



MDSimAid: From Fast Electrostatics to Parallel Scaling

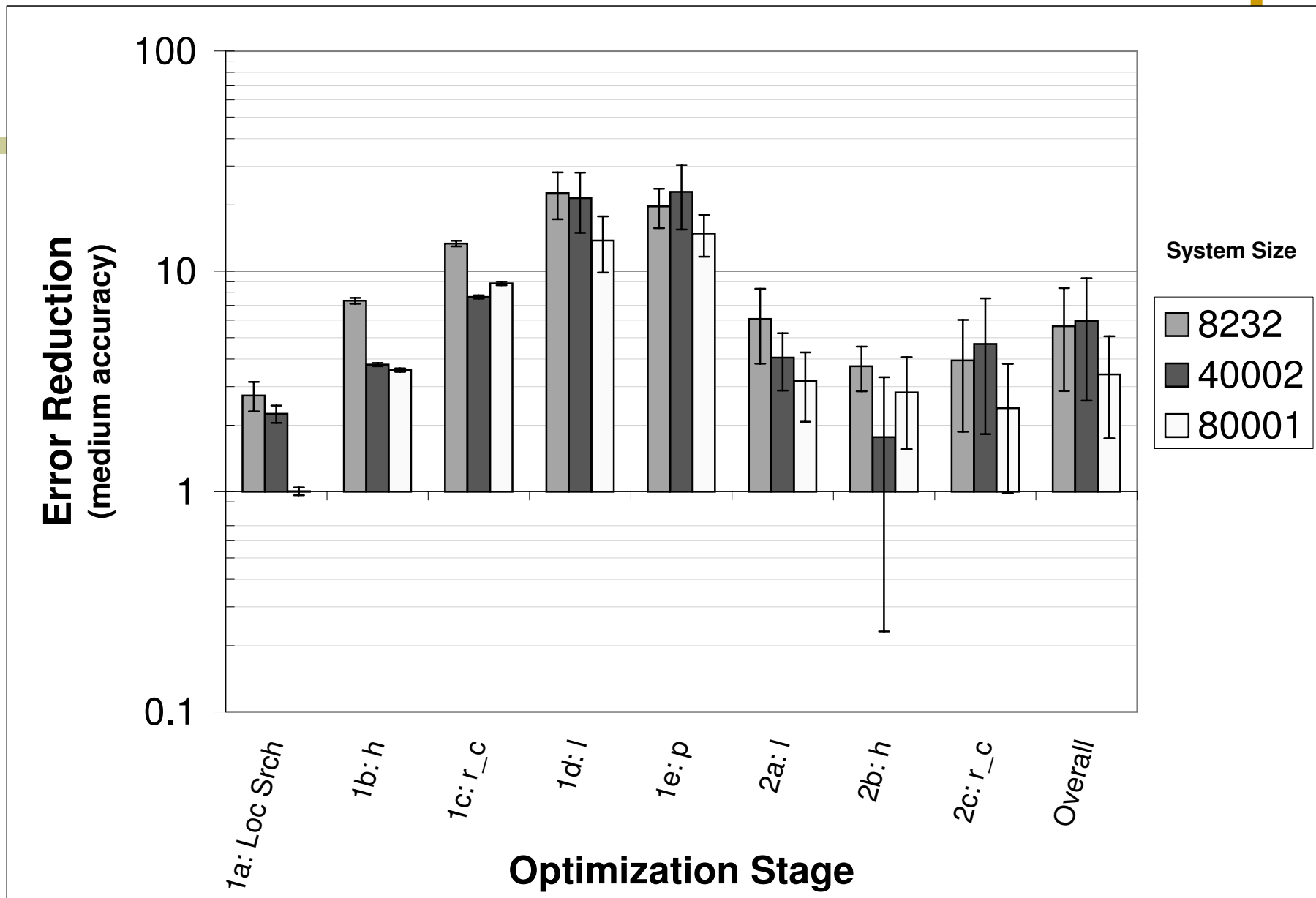
Michael Crocker

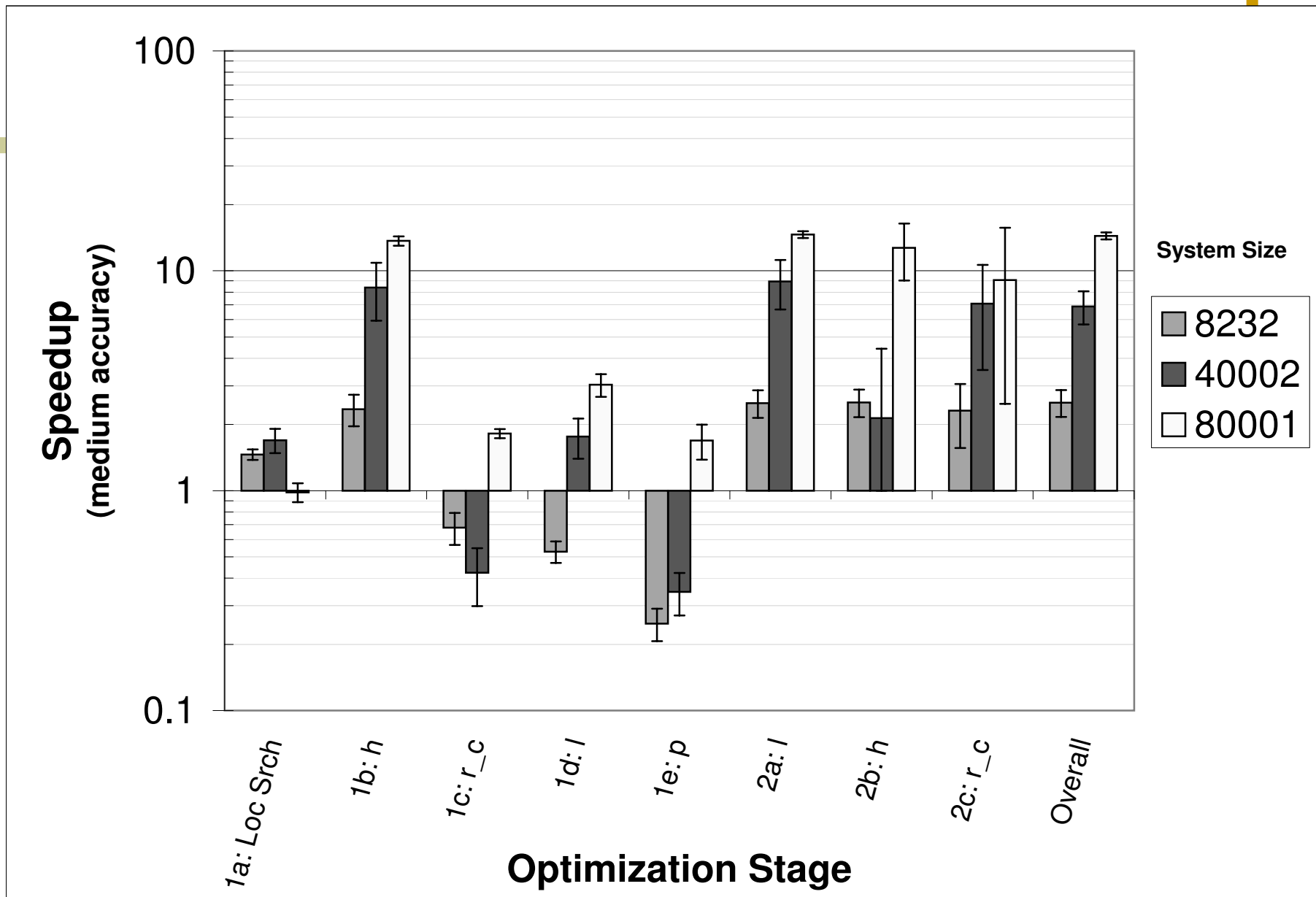
[Optimizing Fast Electrostatics]

- PMEwald
 - cutoff
 - accuracy
- MultiGrid
 - gridsize
 - softening distance
 - levels

[Order of Optimizations (MG)]

- Local Search
- Optimize for Accuracy
 - gridsize
 - softening distance
 - levels
- Optimize for Speed
 - levels
 - gridsize
 - softening distance

