Mentor Introductions

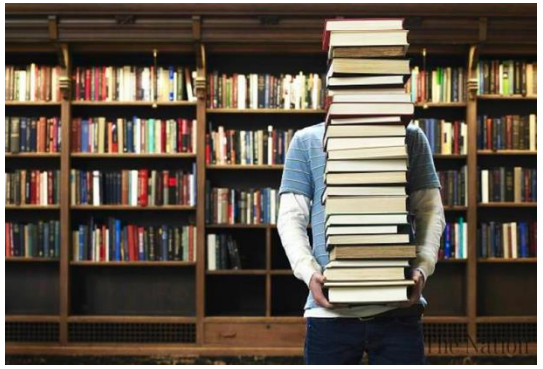
SIMCODES 2025

Qi Li

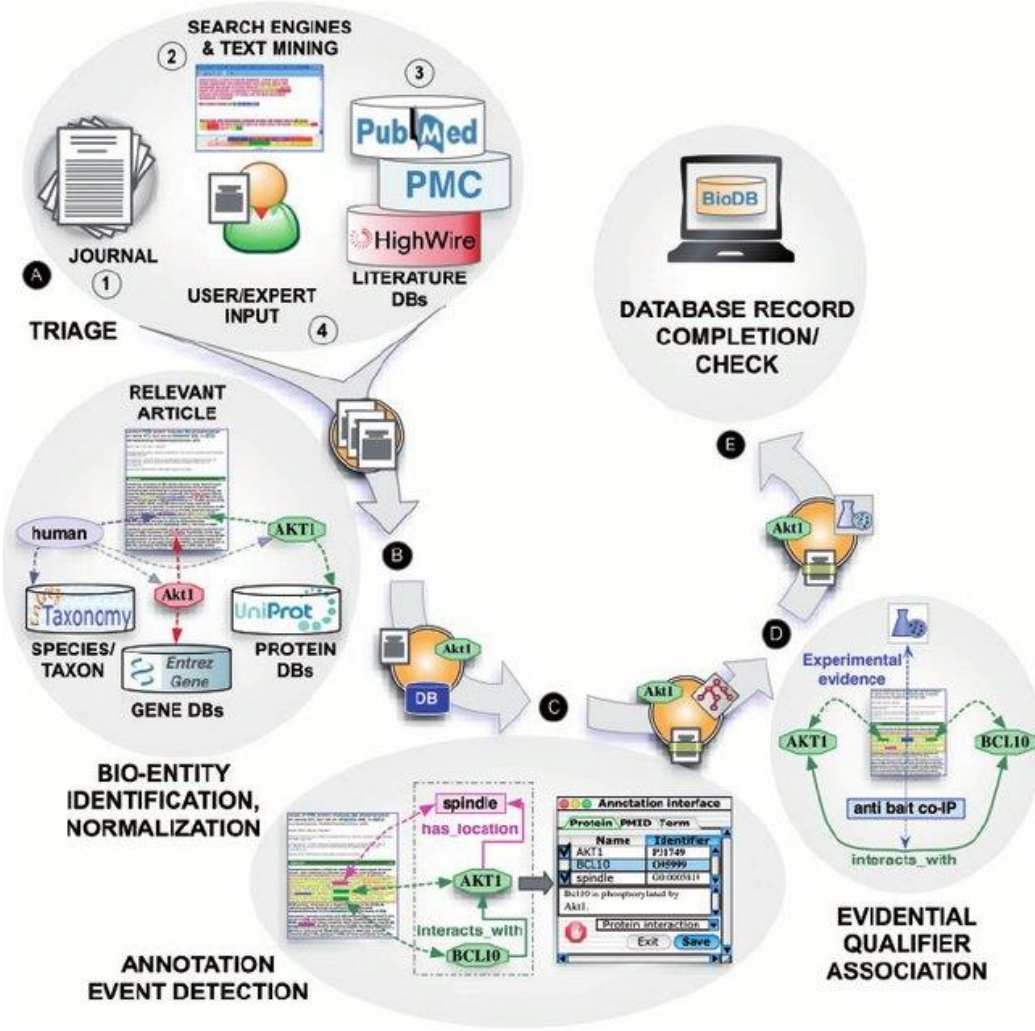
- My name
  - Name can tell a lot
  - Gender, Ethnicity, Age, Religion, …
  - Important feature for many NLP tasks
- My background
  - BS. Math
  - MS. Stats
  - PhD. CS

