Modeling, Simulation and Control of Nanosystems

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- Coupled phenomena, multiple temporal and spatial scales.
  - e.g. the occurrence of a chemical reaction depends on atomic nuclei coming close enough for their electrons to interact and form bonds.
- Computationally expensive at best, analysis also difficult.
- What can be done? Focus on single scales of interest.
  - e.g. density functional theory for electronic structure calculations, molecular dynamics calculations for positions of atoms
- Single scale often not sufficient to understand the system.
- General class of problems termed Multiscale.
- We are investigating methods for modeling, simulating, and controlling multiscale systems with applications in nanotechnology.

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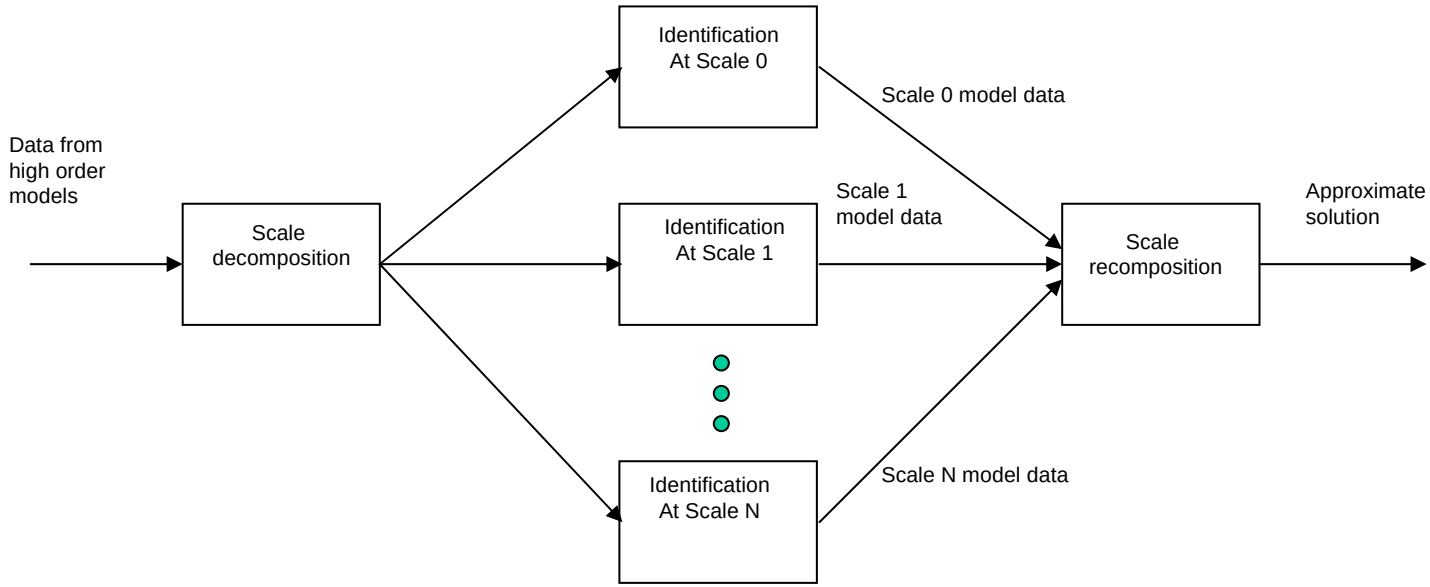
Our Approach

- Data from high order models is used for model reduction by constrained system identification at multiple scales.



- Once accurate models are identified simulation switches to the reduced order model.
- Upon detection of reduced order model failure we switch back to the high order model and identify a new reduced order model.
- Initial work is with a model of the cardiovascular system based on systems of nonlinear ordinary differential equations. We are looking for a nanotechnology example and working on methods for systems of partial differential equations.

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Have a general approach to a class of problems – need a specific nanotechnology example

•Looking for systems where there is a need to control the operation or fabrication of the system, or to otherwise optimize some aspect of the system's performance.

•**The system dynamics occur across multiple distinct time scales**. For example in a semiconductor material, the time scale of changes in the electronic structure is much faster than that of the thermal vibrations of the atoms.

•**The system operates at and/or is influenced by multiple spatial scales**. For example nucleation of nanoparticles on a surface in a CVD reactor, the nanoparticles are the interesting part of the system but their growth is influenced by the environment on the surface and of the macroscale CVD reactor.

•**The dynamics are strongly coupled to the spatial structure**. For example quantum dots possess characteristics unique from what would be observed in a sample of the same material in bulk due to their size.