Team CoMoChEng

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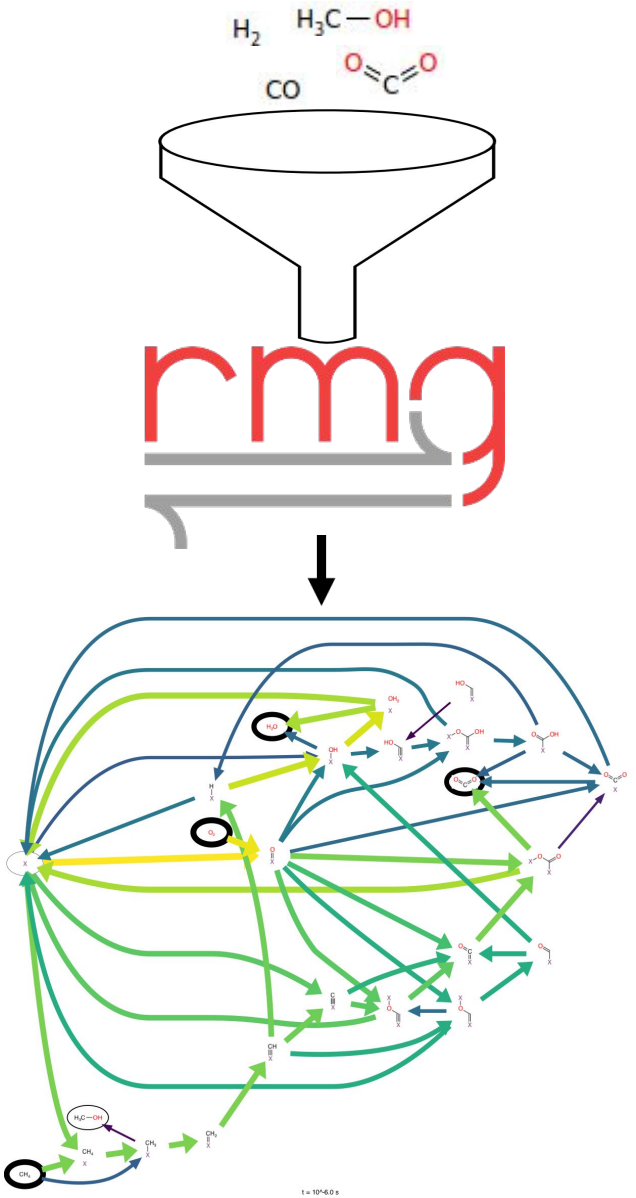
The Reaction Mechanism Generator (RMG)

- Automated chemist: generates complicated chemistry by iteratively including more molecules/reactions in a reactor simulation
- Python-based, with some Julia packages
- Reactor simulation (Julia) and chemical reaction generator (Python) will be focus for speedup.
- GPU port path: Numba, and kernelabstractions.jl, prefer to keep hardware agnostic.



Goals

- What would you like to achieve by the end of the week?
  - Determine *specifically* what code we can improve with GPUs, we've profiled and found where we lose the most time, but need a concrete target.
  - Learn more about GPU acceleration in Python and Julia.