14th World Congress on Computational Mechanics (WCCM XIV)
8th European Congress on Computational Methods in Applied Science and Engineering (ECCOMAS 2020)
July 19- 24, 2020, Paris, France

THE FUTURE ROLE OF DATA ANALYTICS IN COMPUTATIONAL SCIENCE AND ENGINEERING

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Key words: Data Analytics, Computational Mechanics, Fluid Dynamics.

ABSTRACT

The mini-symposium should address recent key trends in using data analytics in the broad area of computational science and Engineering, which can be classified as follows:

Data Analytics & Management (We refer to the use of algorithms to approximately model patterns in data**)**
The pace at which digital technologies are progressing triggers the generation of a tremendous amount of data that can hide important information, if carefully treated. The trend is to invest in the direction of using the newest generation of technologies and architectures to extract value from very large volumes of data produced, using tools for predictive modelling combining statistical analysis and data mining techniques for understanding the trends. The same can indeed be the case in many scientific areas, where the treatment and analysis of data can help conceptualize new theoretical ideas or consolidate known ones

Hybrid Data & Physics Modelling
Turning the massive amount of data into an asset is a trend today. In opposition to this mainstream idea, data analytics maybe be more powerful if tied up with engineering simulation (CAE), towards the so-called 'CAE Digital Twin' concept, where the description of a system is based on both physics modelling and machine learning, using these same simulation data. The concept can be very useful in computational physics problems that cannot cover all the space-time range conditions. Data analytic should use the simulation data for predictive modelling.

Machine Learning in Simulation Processes
In the modelling of the wide range of 1st- principle phenomena, there is a large and endless portion of effort devoted to calibrating model coefficients and constants. In the atomistic scale arena, the same issue faces the modeller as to the prediction of materials' properties governing

various physical-chemical processes. As it has been shown recently in the context of using a genetic algorithm for controlling convergence of CFD simulations [1], machine learning algorithms can be employed within the simulation processes to dynamically infer model coefficients, material/fluid/solid properties, and other parameters.

REFERENCES

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