My research

- NLP -- Information extraction
- Generation models
- Applied ML

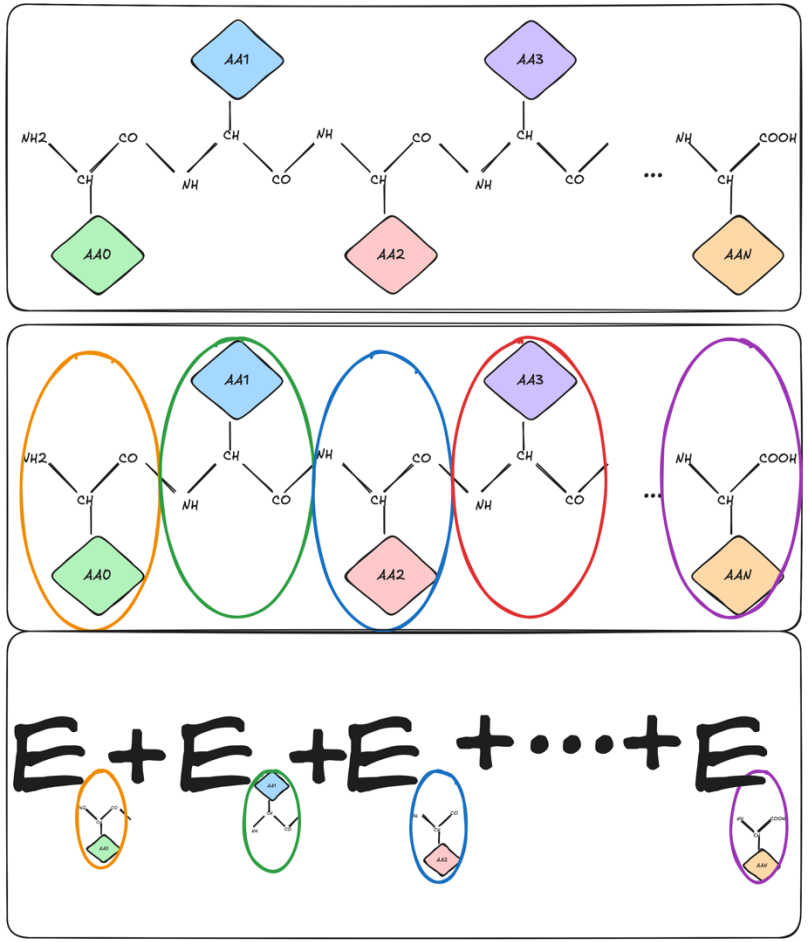


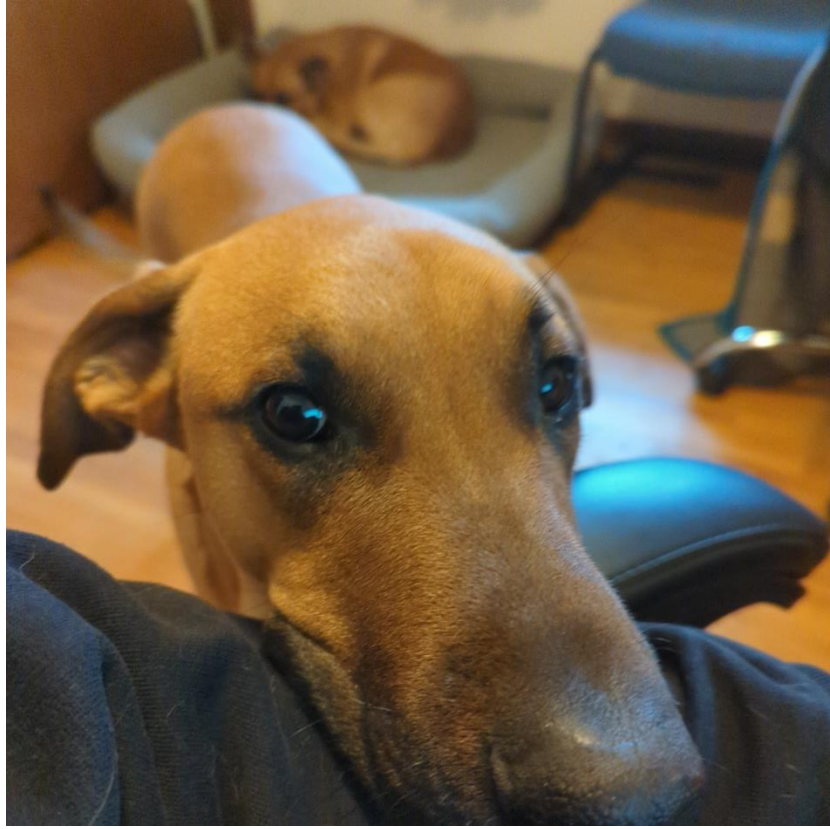
Knowledge
& Insights



SIMCODES Project:
Developing components for automating fragmentation

- Mentee: Gabriela and Devarsh
- Goals:
