# Findings

* Hybrid (global + shared) memory provided best results for all models
* cupSODA was faster than SciPy if at least 1000 simulations were performed (true for all three models)
* Optimal number of threads-per-block depends on the model, number of simulations, and memory choice.

|  |  |  |  |
| --- | --- | --- | --- |
|  | Typical best Tesla K20c  Threads/block | | |
| Number  simulations | Tyson | Ras | EARM |
| 1000 | 8 | 8 | 4 |
| 10000 | 64 | 16 | 8 |

* cupSODA improvements over single CPU for 10,000 simulations:
  + Tyson

|  |  |  |
| --- | --- | --- |
| GPU | Solving time decrease (%) | Total time decrease (%) |
| Tesla K20c | 94 | 78 |
| GTX 760 | 90 | 75 |
| Gt755m (1000 sims) | 75 | 61 |

* + Ras

|  |  |  |
| --- | --- | --- |
| GPU | Solving time decrease (%) | Total time decrease (%) |
| Tesla K20c | 79 | 73 |
| GTX 760 (1000 sims) | 35 | 30 |
| Gt755m (1000 sims) | 10 | -7 |

* + EARM

|  |  |  |
| --- | --- | --- |
| GPU | Solving time decrease (%) | Total time decrease (%) |
| Tesla K20c | 64 | 61 |
| GTX 760 (1000 sims) | 30 | 27 |
| Gt755m (1000 sims) | -57 | -65 |

# Hardware

* Tesla K20c
  + 2496 processor cores
  + 706 MHz processor core clock
  + 5 GB Memory size
  + 20 pieces of 64M x 16 GDDR5, SDRAM
  + 2.6 GHx Memory clock
  + 208 GB/sec Memory bandwidth
  + Peak double-precision 1.17 Tflops
  + Peak single-precision 3.52 Tflops
* GeForce GTX 760
  + 1152 processor cores
  + 980 MHz processor core clock
  + 2 GB Memory size
  + 192.2 GB/sec Memory bandwidth
  + Peak double-precision .99 Tflops
  + Peak single-precision 2.26 Tflops
* GeForce Gt 755M
  + 384 processor cores
  + 980 MHz processor core clock
  + 2 GB Memory size
  + 86.4 GB/sec Memory bandwidth
  + Peak double-precision .99 Tflops
  + Peak single-precision .75 Tflops
* Intel i7- 4820K Ivy Bridge E
  + 4 core
  + 8 threads
  + 3.70 GHz processor base frequency
  + 3.90 GHz Turbo frequency
  + 16GB Memory
  + 10 MB Cache
* Software
  + Python 2.7.6
    - Scipy 0.15.1
    - Numpy 1.9.2
  + gcc (Ubuntu 4.8.2-19ubuntu1) 4.8.2
  + GNU Fortran (Ubuntu 4.8.2-19ubuntu1) 4.8.2

# Methods

Performed simulations of Tyson oscillator (1991), Ras, and EARM.

|  |  |  |  |
| --- | --- | --- | --- |
| Model | Tyson | Ras | EARM |
| Number  of reactions | 7 | 39 | 105 |
| Number  of species | 6 | 33 | 77 |
| Atol | 1e-6 | 1e-6 | 1e-6 |
| Rtol | 1e-6 | 1e-6 | 1e-6 |
| End Time | 100 | 1500 | 20000 |
| Number of  output times | 100 | 100 | 100 |
| Observables | 8 | 33 | 3 |