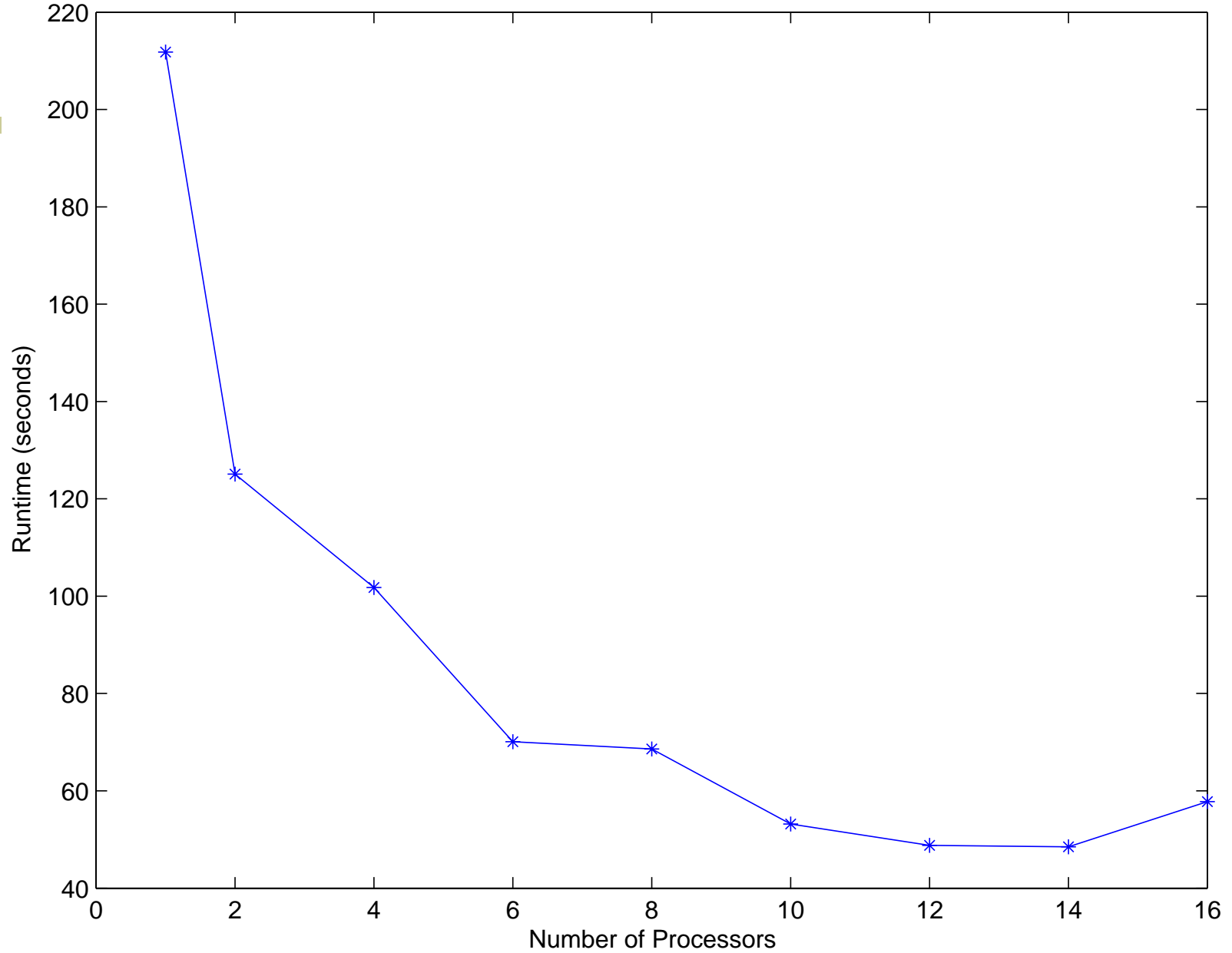




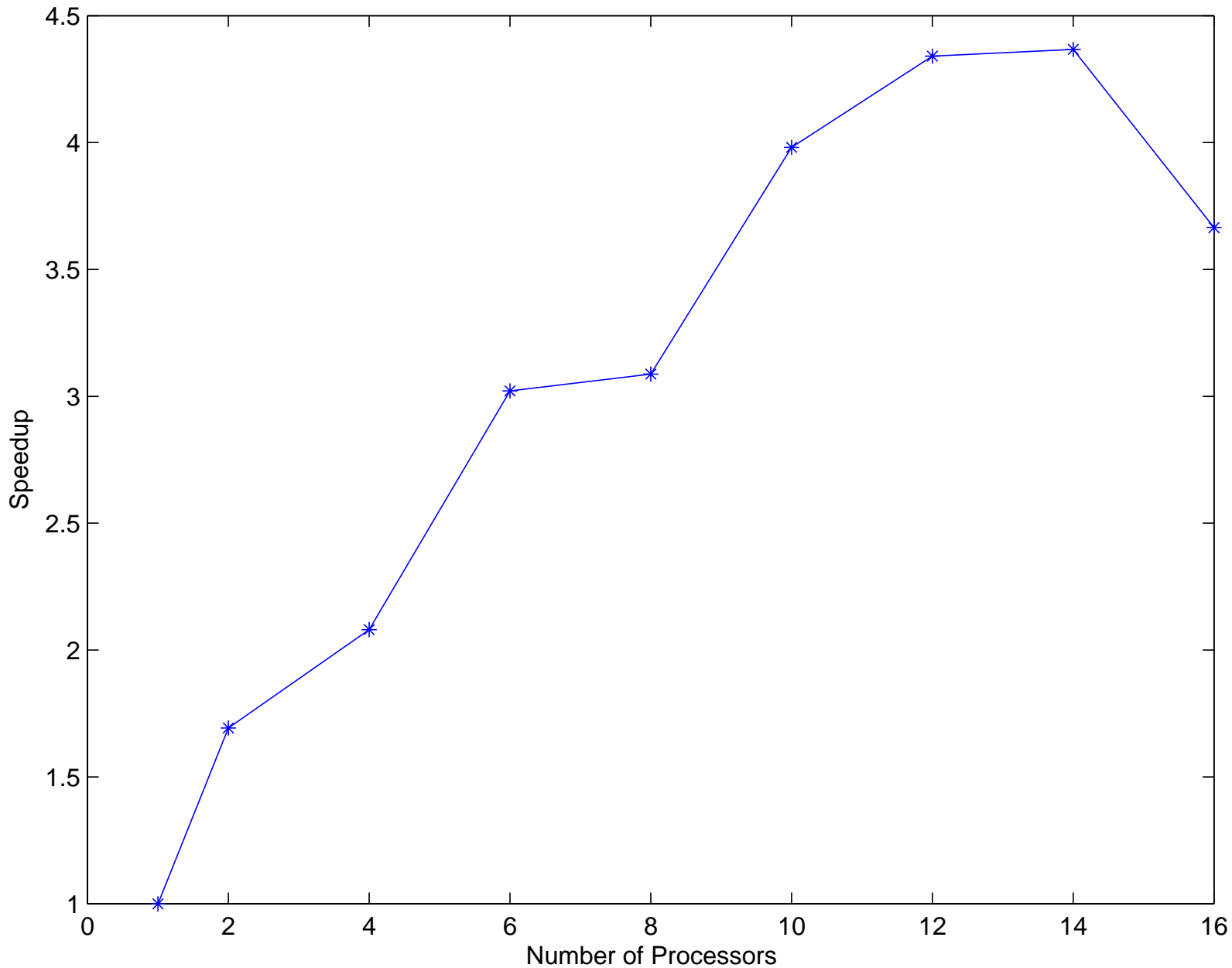
[Optimize for Parallel Execution]

