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THE COMPUTATIONAL MODELLING APPROACH A MULTI-SCALE OVERVIEW

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Abstract: *The revolutionary progress of Computational Methods (CM) involve efficient, user-friendly source to detect the evolution of material behaviour from a multidisciplinary point of view: physical, biological, chemical or mechanical system. Besides, this technique present high level of sustainability due to the cheap price of computational modelling within reasonable times acquired under modern powerful computer.*
A significant advantage rise when this technique is employed at large scale in industrial platform. Thus, in the industrial field the CM transposes the experimental investigations on the numerical simulation, making the possibility to save as well main source of row material. The CM technique is applied in different sectors as: wind energy, aeronautical, naval, automotive, bio-medical, biomechanics industry, power plant assembly, building construction, electromagnetic, electronic field, weather forecasting and etc.
This paper present an summary of general benefit/challenging encountered in CM converted in principal improvement into industrial area, and concludes with an open problem that provides stimulation for further research.
Key words: *Computational Methods (CM), multi-scale algorithm, contact interaction;*

1. INTRODUCTION

The scientific development of CM is recognized as a function of continuous growth of the number of papers published in Journal of specialities (i.e. Computational Mechanics, International Journal for Numerical Methods in Engineering, Theoretical and Computational Fluid Dynamics, Theoretical and Computational Fluid Dynamics, Computational Materials Science and etc.) connected to the industrial field.
The necessity to solve general problem encountered in nature and mostly applicable in industrial area entail the research organization (i.e. Universities and research centres) to imply more energy to obtain new knowledge for solving today's and tomorrow's problems raised from computational algorithm.
Departure algorithm for CM starts from knowledge of the reference coordinate. As location, the position of a particle relative to its coordinate system can be specified by a vector function of time – the position vector x(t). Then, it is normal to define an equation for x(t) to design the trajectory of this particle, and to find its trajectory during time [1]. This border can be considered in order to fix the coordinate of reference system for the stability of the local condition. Besides, if a system undergoing slow time variation in comparison to its time constants can usually be considered to be linear time invariant (LTI) and thus, slow time-variation is often ignored in dealing with systems in practice [2]. The issues arise when time change its sequence, case that is related to time-dependent problems, and planned to be solved with systems of partial differential equations in which the time derivatives are of first order. Moreover, the numerical methods can be used to solve partial differential equations containing higher-order time derivatives by defining new unknown functions equal to the lower-order time derivatives of the original unknown function and expressing the result as a system of partial differential equations in which all time derivatives are of order 1 [3]. The general form of second-order partial differential equation is present in equation 1.

$$\frac{\partial^2 \psi}{\partial t^2} + \psi \frac{\partial \psi}{\partial x} = 0 \tag{1}$$

By setting these basic conditions in the CM, it is possible to go further to implement the algorithm of numerical analysis to detect the evolution of material behaviour from a multidisciplinary point of view: physical, biological, chemical or mechanical system.
In this paper, we present the general benefit/challenging encountered in modelling methods to further improve the efficiency and accuracy of CM within the applicability in industrial sector.

2. CONDITION AND SCENARIOS TO IMPLEMENT THE CM

In the CM, an important step is represented by the validation of the model that entails an accuracy level reliable with the requested application. This procedure can be acquired by a calibration method developed as well as computing code, which can involve an automate regression of the calibration procedure (optimization method) [4]. Figure 1 present the general model for a cycle of CM.

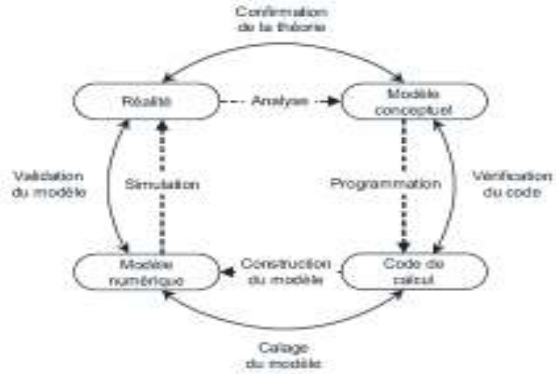

Figure 1. Components of a modeling terminology incorporating the stage of model calibration 4.

