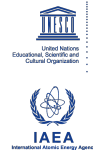




The Abdus Salam  
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**College on Multiscale Computational Modeling of  
Materials for Energy Applications  
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**High-throughput and Multiscale Computing:  
Best Practices and New Approaches**

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Abstract:

Computational materials science has benefitted from recent progress in computing technology, computer science and software engineering. However, current research in this domain faces problems that require adopting even more elaborated and advanced modeling and computational paradigms. The focus of this lecture will be on scalable computational approaches enabling multiscale materials modeling and high-throughput materials design. These approaches are subdivided into model integration, high performance computing, and into more advanced approaches such as model-driven architecture and service-oriented architecture. Furthermore, I will discuss how these techniques can be combined and provide a survey of existing frameworks and tools implementing these concepts. I will also give a general introduction to multiscale modeling and computing. All techniques will be illustrated with examples from materials science and nanoscience research explaining the principal problems and their state-of-the-art solutions.