- Number of Processors
 - nop
- Load Balancing and Communication
 - master/slave or static
 - barrier or no barrier
 - parallel pipe (pipe depth)
 - max. packages

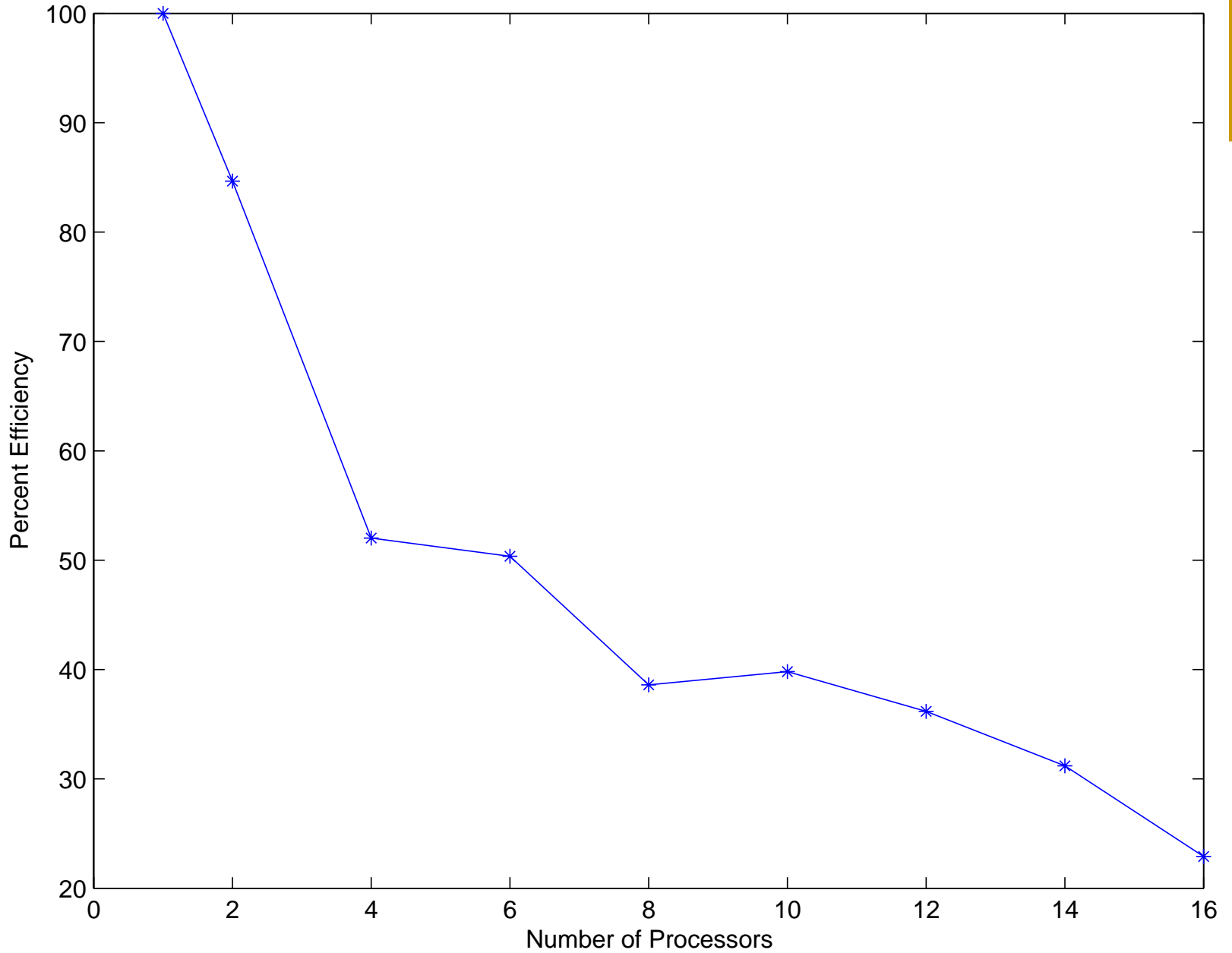
APOA1 run with Master/Slave



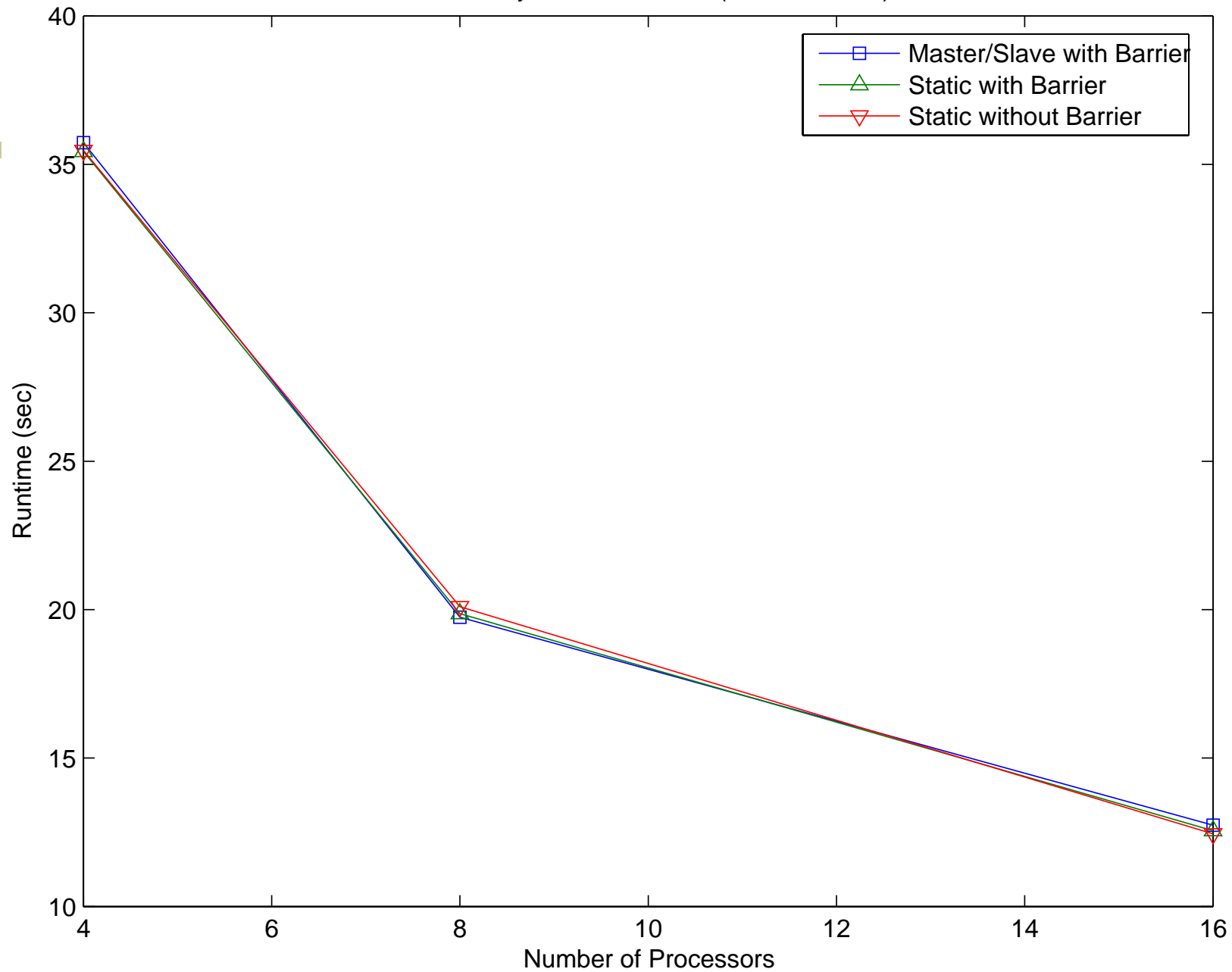
APOA1 run with Master/Slave



