Advancements in Multiscale Modeling

Foundations, Current Status, and Future Prospects

OLUWAFEMI OGUNDARE
Neopathology Corp.

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Outline

* Introduction to MSM
* Importance of MSM
* Key Concepts in MSM
* Integration of HPC and ML
* Historical Milestones
* Applications of MSM
* Challenges
* Future Directions
* Conclusion
* References

Introduction to MSM

- Multiscale modeling (MSM) deals with problems that involve different time and length scales.
- Complex processes in physics, engineering, and biology often span multiple scales, meaning one cannot fully understand them by just looking at one level (e.g., atomic or macroscopic).
- MSM combines different models that work at these various scales to solve such problems.
- For example, simulating a protein's interaction with a drug requires both atomic-level details (microscale) and the behavior of the whole system (macroscale).

Importance of MSM

- MSM is important because it allows scientists to bridge the gap between small, detailed models (e.g., molecular interactions) and larger, broader models (e.g., fluid dynamics). This helps researchers create more accurate simulations that reflect real-world conditions better than simpler models.

Key Concepts in MSM

- Multiphysics: MSM not only deals with multiple scales but often with multiple types of physical processes (e.g., chemical reactions, fluid dynamics).
- Governing Equations: These are foundational mathematical equations (like Newton's laws, Schrodinger's equation) that describe how systems evolve at different scales.
- Data Intensiveness: Modern MSM is data-heavy, requiring sophisticated methods for analyzing and handling large datasets—an area where ML is becoming important.

Integration of HPC and ML

- In recent times, there has been increased application of HPC and ML in MSM.
- Advances in computing allow for much more detailed simulations, while ML is beginning to assist MSM by finding patterns in massive datasets.
- Combining MSM, HPC, and ML could lead to innovative approaches in various fields (e.g., material science, biotechnology), making it possible to tackle even more complex problems than before.

Historical Milestones

- Several mathematical equations and methods form the historical basis of MSM and are essential to appreciate how MSM has reached its current state.
- They include, but are not limited to: Newton's laws of motion, Navier Stokes equation, Boltzmann equation, Schrodinger equation, Markov process, Linear response theory, Fluctuation theorems, and the modern-day computational algorithms.

Applications of MSM

- MSM is applied across disciplines, but especially in chemistry, biology, and engineering.
- For example, in biology, MSM helps simulate cellular processes that involve different scales—like how molecules move within cells (microscale) versus how cells interact with tissues (macroscale).
- In chemistry, MSM assists in understanding reactions at the atomic level while considering macroscopic effects like temperature.

Challenges

- One of the ongoing challenges is combining MSM and ML effectively, as both fields have traditionally developed independently. Another challenge is computational—solving multiscale problems often requires enormous computing resources, which is why advancements in HPC are vital.

Future Directions

- The future of MSM seems to be increasingly tied to the ability to leverage these computational advances to manage the growing complexity of modern problems.

Conclusion

- MSM is used to study problems that span multiple time and length scales due to the complexity of the systems involved.
- MSM involves constructing algorithms at various scales and coupling these scales rigorously to capture the system's behavior accurately. Traditional models are now augmented with advanced computational methods, including HPC and ML, allowing for more efficient simulations of large-scale problems.
- MSM involves creating algorithms that work at different scales and connecting these scales to accurately represent system behavior. By integrating advanced computational techniques like HPC and ML, traditional models can now run more efficient simulations for complex problems.

References

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