A Programmatic Interface for Particle Plasma Simulation in Python

Preliminary Results with PyCUDA

Min Ragan-Kelley (UCB AS&T)

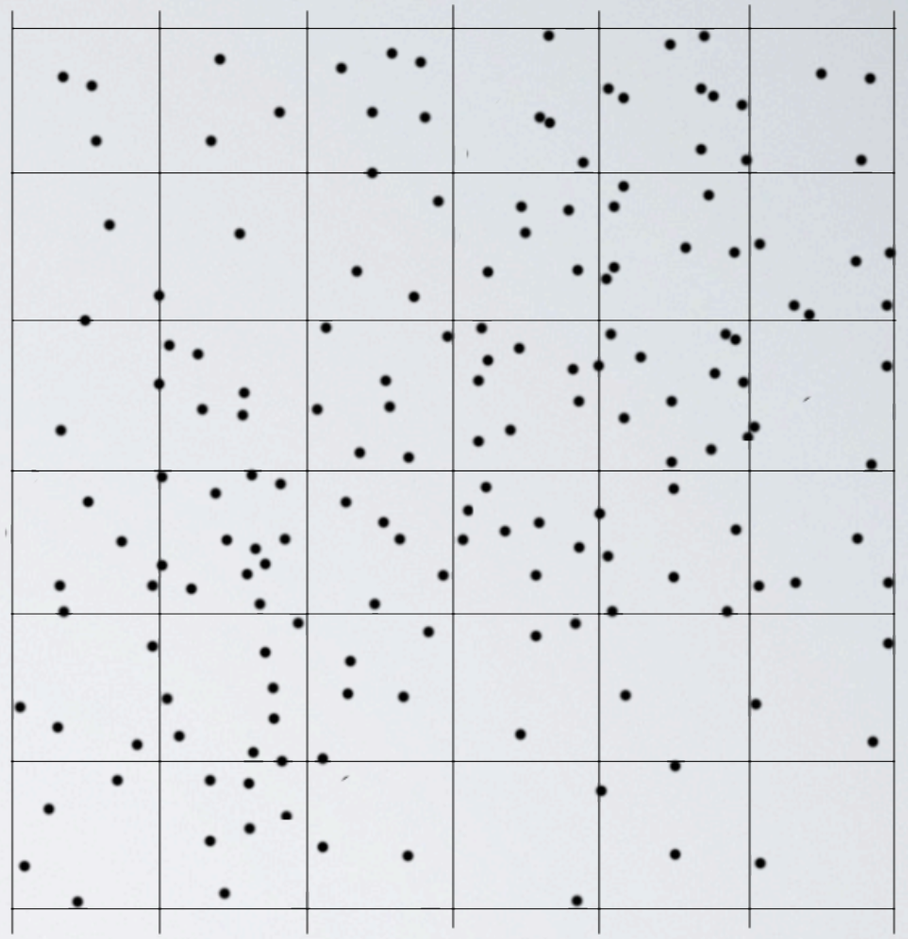
June 30, 2010

Outline

- What is PIC
- Motivations for the Project
- Design Goals of Python PIC
- Interface Design
- Use Cases
- PyCUDA Test Problem and Results

What is PIC

$$\nabla^2 \Phi_{[i,j]} = -\frac{\rho_{[i,j]}}{\epsilon} \qquad \ddot{x}_{(\vec{r})} = -\frac{q}{m} \nabla \Phi_{(\vec{r})}$$



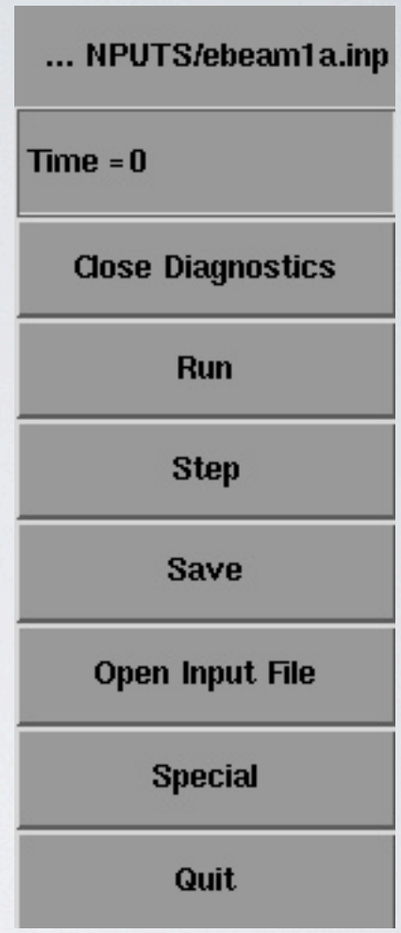
- Particle-In-Cell (PIC) Simulations are popular in plasma physics
- E/M Fields are defined on a discrete grid
- Particles live in continuous space
- Particles do not directly interact, but rather are mediated by the grid
- PIC: Weight (p->g), Solve(g), Interpolate (g->p), Push(p)

