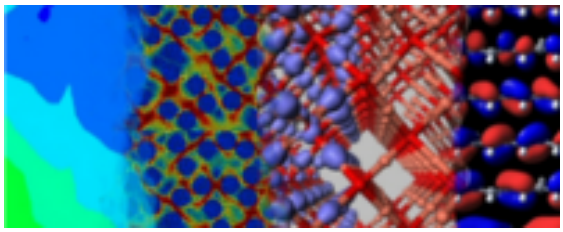

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Multiscale modelling on petascale supercomputers

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The availability of High Performance Computing (HPC) has revolutionized many fields in science and engineering, allowing insights into phenomena which are not obtainable from experiment alone. However, using HPC facilities is daunting for many researchers who find that in order to exploit the resources effectively they must understand concepts of parallel computing and architectures, intricacies of operating systems and working environments unlike those used on common workstations. Further challenges are becoming apparent as Europe, the US, Japan, China and other countries start bringing into production clusters capable of performances extending into the Petaflop range, the so-called "Petascale". For these systems, not only do the application codes have to be parallel but the level of parallelism has to be very high, extending to thousands of cores. Other characteristics of Petascale architectures, such as low core memory and limited I/O bandwidth, are also important and influence the software applications and scientific problems available to researchers. In this study we examine how these factors are affecting users in multiscale modelling where many very different codes are employed. We also discuss the opportunities and implications for application programmers and users as HPC centres move beyond Petascale and in the near future to Exascale systems.

Author: EMERSON, Andrew (CINECA Computer Centre)

Presenter: EMERSON, Andrew (CINECA Computer Centre)

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