  - Function for identifying amino acids in a protein.
  - Function for splitting a protein by amino acid.
  - Idea: protein as an unnatural language



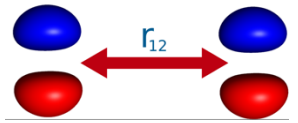


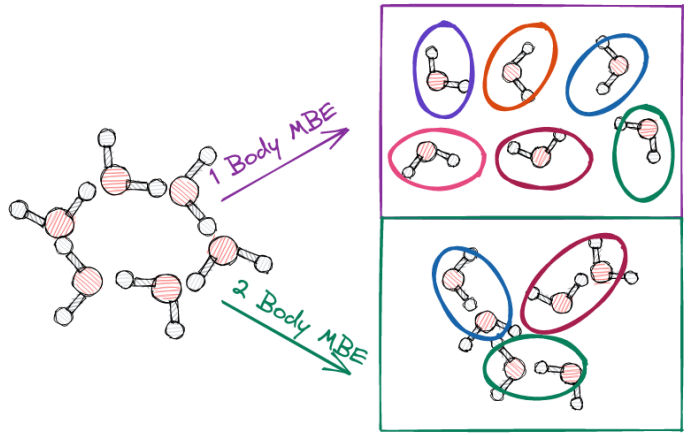
Ryan Richard

- 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.