The calibration procedure can be very difficult task, for example at atomistic scale. The challenge can rise when the required input data represent properties of small-scale volumes, embedded and constrained by other phases, with complex geometry and some internal heterogeneity. Obviously, the properties cannot be directly measured or tested, or might be different from the properties of macro specimens (due to the scale and size effects, constraints by other components, effects of treatment regimes, etc.). The extraction of the data for the phases from the standard or modified tests of materials can become a nontrivial problem, which requires both rather complex experiments and an inverse analysis step [5]. A particular case, that confirms this situation, can by exemplified when is applied the generation of unit cells, as is present in Figure 2, where molecular distribution are very sensitive to CM procedure.

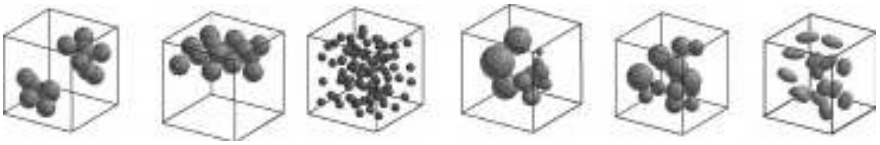

Figure 2. Examples of the unit cells generated with the use of the program Meso3d [5].

Furthermore, at the mesoscale levels are a wide range of configuration that encloses different heterogeneities. Such arrangement can involve a large number of small inclusions, so that a small parameter, the relative size of an inclusion, may compete with a large parameter, represented as an overall number of inclusions. To solve this kind of problem, the method of meso-scale asymptotic approximations is usually applied in order to obtain a uniform approximation to the solution of the Dirichlet problem in the multiply perforated domain [6].
An alternative approach could be considered homogenization techniques [7]. Through this method can analyze the local stress and strain in the constituent material. In this case the grain core (inclusion) and the grain boundaries (matrix) mechanism are engaged. The behavior of the grain core and of the grain boundaries are, respectively, elastic visco-plastic and elastic perfect–plastic.
Besides the heterogeneous nature of the compound, one must consider all kinds of interactions developing at even very different scales. This complex problem that requires careful depth treatment, with accurate and fast numerical methods (i.e. finite difference method, finite volume method, finite element method, mesh-less finite element methods, Discrete Elements Methods, Molecular Dynamics etc.), deal to the contact detection between these particles. In general, the configuration of contact particle is surrounded by two or more body (solid, liquid,

gaseous) established in direct contact as a multi-layered structure comprised of different matters (metal-metal, metal-oxide, sol-gel film, metal-liquid, metal-polymer, polymer-concrete, polymer-textile, rubber/metal composites and polymer-human body) what involve different constraints. The atomistic and/or molecular scale the contact body is considered by the Van der Waals interactions and depends on the geometric configuration of the group of atoms encountered [8]. Figure 3 show the Van der Waals interactions, a schematic representation of the repulsive part of the interaction potential.

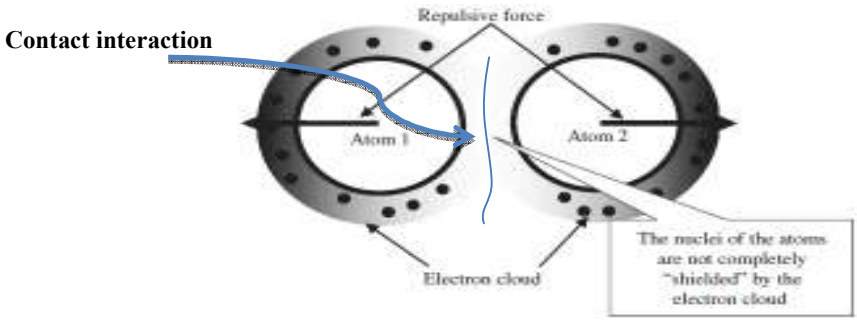

Figure 3. Van der Waals interactions-schematic of the repulsive part of the interaction potential [8].

At the macroscopic scale, the load transfer for interface field is analyzed using molecular structural mechanics method and the matrix deformation by the continuum finite element method. The van der Waals force between interacting atoms is written as:

$$F(r) = -\frac{dU(r)}{dr} = 24\frac{\varepsilon}{\sigma}\left[2\left(\frac{\sigma}{r}\right)^{13} - \left(\frac{\sigma}{r}\right)^{7}\right] \tag{1}$$

where r is the interatomic distance, □ and □ are the Lennard-Jones parameters. For carbon atoms the Lennard-Jones parameters are □= 0.0556 kcal/mole and r= 3.4 A˚.