The Past: XOOPIC

- Object Oriented Particle-In-Cell
- Rebuild the application if you add anything
- Good model, but not scalable
- Mouse-only interface to simulations
- Better tools exist now, that didn't in 1995

Interface Goals

- Represent Device as Python object
- Provide superset of XGrafix controls as methods of that object
- Present existing diagnostics as numpy arrays
- Allow arbitrary derivative diagnostics
- Pure Python for input files (no custom syntax)
- Multiple Backends (PyCUDA, 2D, 3D, etc.)
- Cluster management for parallel simulations (IPython)



Performance Goals

- Exploit ubiquitous parallel hardware to study larger problems
- GPU parallelism
- Multicore/Multi-chip parallelism
- Cluster parallelism
- Short Term: build a model that will use *any* of these
- Long Term: use *all* of them

Interface Design

INTERFACES

- Each type of object provides an Interface
- For extended functionality, subclass an Interface
- All Diagnostics provide IDiagnostic
- All Boundary Diagnostics provide IDiagnostic AND IBoundaryDiagnostic

```
IDevice
¬
IBackend
    IDecomposedBackend
¬
IDiagnostic
    IBoundaryDiagnostic
    IParticleDiagnostic
    IFieldDiagnostic
    ITimeDiagnostic
¬
ISpatialRegion
¬
¬
IFieldSolve
    ISolvePoisson
    ISolveMaxwell
¬
IParticleBin
¬
ISpatialRegion
```

INTERFACES

```
import zope.interface as zi
¬
class IDiagnostic(zi.Interface):¬
    ¬
    data = Attribute("The Data for this diagnostic")¬
    ¬
    interval = Attribute("The update interval")¬
    ¬
    def save(fname=None):¬
        """save me to a file"""¬
    ...¬
¬
class BaseDiagnostic(object):¬
zi.implements(IDiagnostic)¬
¬
@property¬
def interval(self):¬
    return self._interval¬
¬
@interval.setter¬
def interval(self, newinterval):¬
    self._interval=newinterval¬
    self.backend.change_diag_interval(self, newinterval)¬
¬
def save(self, fname):¬
    self.data.tofile(fname)¬
```