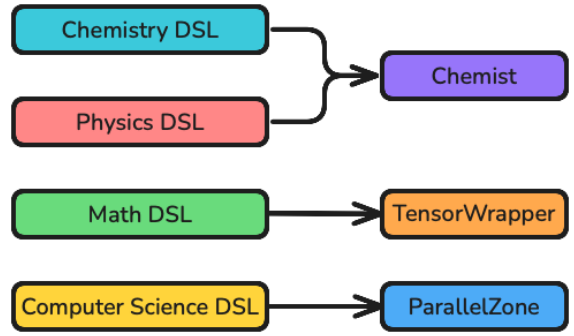




PluginPlay

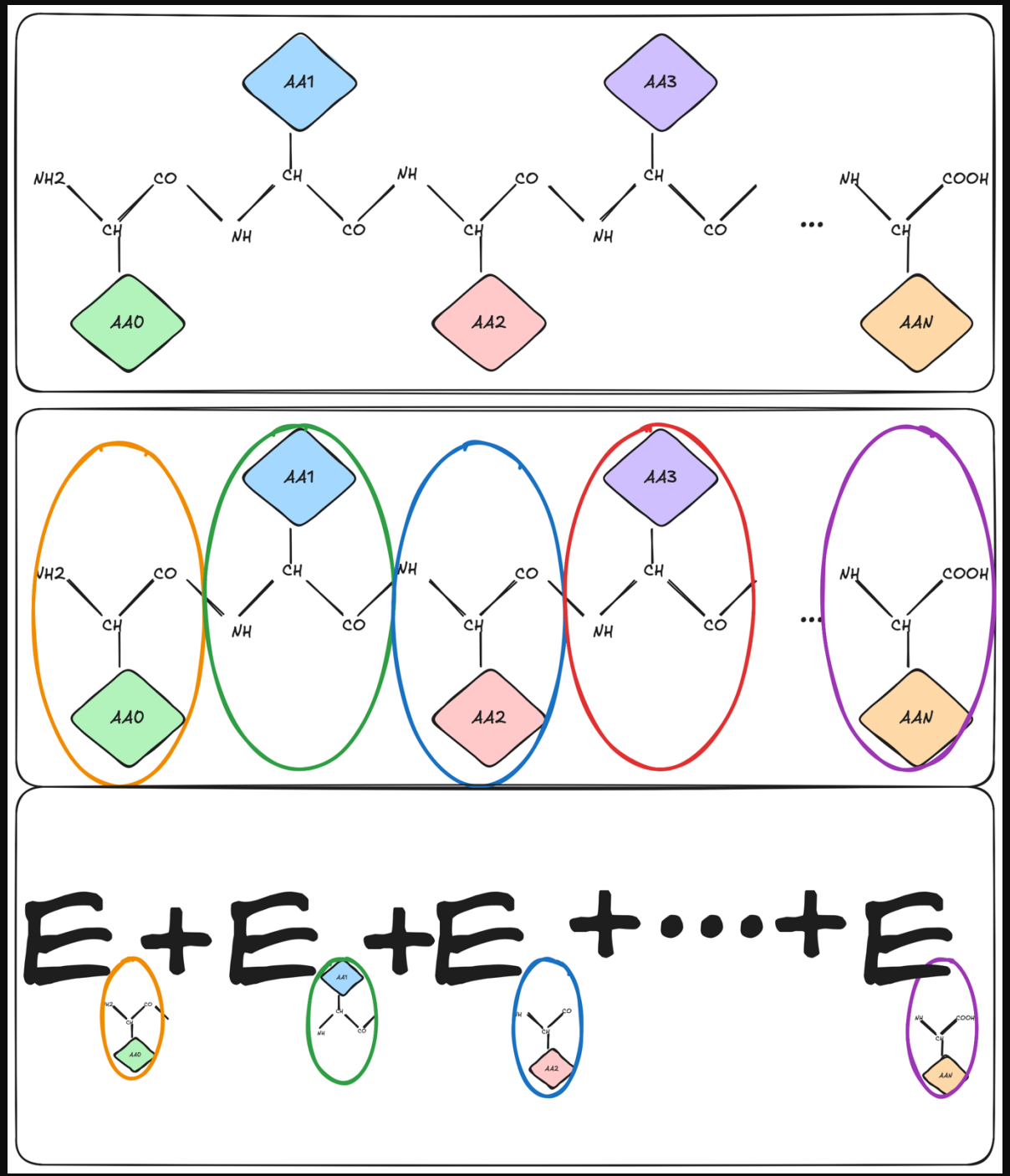
NWChemEx

SimDE



SIMCODES Project: Developing components for automating fragmentation

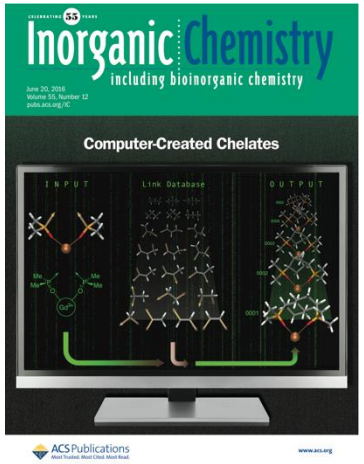
- Mentee: Daniel Woodard
- Summary: Winner-take-all battle between Daniel's chemical intuition and the best AI/ML model Gabriela and Devarsh can make.
- Goals:
  - Develop tools for reading PDF files.
  - Function for identifying amino acids in a protein.
  - Function for splitting a protein by amino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