Panin et al. [9], [10] applied the concept of structural scaling and structural-scaling transition to assess defect on subsystem for a deformed Nano solid. An important functional role in the response of the internal medium to external actions, in multilevel system, is played by the heterogeneous medium. The surface layer substrate interface may be described with fundamental effect of a chessboard-like stress strain distribution model. This effect implies the generation of strain induced defect on the surface of a loaded solid. Plastic flow propagation at meso- and macrobands is localized as well as, and show the behavior of solid under various external actions. The mechanical interface is generating by sinusoidal surface layer due to rotation of constraints successively in tensile and compression in the structure. Described by the following equation:

$$\sigma = A\sigma_y \sin\frac{x - l_x}{t\sqrt{2}} \tag{3}$$

where t, x, σ_y □□A, are the thickness of the coating, distance of crack propagation, stress coefficient and surface area covered by “paper”, respectively.

$$l_x = \frac{1}{\sqrt{2}}\left(\frac{\pi}{2} + n\pi\right)t \tag{4}$$

For macroscopic contact interaction, this complex problem can be discretizing as a function of contactor behavior (elastic, elasto-plactic, and perfect plastic mechanical behavior) and/or contactor shape that act to the specimen sample (i.e. from meso-micro-to macroscale). Generally, the shape of contactor is described by a curve or a segment. It is well know that the numerical approximation of contact interaction is allocated to node to segment surface. For example, the interaction between an segment surface and an disc curve present three situation as is exemplified in Figure 4.

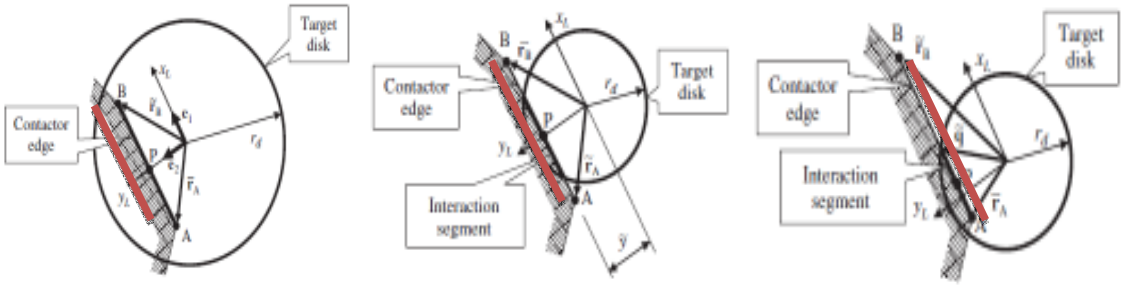

Figure 4. Schematic of interaction between an segment surface and an disc curve for different case a) both nodes of the contactor edge are inside the target disk, b) both nodes of the contactor edge are outside the target disk and c) Node A is inside the target disk while Node B is outside [8].

These types of contact problem showed above surround a large domain of application, from mechanical forming (cold, worm, hot) problem to biomechanics approach (interaction between different implants applied on human body).

Multiple-scale techniques, where the emphasis is made on the latest perspective approaches, such as the bridging scale method, multi-scale boundary conditions, and multi-scale fluidics. As a possible application of studies in bone failure may be detection of milder osteoporotic symptoms.

3. CHALLENGING

Considering the limit when a "numerical model" encloses structure from a unit scale at the quantum level to a model with multiscale processes (see Figure 5) at the Human scale, it is possible to be ideal calibrated to respect the powerful of length scale approach? Or this methodology applied under the philosophy of multiscale analysis has the effects on the upscale after modeling, simulation, and validation occurred at the length scale of interest?

The successfully integration of multiscale approach can lead to a comprehensive industrial solution.

