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