Mathematical Challenges in Multiscale Approaches and Related issues in Nuclear Reactor Simulation

Mihai Anitescu, Argonne

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Structure of talk

- Multiscale example problems examples and challenges (hopefully) relevant for GNEP, based on the speaker’s (small) experience.
- General challenges that can be abstracted from these examples?
Parametric Sensitivity of Large Eddy Simulation (LES)

- A subgrid model for fluid flow seems unavoidable, so its effect on the “reality” should be quantified.
- Parametric sensitivity (Smagorinski, left panel) of LES leads to improved estimates of flow functionals, compared to LES itself (with William Layton, Pitt).
- Our finding: For accurate estimation, the sensitivity needs to be estimated on a finer mesh than LES, but coarser than the one needed for direct numerical simulation.
- Open questions: Other LES, comprehensive error analysis, aposteriori error analysis.

2d drag on fixed cylindrical body
Multiscale Approaches for Problems in Material Science.

- ... inspired by the quasicontinuum approach (Tadmor et al.).
- High resolution model

\[
\begin{align*}
\min_{(O)} & \quad f(x_1, x_2) \\
\text{sbj. to} & \quad g(x_1, x_2) = 0.
\end{align*}
\]

- Representative (coarse-scale) DOF, \( x_1, \dim(x_1) << \dim(x_2) \).
- Key observation: at the solution of the problem we have \( x_2 \approx Tx_1 \), where \( T \) is an interpolation operator.
- Replace \((O)\) with \((RE)\), of much smaller dimension, by writing optimality conditions and using the interpolation rule.

\[
\begin{align*}
(RE) \quad \nabla_{x_1} f(x_1, Tx_1) + \nabla_{x_1} g(x_1, Tx_1) \lambda &= 0, \\
\quad g(x_1, Tx_1) &= 0.
\end{align*}
\]
Fundamental question: is the reduced problem well posed?

- Yes (Anitescu, et al., 2006) … under certain assumptions. There must be a certain local compatibility between the interpolation operator and the energy (or Lagrangian) functional.

\[ x = (x_1, x_2), \quad L(x, \lambda) = f(x) + \lambda g(x) \]

\[ \left\| \nabla^2_{x_2x_2} L(x^*, \lambda^*) T + \nabla^2_{x_2x_1} L(x^*, \lambda^*) \right\| \ll 1 \]

- Related question: Is it better to Optimize and Interpolate (force based) or Interpolated and Optimize (energy based).

\[(RO) \quad \min f(x_1, Tx_1) \]

\[ \text{sbj. to } g(x_1, Tx_1) = 0 \]

- Answer: the latter, but its data are harder to compute.

- Open questions: Improved reduction of Interpolate and Optimize, the case of inequality constraints, aposteriori error estimation, efficient solvers for the subproblems.
A multiscale approach for orbital free density functional theory

- Representative variables: The density in the representative domains

\[ Y_\alpha, \quad \alpha = 1, 2, \ldots, P \]

- The interpolation operator is constructed with respect to a reference crystalline mesh (2005, in print)

\[ \rho_i(\Phi(r^0, t)) = \sum_{\alpha=1}^{p} g_\alpha(i) \rho_\alpha(\Phi(r^0 + T_{i\alpha}, t)). \]

- In material problems appearing in radiation damage, accurate potentials are not available so DFT is an essential.

- We have proved that the approach is well posed.
How well does it do?

- Parallel solver, based on PETSC/TAO, created in the last 3 months.
- Example for 11 hydrogen atoms, 1D and 3D
- Open questions:
  - How to extend to the case the energy functional is not explicit? (Kohn-Sham)
  - Efficient ways to compute, store and use the reduced Hessian matrix?
  - What are useful optimization algorithms that exhibit minimal communication (the domain decomposition angle? What are appropriate boundary conditions?)
General open questions applicable to multiscale model reduction.

- Parametric sensitivity equations and a posteriori error estimation for homogeneous multiscale method reduction.
- What are consistent model reduction of and efficient algorithms for multiscale models with constraints (e.g. total charge and nonnegativity constraints), when only representative subdomain solves are considered?
- What is a consistent mathematical framework for multiscale model reduction, which is useful for uncertainty quantification? For example deterministic high resolution deterministic problem reduced to stochastic differential equation (e.g. molecular dynamics -> Langevin, with high resolution solves to compute the reduced parameters).
- Can this framework be used to define a domain-specific language for nuclear reactors that would accelerate component integration and HPC performance (freeFEM and Sundance for FEM). That is essential for efficient development of future workforce.
- For back-end sensitivity calculations, how does one do accelerated sampling? If answer is randomized quasi Monte Carlo, can we prove convergence in distribution that is essential in statistical estimation?