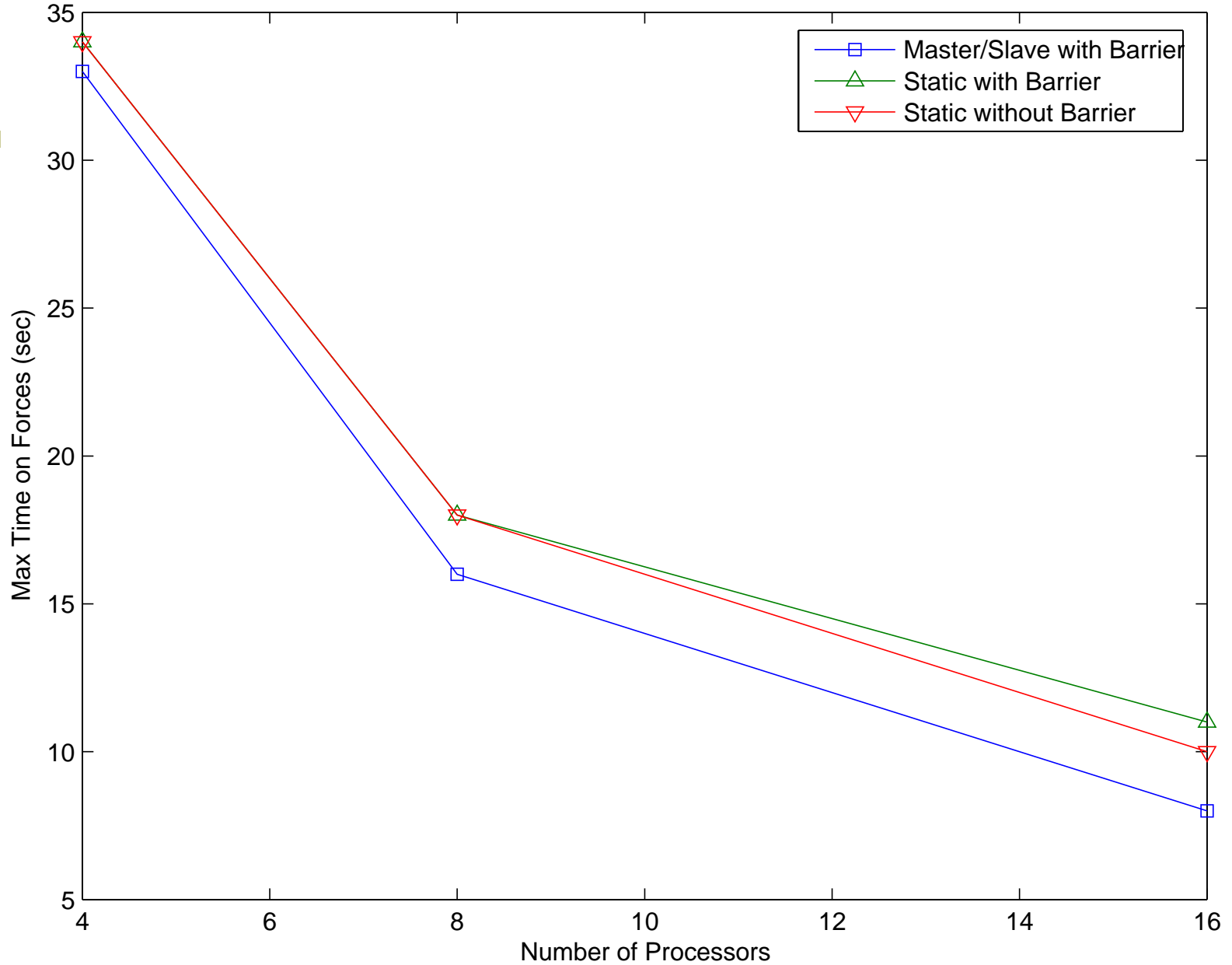
APOA1 run with Master/Slave



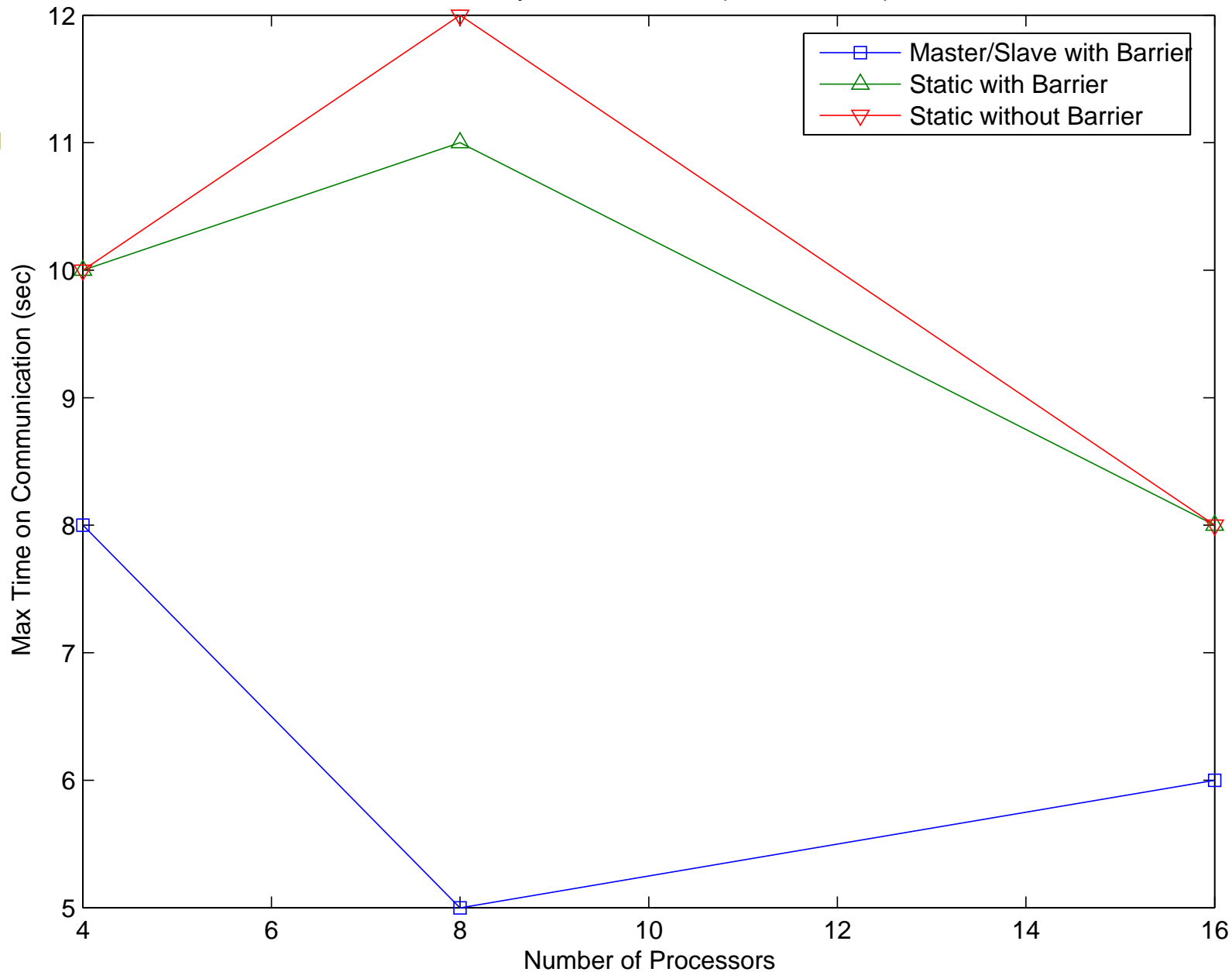
APOA1 System with Water (92,224 Atoms)