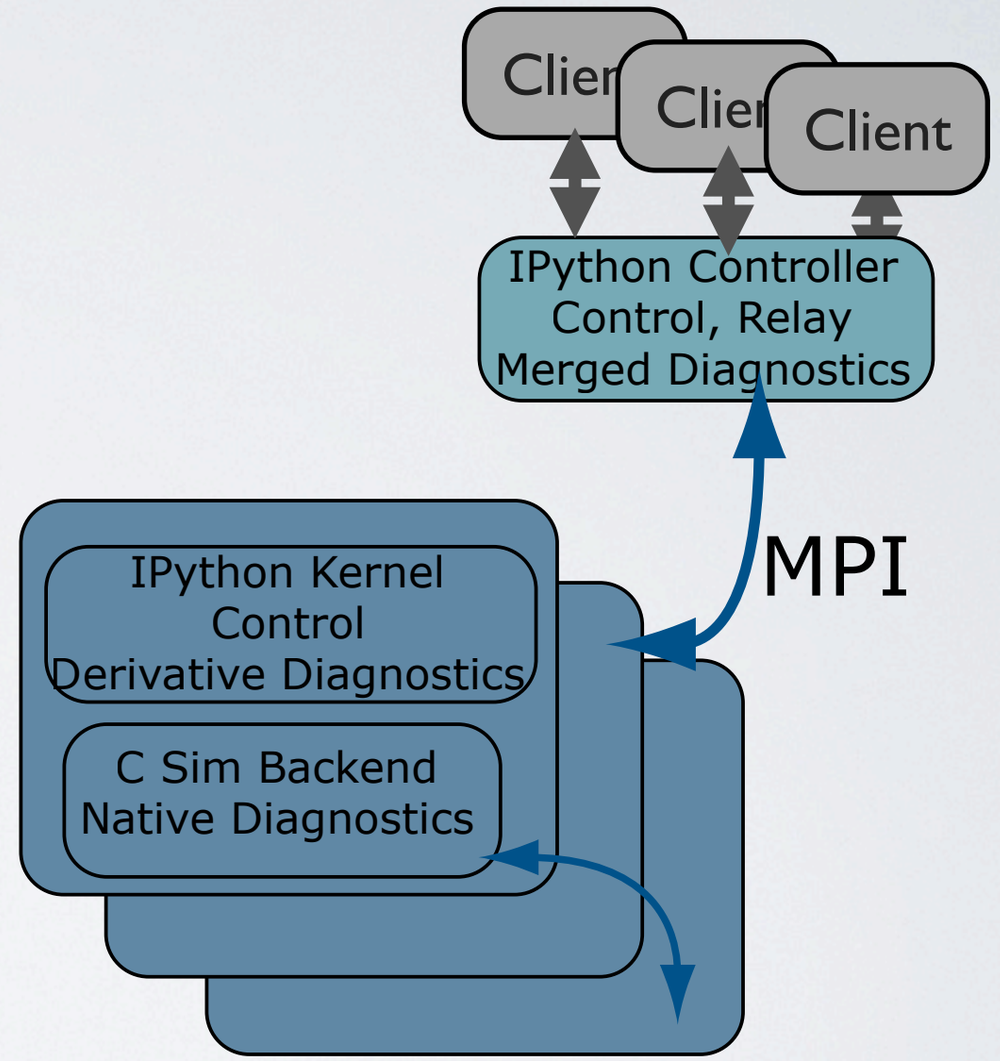
INTERFACES

- Rather than writing a parser, input files are Python scripts, executed in a namespace.
- That namespace is scanned for **Objects** providing **Interfaces**, and a Simulation is built from them.

The Design

Use Model

- User builds Logical Model in Python
- Python Backend builds Native Simulation Objects (C/CUDA)
- Control and Derivative Diagnostics in Python
- Inner Loops and Native Diagnostics in C/CUDA



Workflow

- Solve Field
    - Compute Field Diagnostics
- Push Particles
    - Particle Diagnostics
- Weight Particles

- defer to Python for Control

Backend

- start next step(s)

Python

- Collect Derivative Diagnostic dependencies
- Make adjustments
- defer to parent for Control
- <resume worker>
    - Compute Derivative Diagnostics

Proxy Objects

- In parallel Sims: diagnostics, etc. will actually be Proxy Objects, relaying instructions to Spatial Regions

- Data will not be retrieved unless explicitly requested

- Due to data moving, diagnostics will have update intervals at *each* level

NumPy Diagnostics

- The basic data structure of all Diagnostics will be NumPy Arrays.

- This gives us (and users) free access to:
  - slicing
  - native BLAS,FFT,etc.
  - rich analysis tools with SciPy etc.
  - all major Python plotting tools - Matplotlib, Gnuplot, Chaco, etc.

Use Cases

API

```
from OOPIC import *
sim = Simulation("/path/to/inputfile.inp")
defaultDiags = sim.diagnostics
sim.run() # run simulation until interrupt
sim.run(10) # run 10 steps
sim.step() # step forward once
J = sim.diagnostics["Current"]
B = sim.diagnostics["Magnetic Field"]
JcrossB = cross(J[:,6], B[:,6]) # adds JxB Diagnostic
JcrossB.interval = 10 # update every 10 timesteps
pylab.plot(sim.X, JcrossB)

def f(N):
    return N > 1e9
n = sim.diagnostics["Number"]
sim.runUntil(f, (n,)) # runs until there are 1e9 particles
```

Multiple Simulations

- As long as you can define your analysis, you can do it.
- Second simulation depends on results of first (sim2 could be DSMC or anybody else's code)

```
from mystuff import *
¬
sim1 = Simulation("sim1.py")¬
def stop_condition(sim):¬
    metric = check_some_stats(sim.diagnostics)¬
    if metric > threshold:¬
        return True¬
sim1.run_until(stop_condition, (sim1,))¬
¬
analysis = perform_analysis(sim1)¬
del sim1¬
sim2 = Simulation("sim2.py")¬
update_with_analysis(sim2, analysis)¬
sim2.run()¬
```

Search Parameter Space

- here we have a set of parameters that we want to find
- run a simulation, and get new input parameters from analysis
- start again with new parameters
- repeat until new parameters are close enough to the most recent input.

```
sim = Simulation("sim0.py")
prev = None
next = init_parameters()
while prev is not None and \
    norm(next-prev) > tol:
sim.reset()
configure(sim,next)
sim.run_until(stop_condition)
prev = next
next = analyze(sim)
```

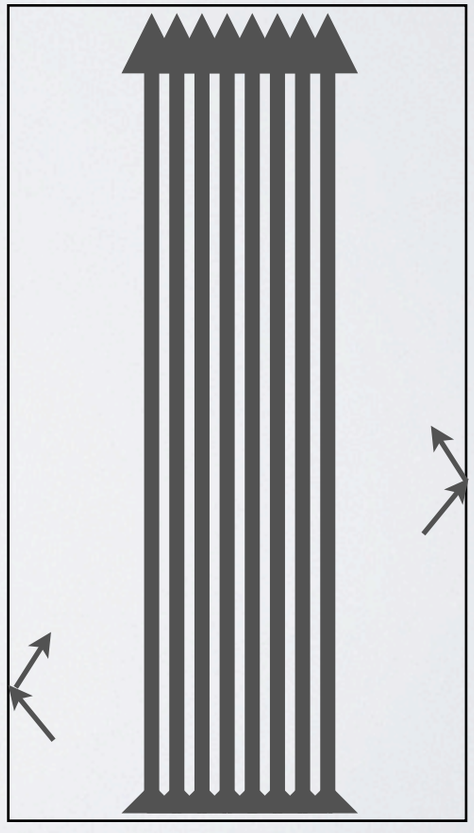
Summary

- The UI and the Analysis systems are *the same*.
- Interfaced Based Backend model facilitates extensions of Physics
- Python provides intuitive, extensive Sim building tools
- Ground up Parallel design will scale better than XOOPIC
- PyCUDA is the first Backend

