DIRECT Capstone Project -

Neural networks for fast analysis of complex chemical reaction mechanisms

- 1 Slide Updates -

Ivan Cui
Daniel Pan
Jiayuan Guo
Yu Liu

UNIVERSITY of WASHINGTON

Neural networks for fast analysis of complex chemical reaction mechanisms

Project sponsors: David Beck, Jim Pfaendtner

- **Tasks and Methods:** Mathematical analysis and implementation of ODE solvers for lignin pyrolysis in both Cantera and scipy.integrate packages
- **Data description:** 3 files defining kinetic parameters in 406 reactions, and the initial composition of 93 lignin species
- **Preliminary results:** Using LSODA in scipy.integrate to solve ODE sets and find the running time is long.

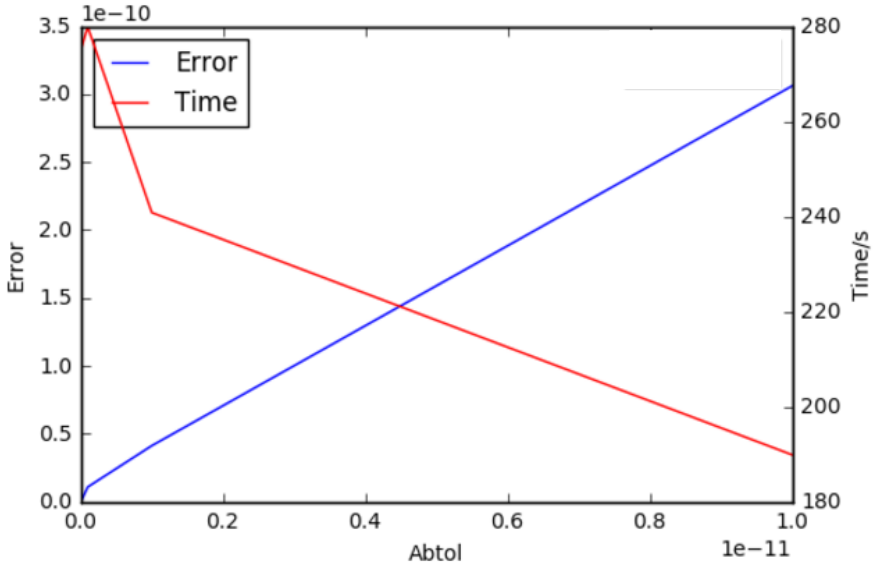

Figure. Error-Time tradeoff for LSODA ODE Solver