

Frontiers in Materials Modelling

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As in many other scientific areas, computer simulations have become an indispensable tool in materials science. Our present ability to simulate accurately and precisely the behavior of complex materials is unprecedented, due to the combination of the development of theoretical tools and numerical algorithms to solve the underlying basic physical equations, and to the overwhelming (and constantly growing) computing power of present-day supercomputers. The challenges that still need to be overcome to have a truly predictive simulation-based materials discovery tool, which can be used even in the industrial environment, are many. Their solution will require solving hard scientific problems, but also hardware and software engineering tools to be developed in the context of the forthcoming exascale computing facilities, and new approaches like artificial intelligence and big data. Europe has been in the forefront of this scientific area, and recent initiatives aim to maintain this situation in the future.