving domain with its micro solidification zone utilising Neper tool; b) smart multi-resolution framework representation; c) graphical tree-diagram for GASR multi-dimensional search-space optimisation for CPU-time and; d) its resulting function for computational time versus mesh size & number of seeds

When completed, the smart multi-scale/resolution framework is planned to deliver an optimised material through process simulations suitable for industrial applications.

5. Concluding Remarks

One of the biggest challenges for today’s sophisticated computational frameworks is how to simulate multi-physical and multi-scale material processes in accurate manner with affordable computational time. Some of these processes have a very dynamic nature and the variations of parameters and thermal boundaries in time and space causes a huge challenge for industrial-based simulation tools. Some novel techniques have eagerly been developed recently to implement new dynamic techniques into the mainstream software tools which enables the accurate simulation of dynamic systems in both spatial & transient manner using hybrid physical & data-driven scheme. Some of these physical and data-driven trends in material & process simulations of industrial production chains have briefly been presented herein. The integration of hybrid modelling and utilization of ML & AI technologies into computational material science is one of the new challenges for scientist and material engineers in the horizon of digitization revolution.

Some technical aspects of new evolving domain and dynamic mesh technique with its new zonal discretization method has shortly been presented and the introduction of hybrid models for material and process simulation were discussed. In the final part of the paper, the contagious concepts of multi-scaling and multi-resolution modelling combined with its genetically-algorithm ML tool have briefly been scrutinized and the potential application of the method for industrial material processes are highlighted using a simple case study. As a final statement, the intention herein is to promote and encourage the use of necessary new inter-disciplinary technologies to upgrade the computational material science into next level, ready for the challenges of 21st century. The opportunity to follow the trend on new hybrid modelling schemes for further material processes would be taken and this would be the subject for extension of the research work presented herein.

6. References

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