Using Optimization to Drive Materials Design

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Scientific Achievement

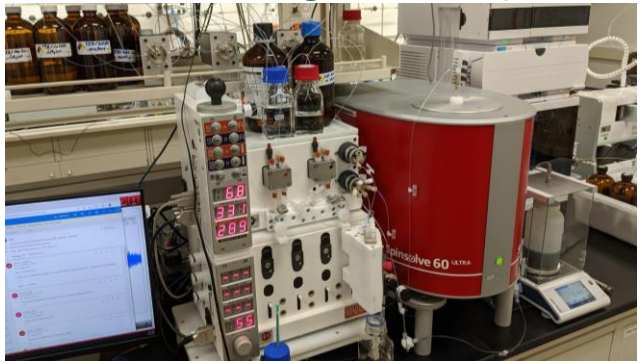
Optimization software is backbone for self-driving continuous-flow chemistry lab for materials design and manufacturing

Significance and Impact

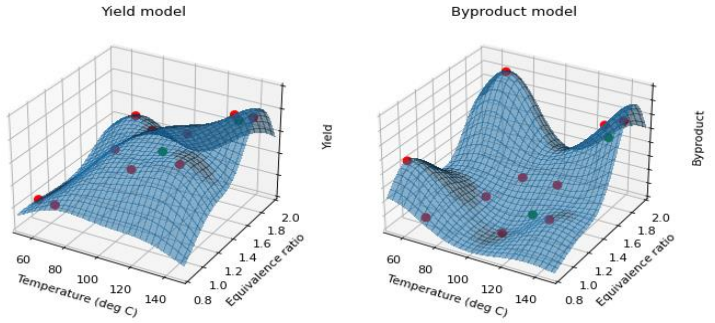
By integrating multiobjective optimization with a continuous-flow reactor (CFR) and nuclear magnetic resonance (NMR) spectroscopy, we save significant time and resources in materials design and discovery

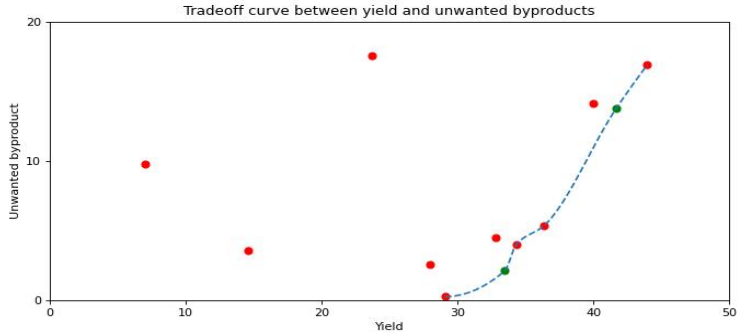
Research Details

- *Multiobjective optimization* software **ParMOO** was originally designed to support parallel, computationally expensive simulations in SciDAC
  - Deployed here in a time-expensive synthesis and characterization loop
- Traditionally, material scientists choose manufacturing conditions via trial/error:
  - Expensive, in terms of time and raw material requirements
  - Involves *tradeoffs* between maximizing yield and minimizing unwanted byproducts
- **ParMOO** generates CFR configurations in a closed, operator-free loop:
  - ParMOO sends candidates directly to CFR controller
  - CFR performs material synthesis and sends output to NMR
  - NMR characterization results sent to ParMOO



Setup: lab computer (left) with ParMOO generates design, CFR (middle) performs synthesis, NMR (right) processes output, which is returned to ParMOO





ParMOO dynamically updates yield and byproduct surrogates, then uses these models to balance tradeoffs

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parMOO

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