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

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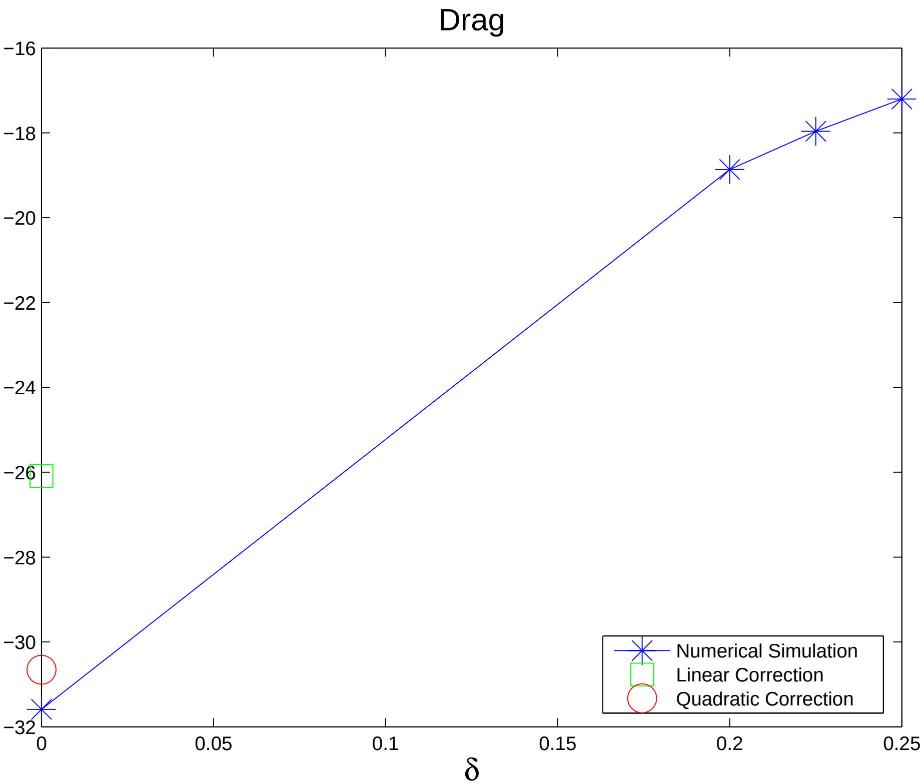
Structure of talk

- 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)



2d drag on fixed cylindrical body

- 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**

Multiscale Approaches for Problems in Material Science.

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

$$(O)\quad \begin{array}{ll} \min & f(x_1,x_2) \\ \text{sbj. to} & g(x_1,x_2)=0. \end{array}$$

- 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.

$$(RE)\quad \begin{array}{rcl} \nabla_{x_1} f(x_1,Tx_1) + \nabla_{x_1} g(x_1,Tx_1)\lambda & = & 0, \\ g(x_1,Tx_1) & = & 0. \end{array}$$

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.

$$x = (x_1, x_2), \qquad L(x,\lambda) = f(x) + \lambda g(x)$$

$$\left\| \nabla^2_{x_2 x_2} L(x^*,\lambda^*) T + \nabla^2_{x_2 x_1} L(x^*,\lambda^*) \right\| << 1$$

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

$$(RO) \quad \begin{array}{ll} \min & f(x_1, Tx_1) \\ \text{sbj. to} & g(x_1, Tx_1) \quad = 0 \end{array}$$

- 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

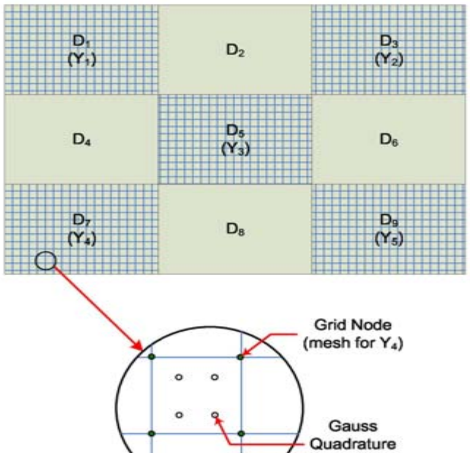
$$Y_\alpha, \quad \alpha = 1, 2, \ldots, P$$

