Determination of Kinetic Parameters for Heterogeneous Reaction System Employing Discrete Element Methods under HPC Platforms

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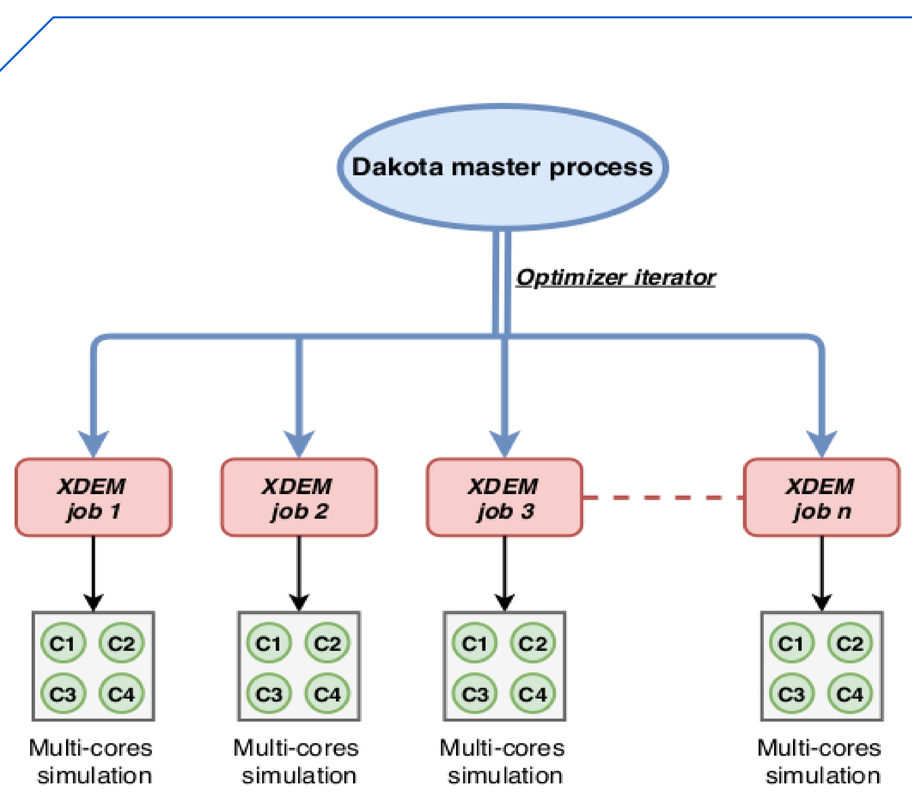
Introduction

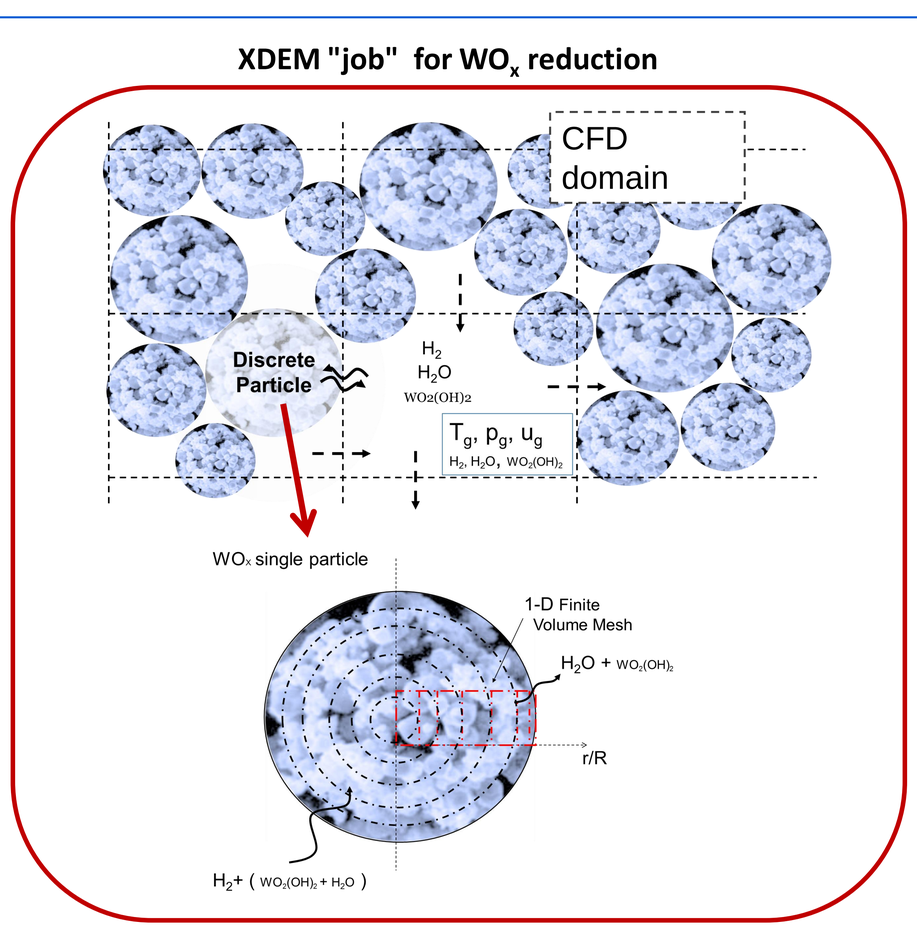
Heterogeneous reactions of granular materials, such as those involved in metals ore reduction or biomass gasification, are complex processes that involve numerous physical phenomena. The combination of elevated temperature, complex flow, aggressive atmosphere, and heterogeneous chemistry make it difficult to study these industrial processes. One of the most important aspects of these reactions is to understand and quantify the evolution of the different transformations, such as the rate at which pure metal is formed during metal-oxides reduction processes. However, it is almost impossible to accurately quantify and gain insight into these mingled nonlinear physical and chemical processes solely through experimental means. In the past decade, numerical simulation tools for particulate processes, such as the eXtended Discrete Element Method (XDEM) [1], have become indispensable for studying heterogeneous reaction systems without the need for costly experimental practices. However, the employed reaction rate parameters are often interpreted from lumped or empirical models bonded to specific experimental conditions resulting in differing kinetic data. To address this issue, we present an optimization problem for finding accurate kinetic parameters for the hydrogen reduction of tungsten trioxide system. We employed different algorithms implemented in a Dakota optimization toolkit [2] under High Performance Computing (HPC) platforms. The results show that this methodology can be extended to other complex industrial processes where resolved simulations are required.