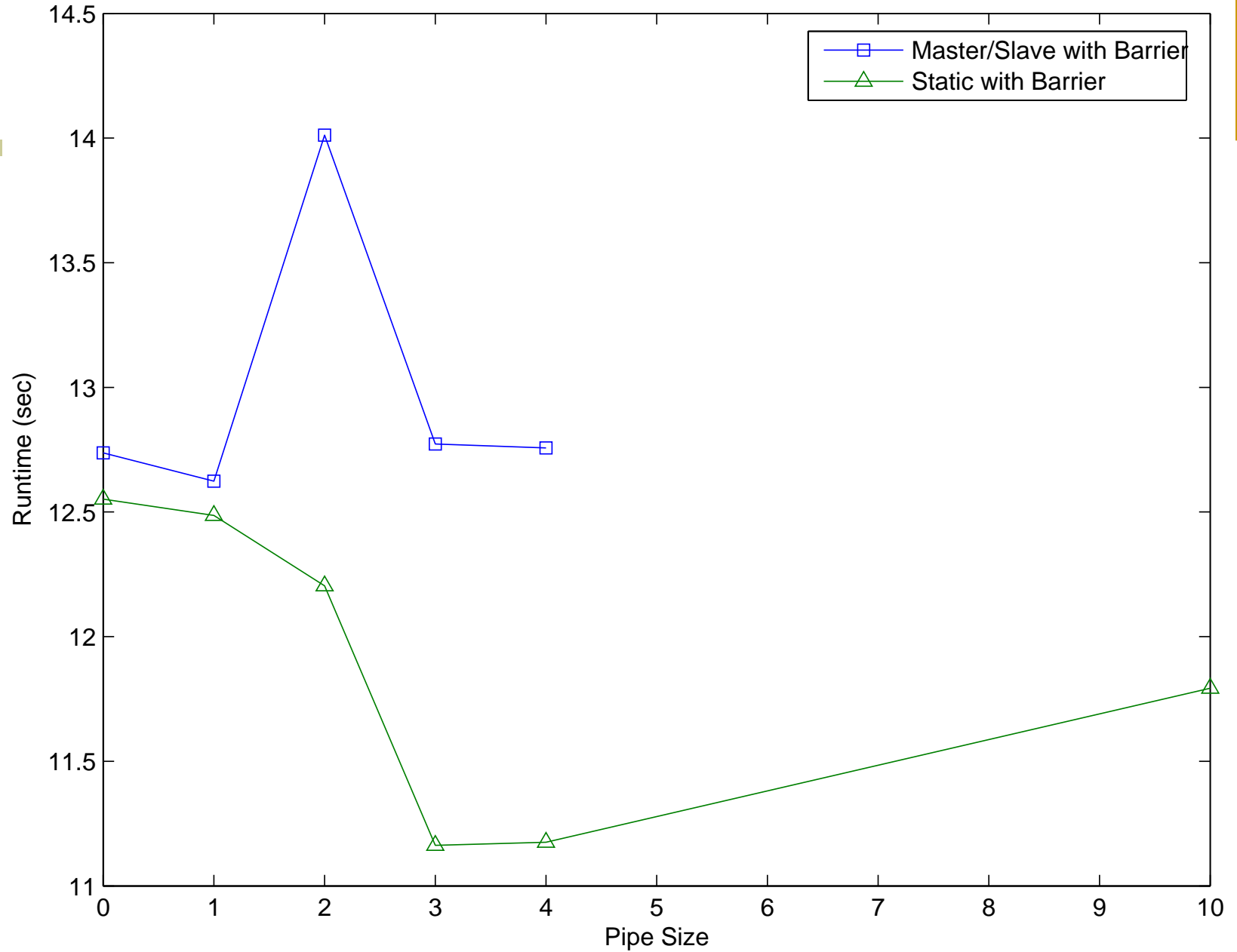
APOA1 System with Water (92,224 Atoms)