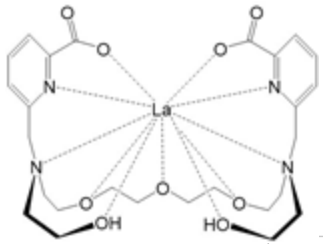


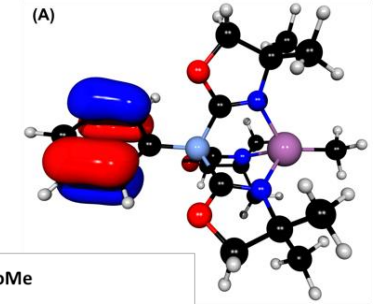
The Richard and Windus Groups

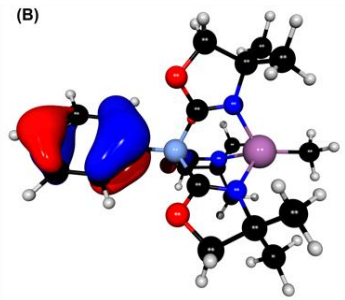
The Windus Group

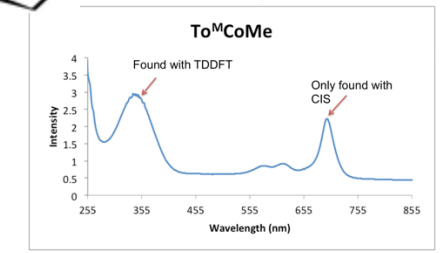
Separations and catalysis challenges



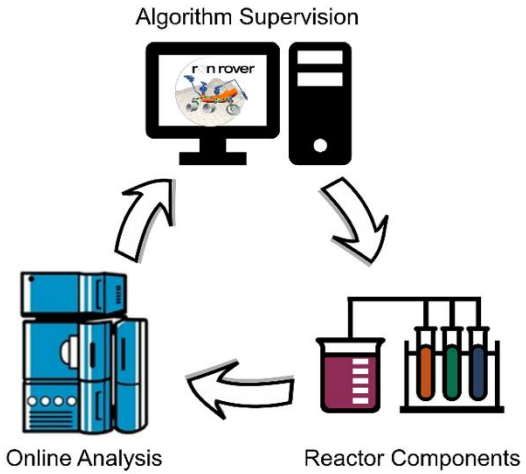




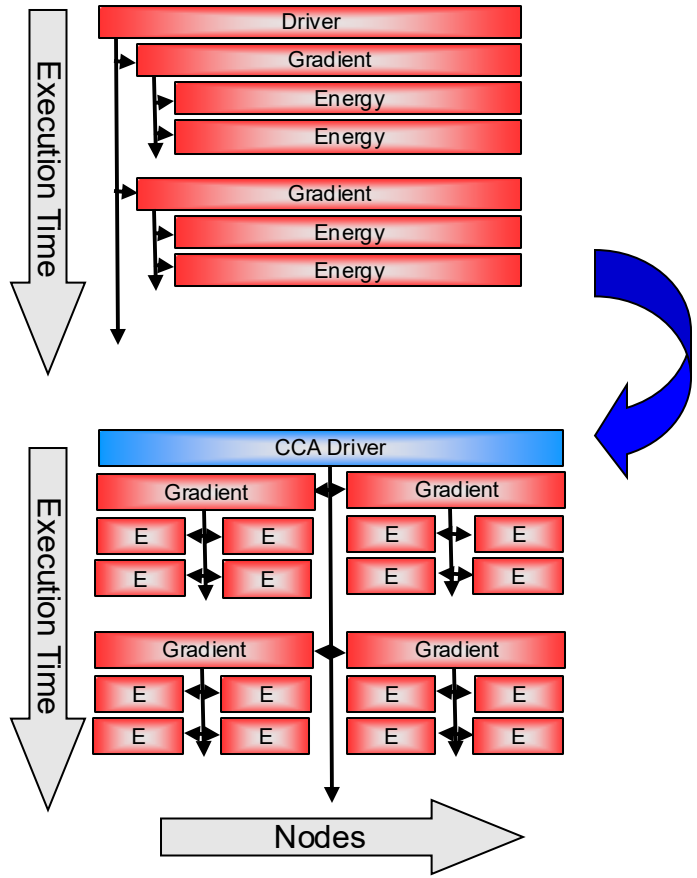




Reaction optimization and lab automation



High performance, exascale computing



The Windus Group and Funding

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CMI Accelerating Energy Innovations

NWChemEx

Department of Energy

Air Force Office of Scientific Research

NSF

AMES National Laboratory 1947 75 2022

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