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HPC in all the right places – accelerating modelling workflows in metallurgical engineering applications

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Our modern technological societies depend critically on metals and alloys. Producing these materials from their original sources, which can be either natural (mined ores) or man-made (recycled wastes), is an expensive and energy-intensive process. In addition, it is damaging to the environment – production of steel alone currently contributes about 8% to the world's total carbon dioxide emissions. Due to the phenomenological complexity of many metallurgical engineering applications, computational modelling tools play an important role in the optimisation of existing processes and the design of new ones. This is especially true today when parts of the industry are under pressure to change rapidly to address their environmental impact while continuing to deliver on important economic, social, and governance targets.

Unfortunately there are no "one size fits all" tools when it comes to modelling of metallurgical processes, and a variety of different pieces of software must often be brought to bear on a particular problem. Apart from data formatting and translation issues, this can pose some interesting challenges in assembling workflows that take advantage of high performance computing (HPC) in appropriate parts of the overall solution.

In this presentation, we will discuss a simple application of this workflow approach in the assessment of electrical performance of large-scale direct-current (DC) plasma arc furnaces used for the production of ferroalloys. Magnetohydrodynamic multiphysics models of high current DC arcs give insight into the electrical behaviour of the furnace, but they require information about the thermophysical properties of the plasma fluid, and this in turn requires knowledge of the gas compositions in the furnace while it is operating. The HPC needs of each calculation step vary widely, and providing appropriate acceleration at each step is the key to obtaining an overall workflow that runs in reasonable times.

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