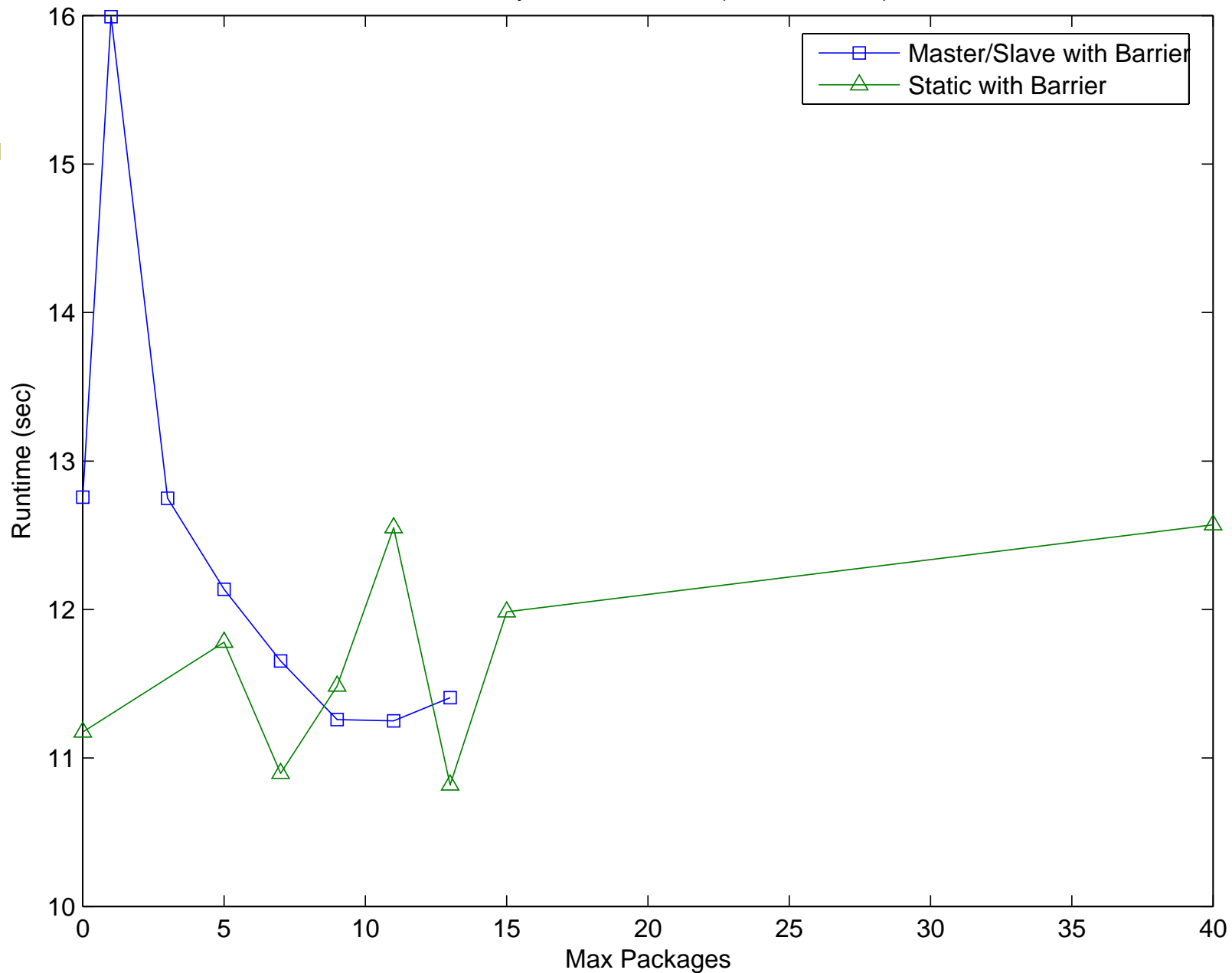
APOA1 System with Water (92,224 Atoms)



APOA1 System with Water (92,224 Atoms)



APOA1 System with Water (92,224 Atoms)



[What does this data tell us?]

- The data is inconclusive in terms of determining performance.
- More tests are needed.
- Creating an automated script for testing these parameters, like for MG and PME, would be great.
- Still need to fix some mpirun issues.
- Don't want to crash iss again.