

Mentor Introductions

SIMCODES 2025



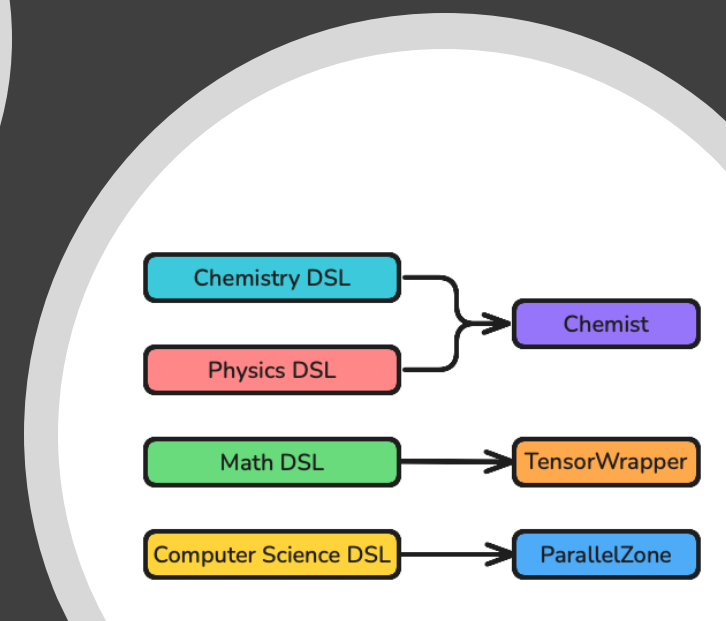
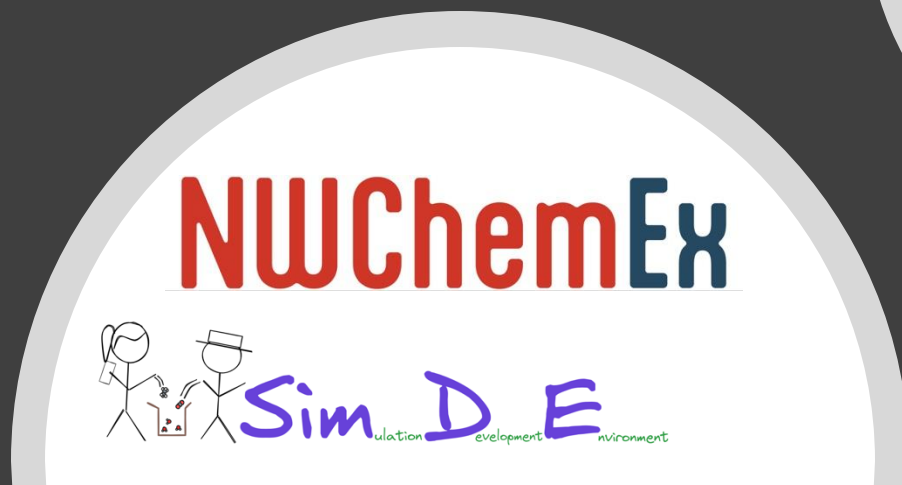
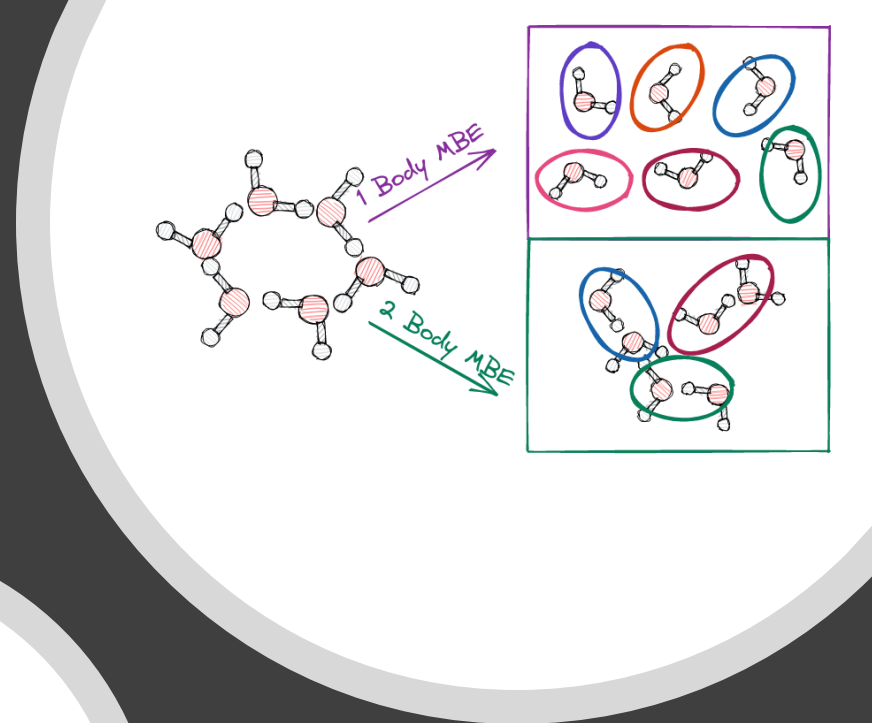
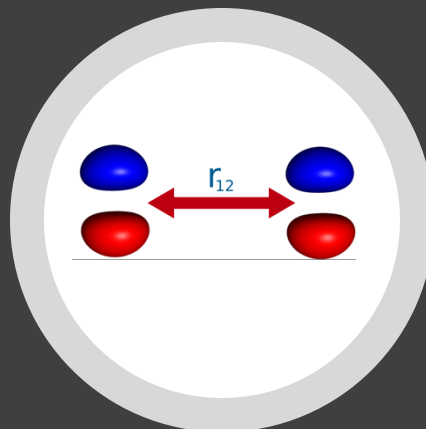
Ryan Richard

- Scientist at Ames National Laboratory and Adjunct Professor of Chemistry at Iowa State University.
- Background: Grew up in Ohio, PhD in chemistry from “The” Ohio State University.
- Interests: travel, technology, video games, exercise, being told what to do by my dogs.