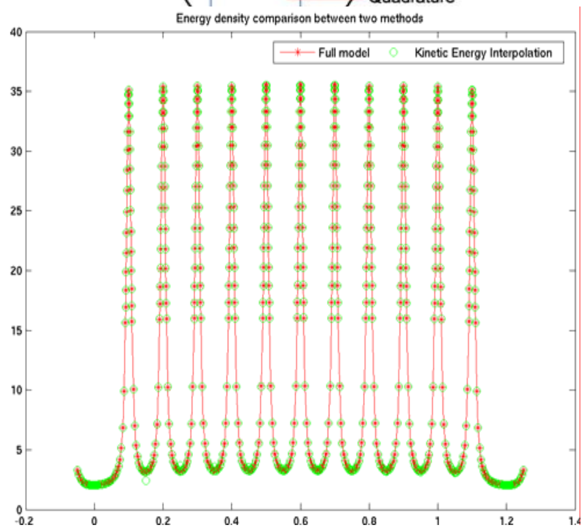
- The interpolation operator is constructed with respect to a reference crystalline mesh (2005, in print)

$$\rho_i(\Phi(\mathbf{r}^0, t)) = \sum_{\alpha=1}^{p} \vartheta_\alpha(i)\rho_\alpha(\Phi(\mathbf{r}^0 + \mathbf{T}_{i\alpha}, t)).$$

- 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.

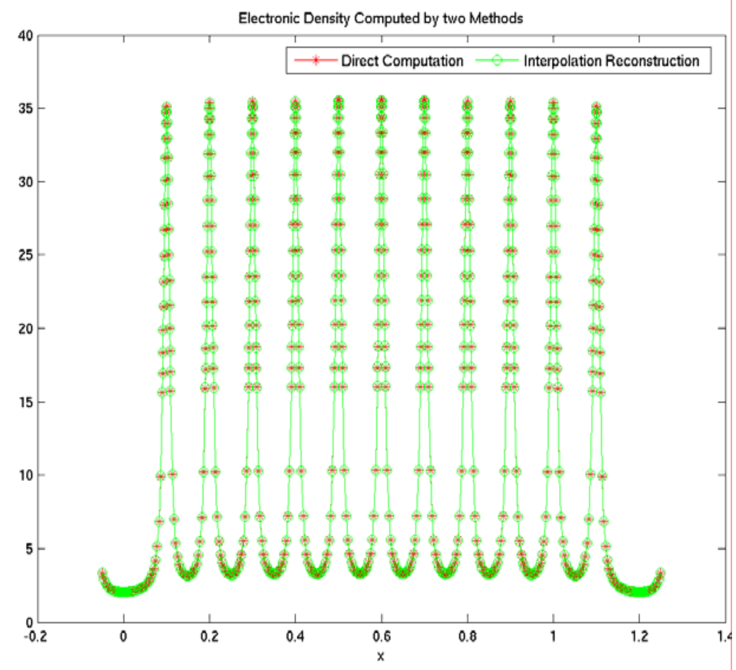
$Y_\alpha , \alpha = 1 , 2$

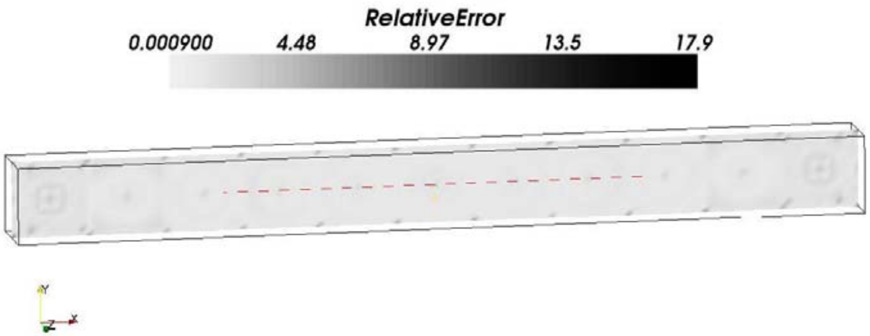




How well does it do?

- 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 aposteriori 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?