Theory to Software Translation: Different challenges for different aspects

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My background

- PhD in Quantum Chemistry
- Worked
  - GAMESS-UK (and ChemShell)
  - NWChem
  - Currently
    - NWChemEx
    - Comsuite

Interesting challenges

- Scientific
  - Validate models by comparing to experiment
  - Mapping experimental results to computed results not always unambiguous
- Models
  - ChemShell tried combining arbitrary QM to arbitrary MM codes
  - Same high level concepts are differently implemented in detail
- Culturally
  - Some groups will coordinate everything through a common github repository
  - Some individual will just fork a code and go off on their own
- Technical
  - Difference between running on your desktop vs. compute cluster
- Data
  - Growth of machine learning increases needs for long term data storage
  - Individual research groups don’t have the resources