The Test Case

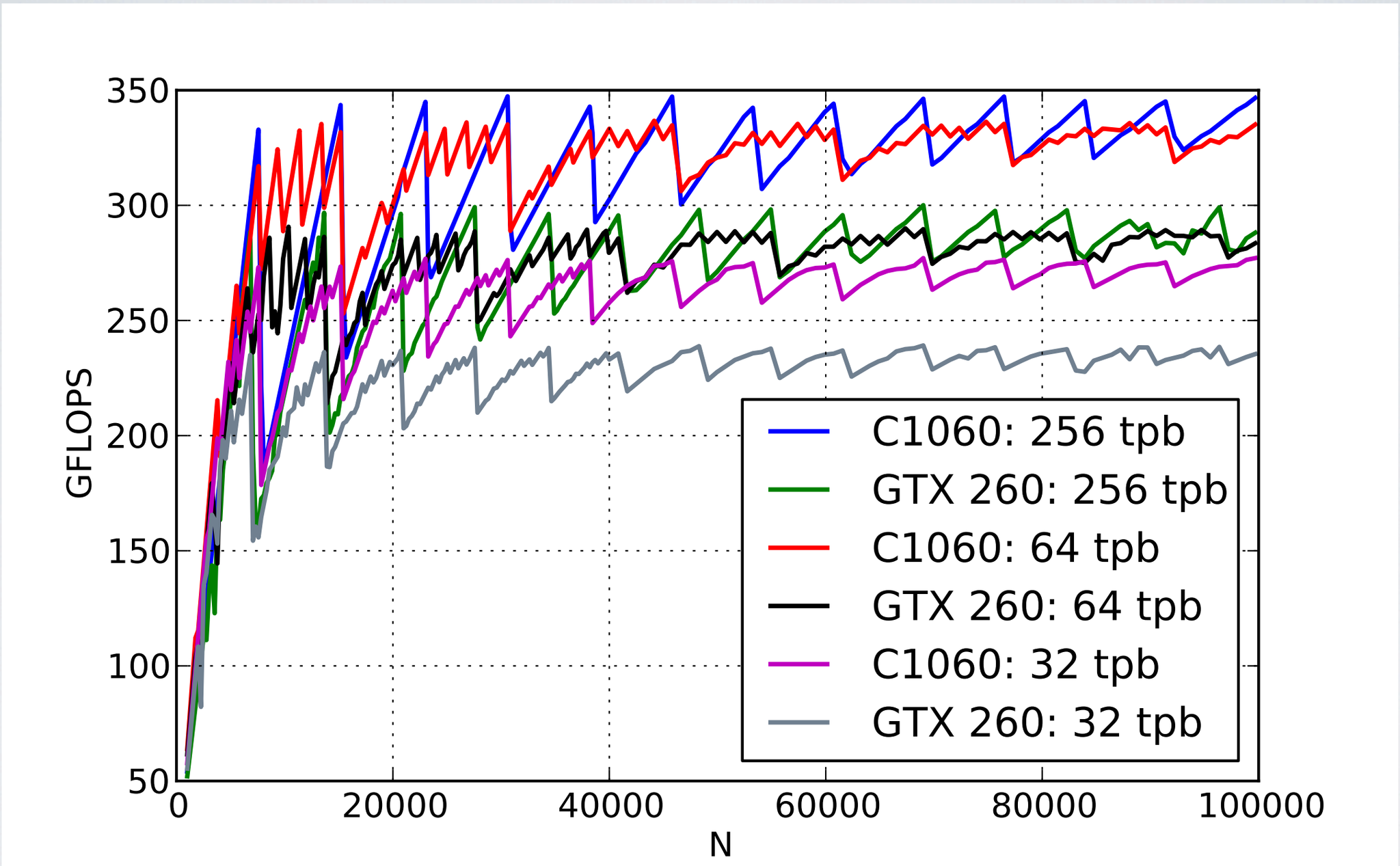
Test Case: Sheet Beam

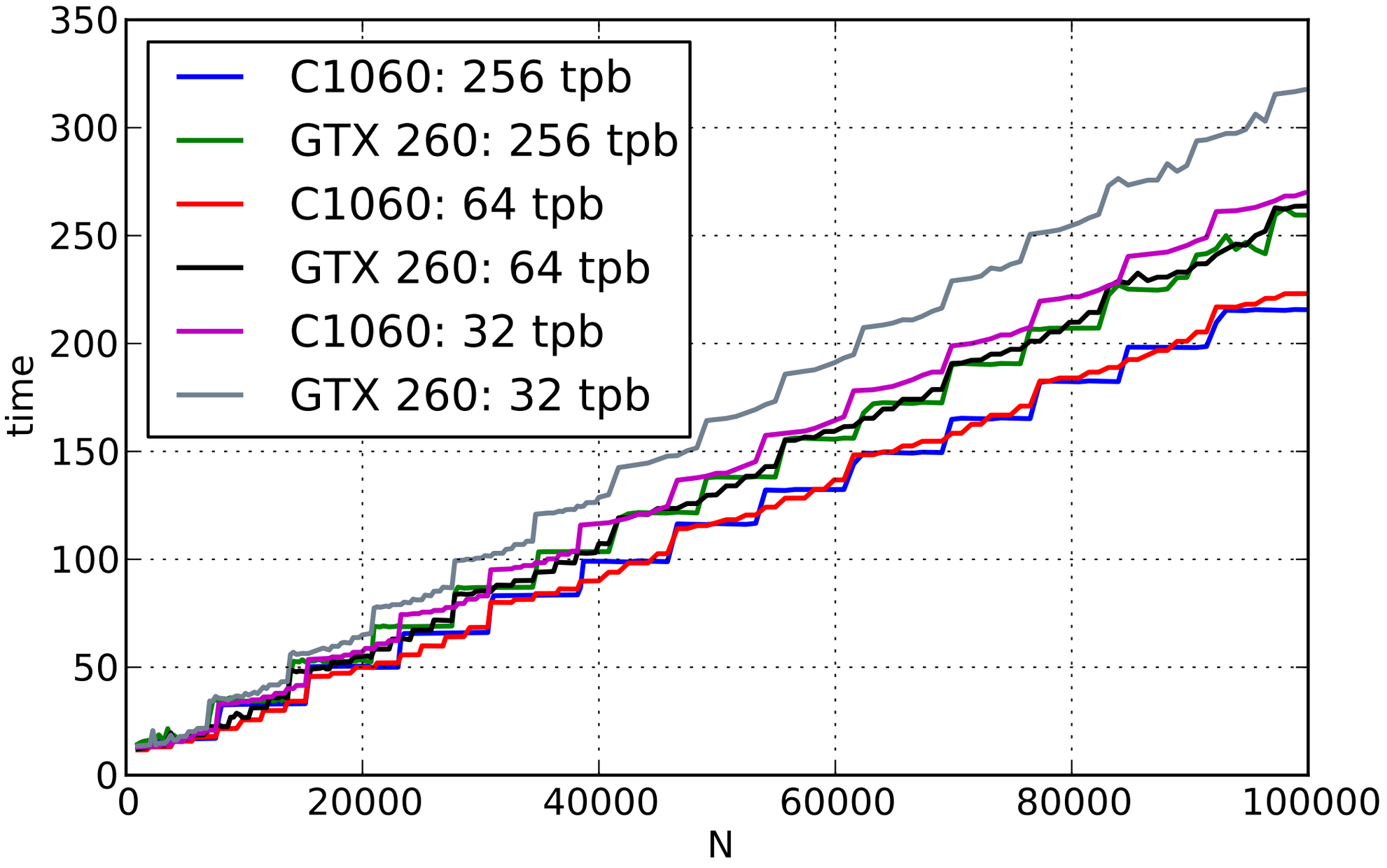
- Goal: Simulate a number of particles with PyCUDA (2D Cartesian)
- Direct Coulomb repulsion (short-range approximation)
- Initial Drift in +Y
- Specular bounce off X walls
- Periodic in Y (continuous infinite beam)

