

Feedback

Q1: Onion approach: Is there any priority which layer goes first?

A1: It really depends on the application: The coarser model might have to feed the finer model first or vice versa.

Q2: What is the advantage of the Onion approach?

A2: Vastly varying temporal and spatial scales (complexity!) render us unable to use “brute force” molecular simulation of entire processes. In these cases, the application of different models and tools at different scales, so-called onion-type hybrid multi-scale models, is essential.

Feedback

Q3: How to determine the level of granularity required for modelling a system accurately?

A3: That depends on the phenomena and the scale of interest (reference scale): The finer the granularity the more accurate is the model. Of course, there is a minimum granularity to capture the phenomena. However, the finer we grain, the more computational intensive is the simulation. In other words, we have to find a balance between computational costs and the level of granularity.

Q4: If multi-scale modelling requires some sort of interaction between the models at different levels of granularity, how do you go from course-grained models to finer grained models?

A4: Therefore we perform one course time step and pass the information as an initial condition to the finer grained level.

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Q5: Would you examine the macro view just to gain context for the micro view or could you be looking for behaviour emerging at each level?

A5: Sure, you can do both. But emerging behaviour on a coarser grained level depends on the dynamics on finer grained levels. However, you can see the different levels as different processes, especially when they are separated by several orders of magnitude.