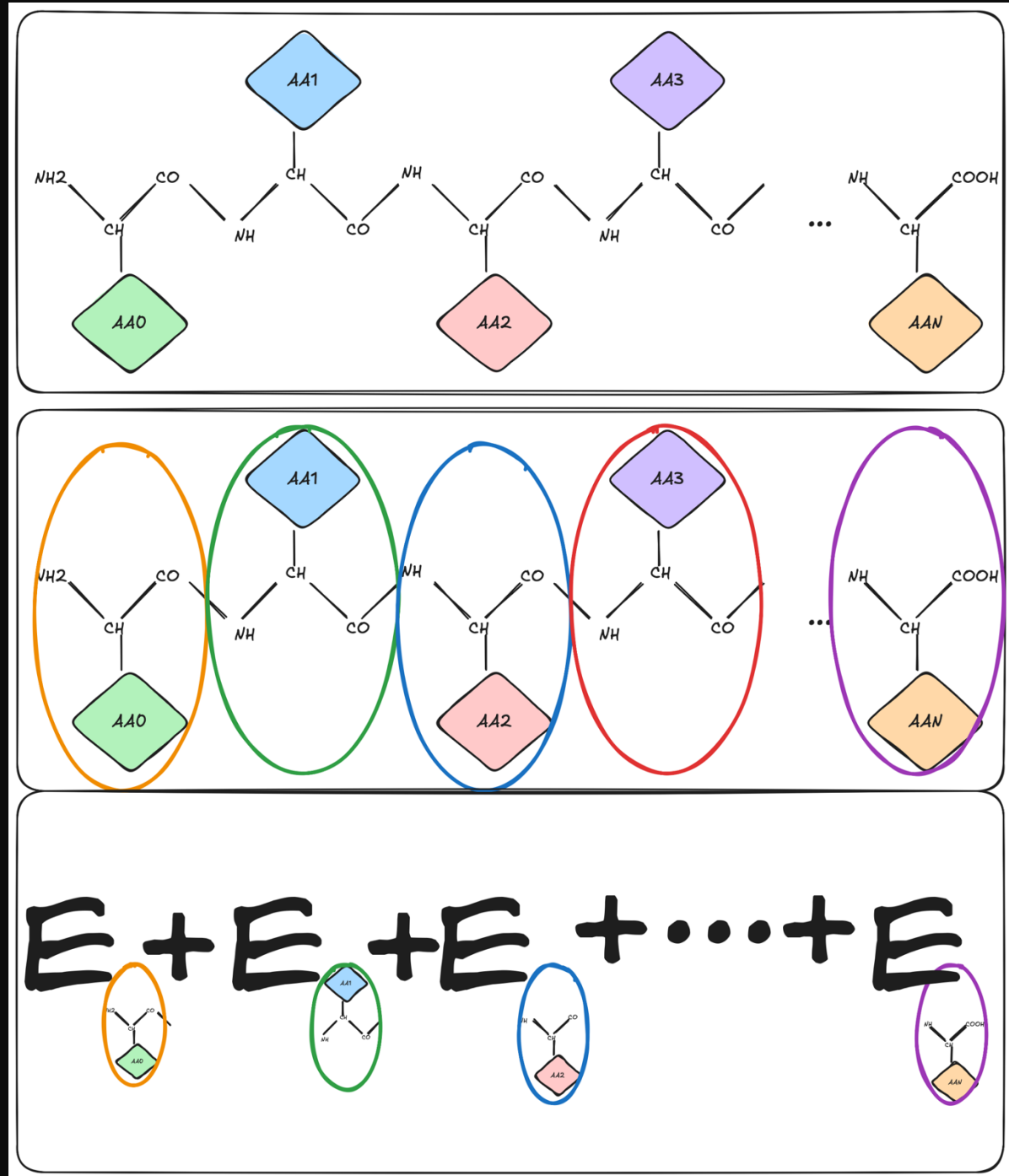
Research in the Richard Group

- Research interests: Sustainable scientific software development, high-performance computing, reduced scaling electronic structure theory.
- Develop for NWChemEx ecosystem.
- Strong emphasis on software engineering applied to theoretical chemistry.



SIMCODES Project: Developing components for automating fragmentation

- Mentee: Daniel Woodard
- Summary: Winner-take-all battle between Daniel's chemical intuition and the best AI/ML model Gabriela and Devarsh can make.
- Goals:
 - Develop tools for reading PDF files.
 - Function for identifying amino acids in a protein.
 - Function for splitting a protein by amino acid.





The Richard and Windus Groups