



Team CoMoChEng

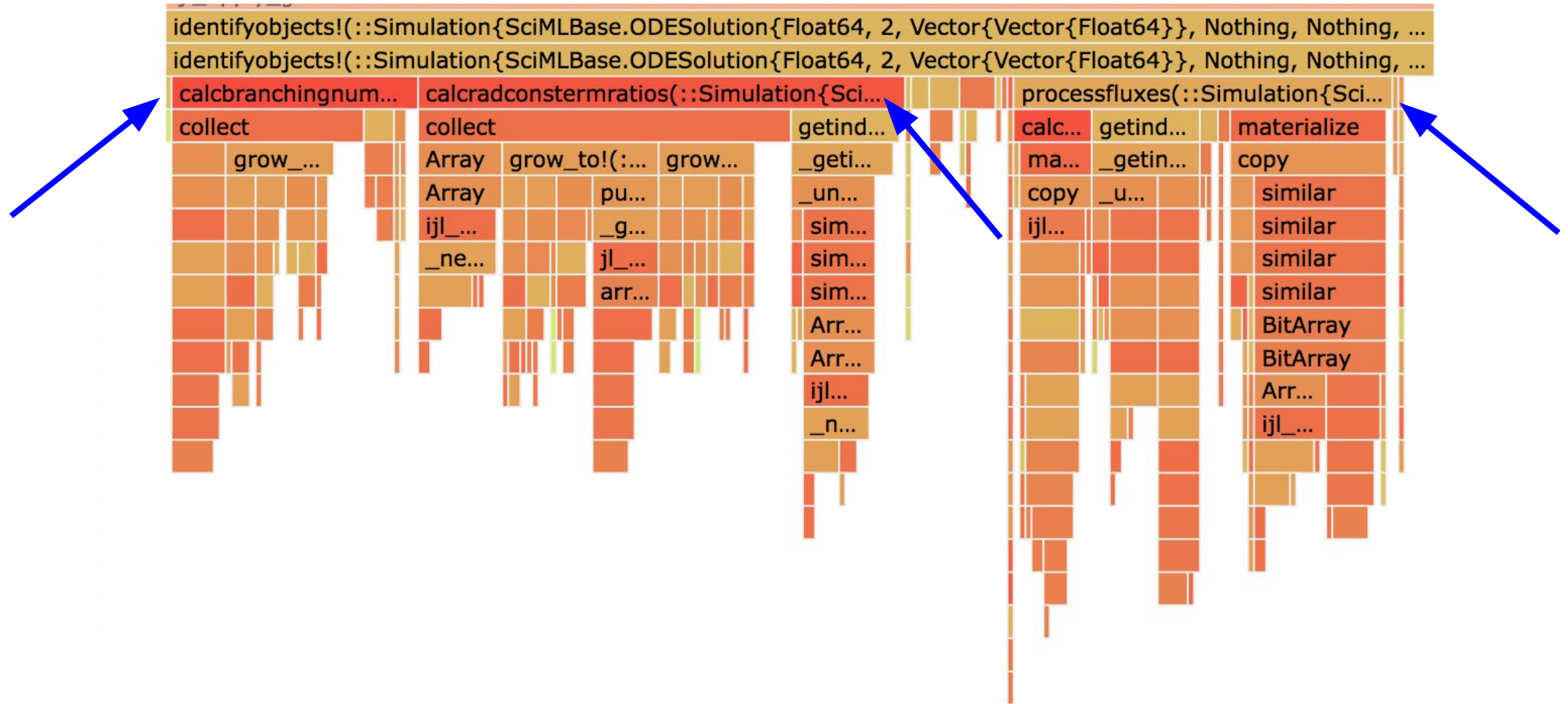
Chris Blais, Chao Xu, Sevy Harris, Su Sun, Nora Khalil
(Northeastern University)

Mentors:

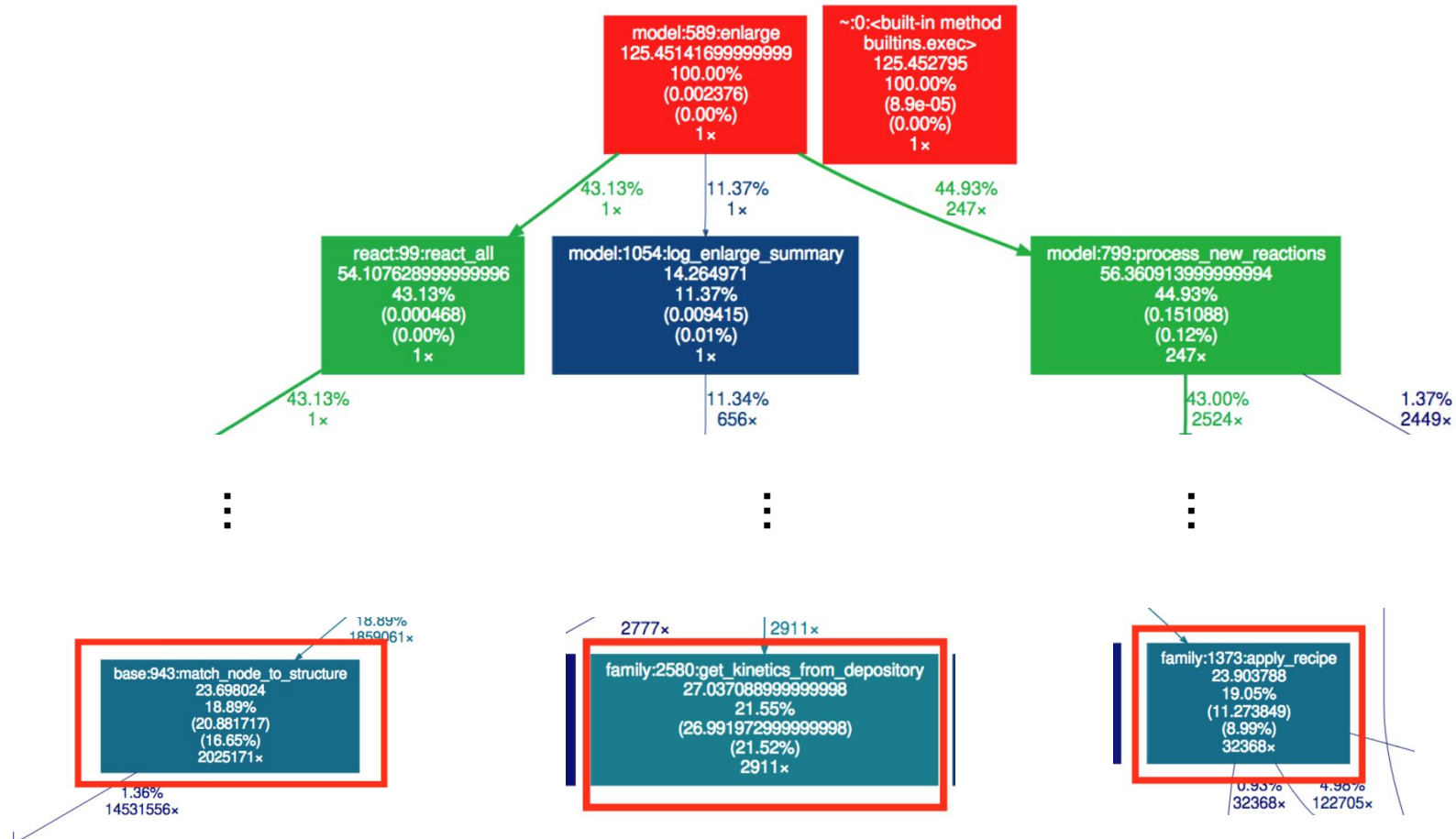
Johannes Blaschke, Weile Wei, Dhruva Kulkarni
(NERSC)

Profiler Output

Julia Profile:



Python Profile (cprofile):



Progress and Goals

- What have you accomplished since yesterday?
 - we have profiled our julia code, and determined specific spots in the julia code that can be sped up using a gpu.
 - we have profiled the python portion of our code that was using the most overhead. We do not have a target yet, it may be impossible.
- What are your goals for the day?
 - use `cuda.jl` as a first pass for speeding up the julia portion of our code.
 - investigate VF2 isomorphism checks on the python side and see if there is a path forward there.

Problems and Solutions

- What problems are you currently facing?
 - julia portion has many memory allocation operations. speeding it up on a GPU may not give us a significant speedup if we can't cleverly write data to the gpu at the beginning.
 - may be impossible to speed up python portion with gpus without refactoring large portions of the code.
- Have you resolved any problems (or found bugs) that others might find useful?
 - Most issues we've encountered so far have been addressed. Like most other execution issues, CUDA.jl test suite needs to be run from the scratch folder.