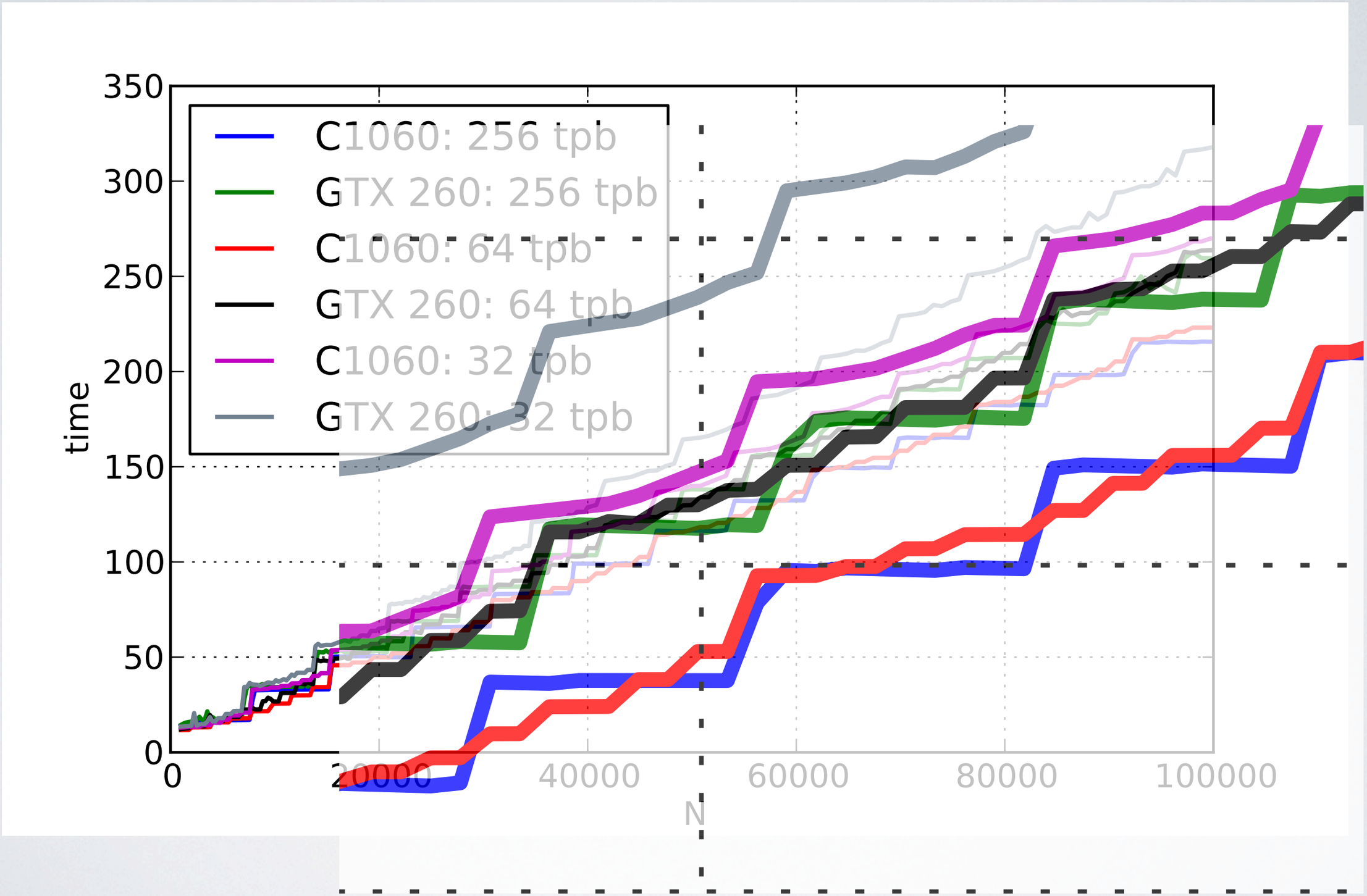


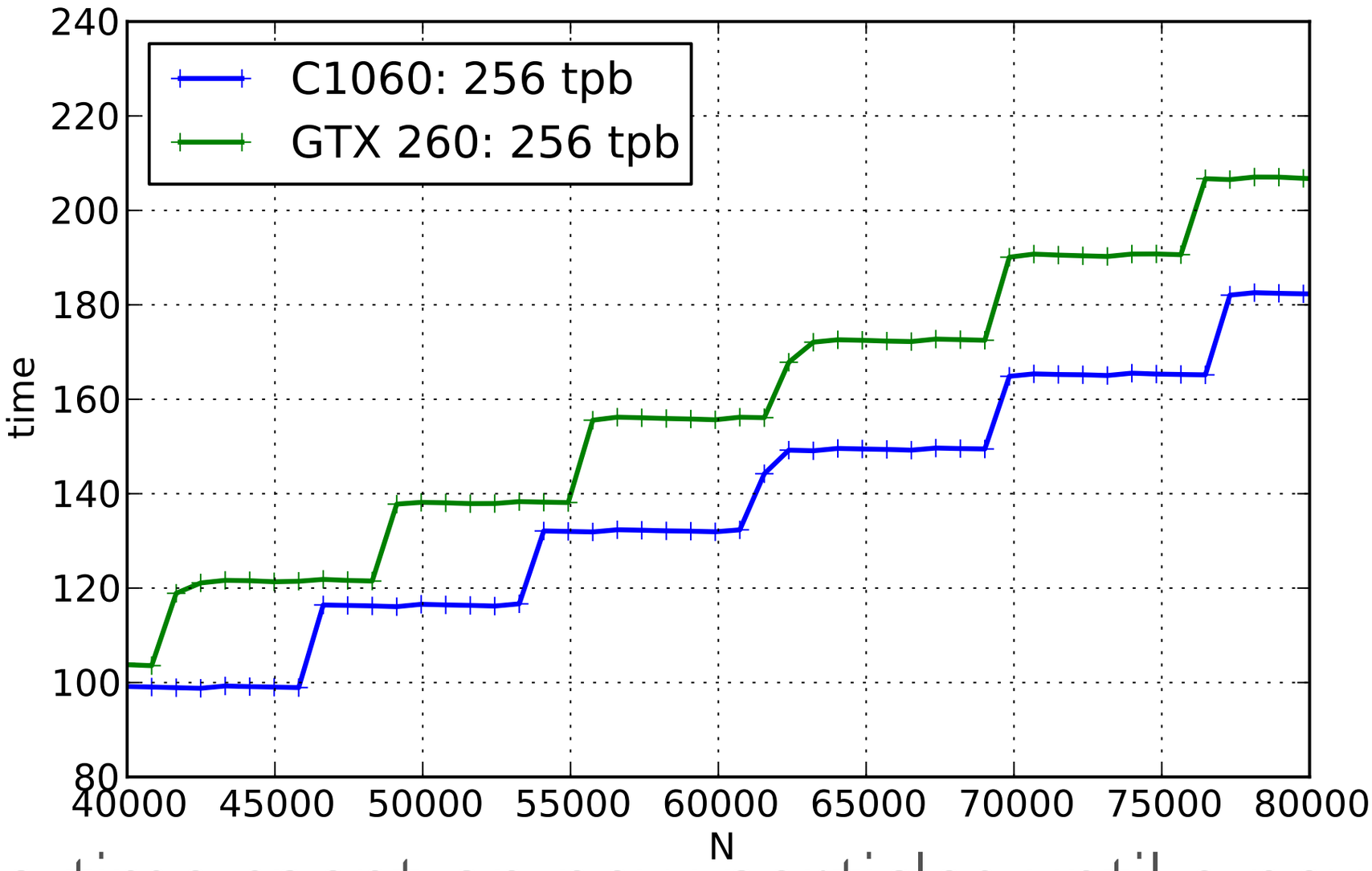
Results

Performance

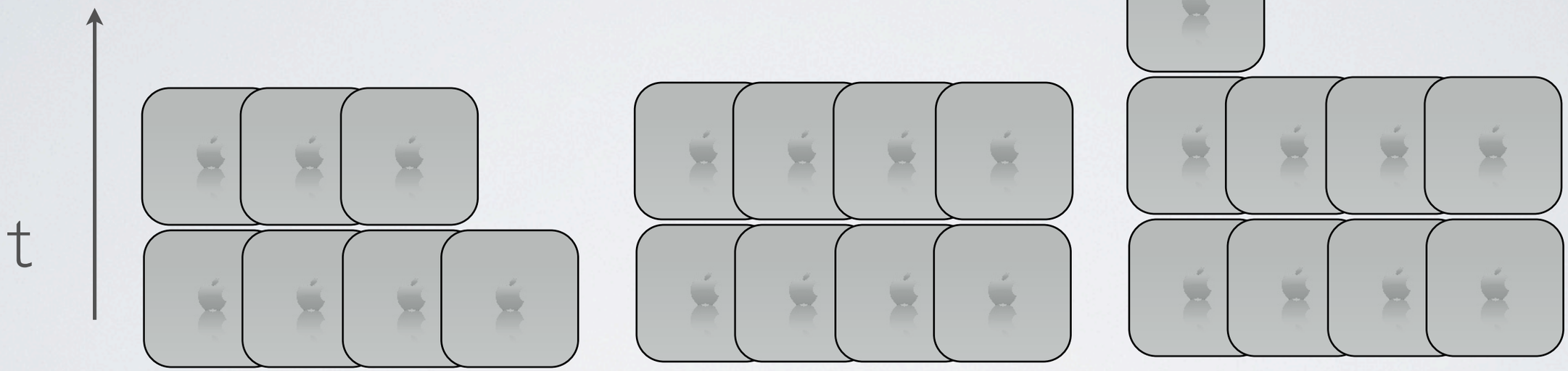



C1060: 256 tpb
GTX 260: 256 tpb
C1060: 64 tpb
GTX 260: 64 tpb
C1060: 32 tpb
GTX 260: 32 tpb
time
N
0
50
100
150
200
250
300
350
0
20000
40000
60000
80000
100000