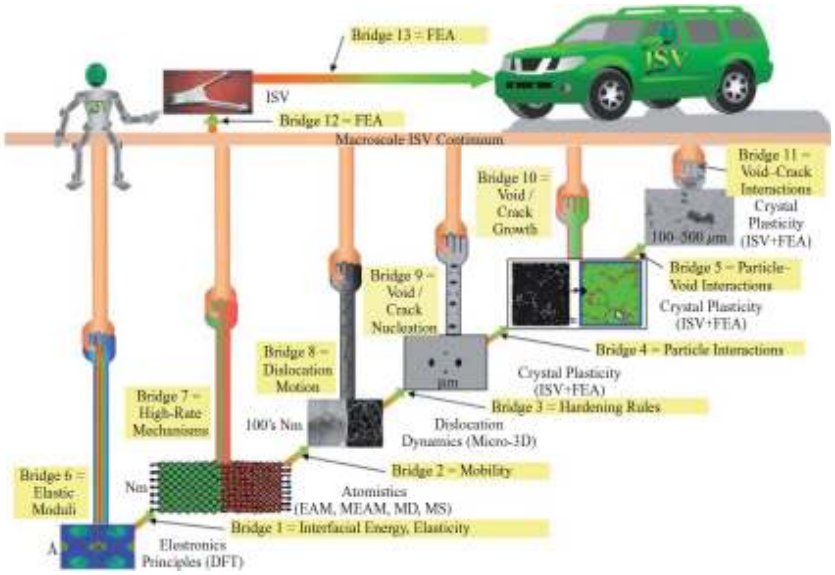

Figure 5. Multiscale approach applied in a metal alloy process for design an automotive component. The structured methodology present different length scale analyses used through various bridges within CM. ISV, internal state variable; FEA, finite element analysis; EAM, embedded atom method; MEAM, modified embedded atom method; MD, molecular dynamics; MS, molecular statics; DFT, density functional theory [11].

4. CONCLUSION

This paper cover the main issue generated when the CM are applied to predict the behaviour of material behaviour, and point out the boundary condition (knowledge the time and the reference coordinate) necessary to

implement the CM processes. Besides, a multiscale approach is called for consideration as further application on the industrial management.

REFERENCES

[1] O.L. de Lange and J. Pierrus. *Solved Problems in Classical Mechanics.* ISBN 978–0–19–958252–5, Oxford University Press Inc., New York, 2010.

[2] DongBin Lee and C. Nataraj. Model-Based Adaptive Tracking Control of Linear Time-Varying System with Uncertainties. Mikhaylo Andriychuk. *Numerical Simulation – From Theory to Industry.* Janeza Trdine 9, 51000 Rijeka, Croatia, 2012.

[3] Dale R. Durran. *Numerical Methods for Fluid Dynamics.* ISSN 0939-2475, Springer Science+Business Media, LLC 1999, 2010.

[4] Denis Dartus. Feedback on the Notion of a Model and the Need for Calibration. [auteur du livre] Jean-Michel Tanguy. *Environmental Hydraulics Numerical Methods, Volume 3.* ISBN 978-1-84821-155-1 (v. 3), © ISTE Ltd, 2010.

[5] Leon L. Mishnaevsky. Computational experiments in the mechanics of materials: concepts and tools. *Computational Mesomechanics of Composites Numerical Analysis of the Effect of Microstructures of Composites of Strength and Damage Resistance.* ISBN 978-0-470-02764-6, John Wiley & Sons Ltd, England, 2007.

[6] Vladimir Maz'ya, Alexander Movchan, Michael Nieves. *Green's Kernels and Meso-Scale Approximations in Perforated Domains.* ISBN 978-3-319-00356-6, © Springer International Publishing Switzerland, 2013.

[7] L. Capolungo, C. Jochum, M. Cherkaoui, J.Qu. Homogenization method for strength and inelastic behavior of nanocrystalline materials. International Journal of Plasticity 21 (2005) 67–82.

[8] Antonio A. Munjiza, Earl E. Knight, Esteban Rougier. *Computational Mechanics of Discontinua.* ISBN: 978-0-470-97080-5, Wiley Series in Computational Mechanics, November, 2011.

[9] V.E. Panin, A.V. Panin, V.P. Sergeev, A.R. Shugurov. Scaling effects in structural-phase self-organization at the "thin film - substrate" interface. Physical Mesomechanics, Volume 10, Issues 3–4, May–August 2007, Pages 117–128.

[10] V.E. Panin, V.A. Panin and D.D. Moissenko. Physical mesomechanics of a deformed solid as a multilevel system. II. Chessboard-like mesoeffect of the interface in heterogeneous media in external fields. Physical mesomechanics, 5-14 (20), 2007.

[11] Mark F. Horstemeyer. Integrated Computational Materials Engineering (ICME) for Metals Using Multiscale Modeling to Invigorate Engineering Design with Science. The Minerals, Metals & Materials Society, 2012.