Methodology

1. Simulation setup: Set up the XDEM simulation by defining the system's geometry, initial and boundary conditions, particle properties, and chemical reaction models. These models should consider mass, energy, and momentum transport, as well as thermochemical interactions between the particles and their environment.
2. Data acquisition: Perform simulations to obtain particle-level data such as species formation, transport, and reaction rates as a function of time.
3. Parameterization: Develop an objective function that evaluates the XDEM predictions [1] by comparison to experimental data. Define the kinetic parameters of the chemical reactions in the objective function, which are the variables that will be optimized using the algorithms. Namely, the *pre-exponential factor* and the *Activation energy* for the Arrhenius type of reaction rates.
4. Optimization: To optimize the kinetic parameters of WO_3 hydrogen reduction, we used, in Dakota [2], a combination of genetic algorithm and non-linear Newton least-squares local search. Specifically, we employed c*oliny_ea* for global search strategy and *optpp_newton* for full Newton method.
5. Evaluation: Evaluate the performance of the optimization algorithms by comparing the optimized results with experimental data. Assess the quality of the results and the convergence rate of the algorithms.
6. High-Performance Computing (HPC): The optimization tasks were performed on the UL HPC platform [3], which were necessary to handle the large number of function evaluations generated by the optimization algorithms in Dakota and to manage the extensive amounts of data generated by the XDEM simulations.



Source: Dr. A. Rousset, FNR grant *Grant 2018-2/13318107-VP4HPC*



Results

Explore our optimization results and other complex simulations for heterogeneous reaction systems by scanning the QR code provided:

Conclusions

- The combination of XDEM and optimization algorithms provides a powerful tool for optimizing complex processes in heterogeneous reactions.
- The utilization of High-Performance Computing (HPC) platforms has allowed us to efficiently handle the large amounts of computation required by the XDEM simulations and the optimization algorithms.
- Optimization Solution: Hybrid Genetic Algorithm coupled With Newton presented the fastest convergence and best performance relative to cpu cost.
- This approach can be extended to other complex processes in heterogeneous reactions, making it a valuable tool in industrial applications.

References

[1] B. Peters, et al., XDEM multi-physics and multi-scale simulation technology: Review of DEM–CFD coupling, methodology and engineering applications, Particuology, Volume 44, 2019

[2] B.M Adams et al., Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.15 User's Manual, Sandia Technical Report SAND2020-12495, November 2021

[3] S. Varrette et al., Management of an Academic HPC Cluster: The UL Experience, Proc. of the 2014 Intl. Conf. on High Performance Computing & Simulation, 2014

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