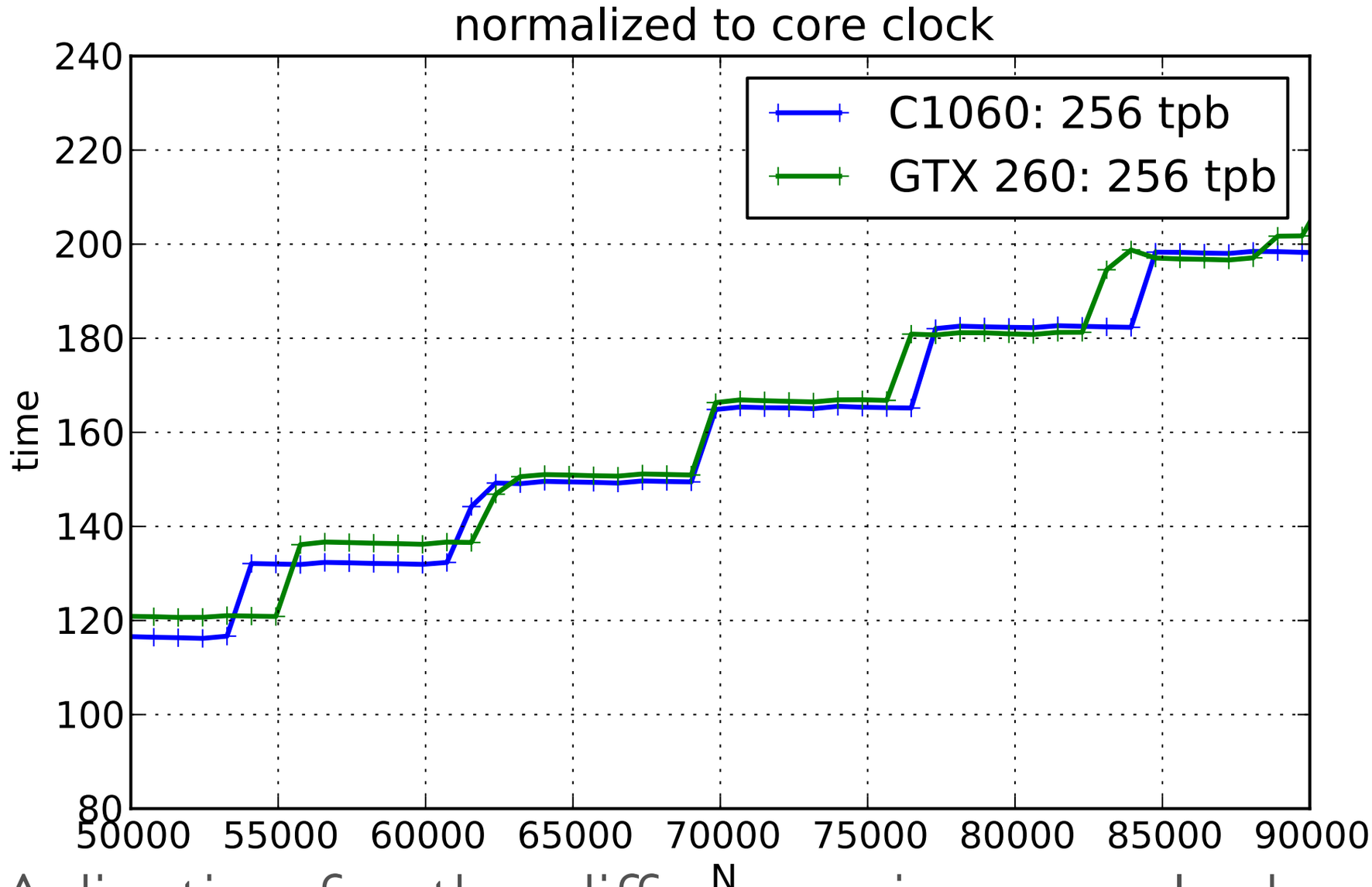

C1060: 256 tpb
GTX 260: 256 tpb
C1060: 64 tpb
GTX 260: 64 tpb
C1060: 32 tpb
GTX 260: 32 tpb
time
N
0
50
100
150
200
250
300
350
0
20000
40000
60000
80000
100000



Zero time spent on new particles until a new set of blocks is needed



N/tpb = 7 8 9



Adjusting for the difference in core clock, performance of the two chips is very similar.

Results

- Performance is periodic in (threads/block * GPU cores)
- The GPU is most fully loaded when the work can be broken into full-sized work groups
- when the work doesn't fit, some of the time is spent with the GPU not fully utilized

Results

- Did achieve good (30% of 1TFlop peak for C1060) performance on simple test case
- Did not get as far in exploring the problem as originally intended (comparing multiple schemes)

Next Steps

- Develop test code into full PIC Backend kernel
- Plug the PyCUDA simulation into the Python Diagnostics and steering part of the code
- Eventually: Port PyCUDA backend to PyOpenCL in order to use MultiCore CPU as well

SOURCES

- CS267
- ParLab Bootcamp videos and pdfs
  http://parlab.eecs.berkeley.edu/bootcampagenda
  Specifically Demmel, Catanzaro, Mattson

- NVIDIA GPU Gems
  http://developer.nvidia.com/object/gpu_gems_home.html

- NVIDIA CUDA/OpenCL Docs
  http://www.nvidia.com/object/cuda_develop.html

- HPG/SIGGRAPH 2009

Thanks

- Fernando Perez & Brian Granger (IPython)
- Andreas Klöckner (PyCUDA/PyOpenCL)
- John Verboncoeur (Advisor)
- You (for coming)