CharmPy: Parallel Programming with Python Objects

Juan Galvez

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Parallel Programming Laboratory

Illinois
University of Illinois at Urbana-Champaign

What is CharmPy?

- Parallel/distributed programming framework for Python
- Charm++ programming model (Charm++ for Python)
- High-level, general purpose
- Runs on top of Charm++ runtime (C++)
- Good runtime performance
- Adaptive runtime features: asynchronous remote method invocation, dynamic load balancing, automatic communication/computation overlap

Why CharmPy?

- Python+Charmpy easy to learn/use, many productivity benefits
- Bring Charm++ to Python community
  - No high-level & fast & highly-scalable parallel frameworks for Python
- Benefit from Python software stack
  - Python widely used for data analytics, machine learning
  - Opportunity to bring data and HPC closer
- Cons?
  - Potentially, performance, BUT performance can be similar to C++

Charmpy Python-derived benefits

- Productivity (high-level, less lines of code, easy to debug)
- Automatic memory management
- Automatic object serialization
  - No need to define serialization (PUP) routines
  - Can customize serialization if needed
- Easy access to Python software libraries (numpy, pandas, scikit-learn, TensorFlow, etc)

Charmpy-specific features

- Simplifies Charm++ programming
  - Much simpler, more intuitive API
- No specialized languages, preprocessing or compilation
  - Using reflection/introspection
  - Everything can be expressed in Python
  - **No interface (ci) files!**

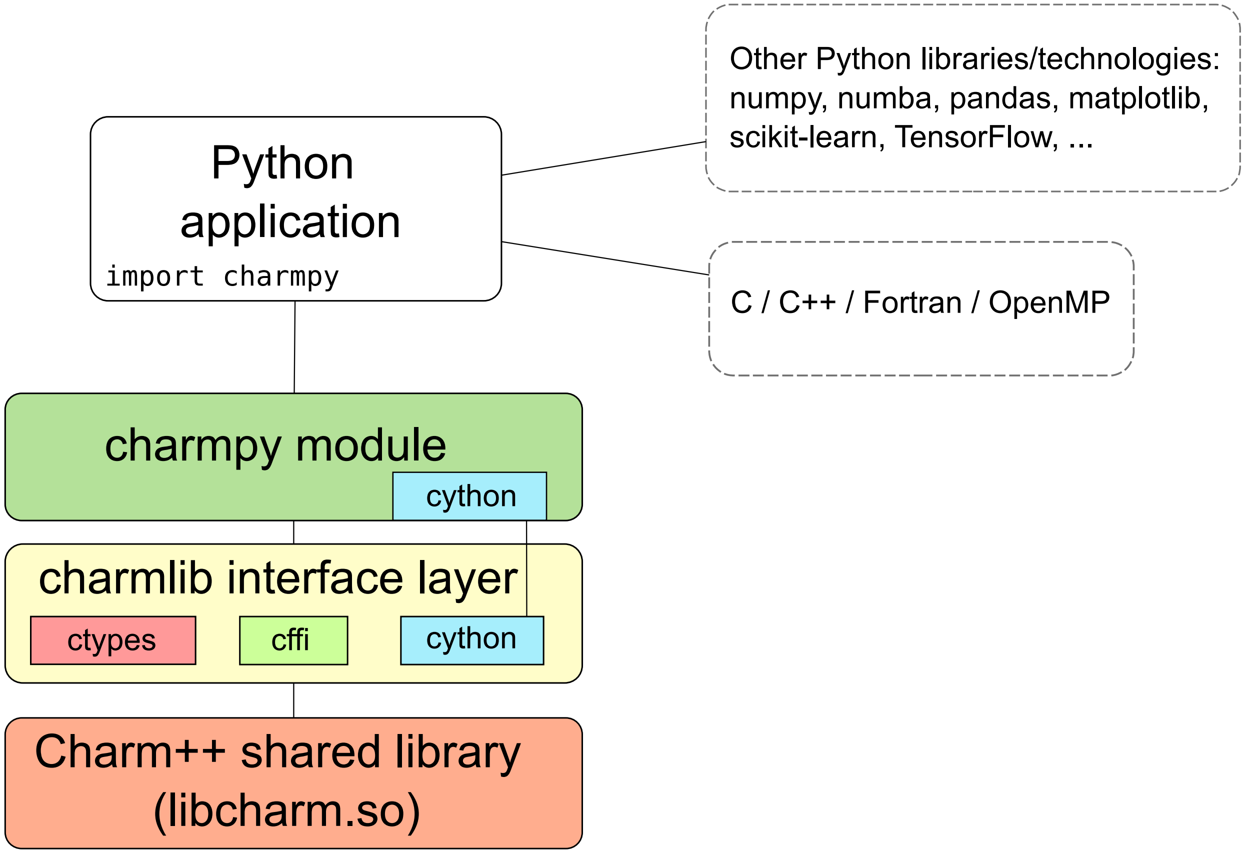
Hello World

```python
#hello_world.py
from charmpy import charm, Chare, Group

class Hello(Chare):
    def sayHi(self, vals):
        print('Hello from PE', charm.myPe(), 'vals=', vals)
        self.contribute(None, None, self.thisProxy[0].done)

    def done(self): charm.exit()

def main(args):
    g = Group(Hello)  # create a Group of Hello chares
    g.sayHi([1, 2.33, 'hi'])

charm.start(entry=main)
```

Run Hello World

```
$ ./charmrun +p4 /usr/bin/python3 hello_world.py
# similarly on a supercomputer with aprun/srun/…


Hello from PE 0 vals= [1, 2.33, 'hi']
Hello from PE 3 vals= [1, 2.33, 'hi']
Hello from PE 1 vals= [1, 2.33, 'hi']
Hello from PE 2 vals= [1, 2.33, 'hi']
```

Charmpy components



What about performance?

- Many (compiled) parallel programming languages proposed over the years for HPC
- Use Python in same way: high-level language driving machine-optimized compiled code
  - Numpy (high-level arrays/matrices API, native implementation)
  - Numba (JIT compiles Python “math/array” code)
  - Cython (compile generic Python to C)

Numba

- Compiles Python to native machine using LLVM compiler
  - Good for loops and numpy array code

(from http://numba.pydata.org)

```
@numba.jit
def sum2d(arr):
    M, N = arr.shape
    result = 0.0
    for i in range(M):
        for j in range(N):
            result += arr[i,j]
    return result

a = arange(9).reshape(3,3)
print(sum2d(a))
```

Numba

- Interesting feature:
  - Input parameters that are normally variables can be compiled as constants thanks to JIT compilation

```
@numba.jit
def compute(arr, ...)
for x in range(block_size_x):
    for y in range(block_size_y):
        arr[x,y] = ...
```

Values can be supplied at launch, but be compiled as constants

- Can write CUDA kernels

Chares are distributed Python objects

- Remote methods invoked like regular Python objects, via proxy: `obj_proxy.doWork(x, y)`
- Objects are migratable (handled by Charm++ runtime)
- Method invocation asynchronous in general (good for performance)
- Can also do: `ret = obj_proxy.getVal(block=True)`
  - Caller gets value returned by remote method
  - Entry method on which call is made needs to be marked as @threaded (runtime will inform)

Distributed collections (Groups, Arrays)

```
group = Group(MyChare)  # one instance per PE

array = Array(MyChare, (100,100))  # 2D array, 100x100
                                   # instances

array.work(x,y,z)  # invoke method on all objects in
                   # array
array[3,10].work(x,y,z) # invoke method on object with
                        # index (3,10)
```

Reductions

- Reduction (e.g. sum) by elements in a collection:

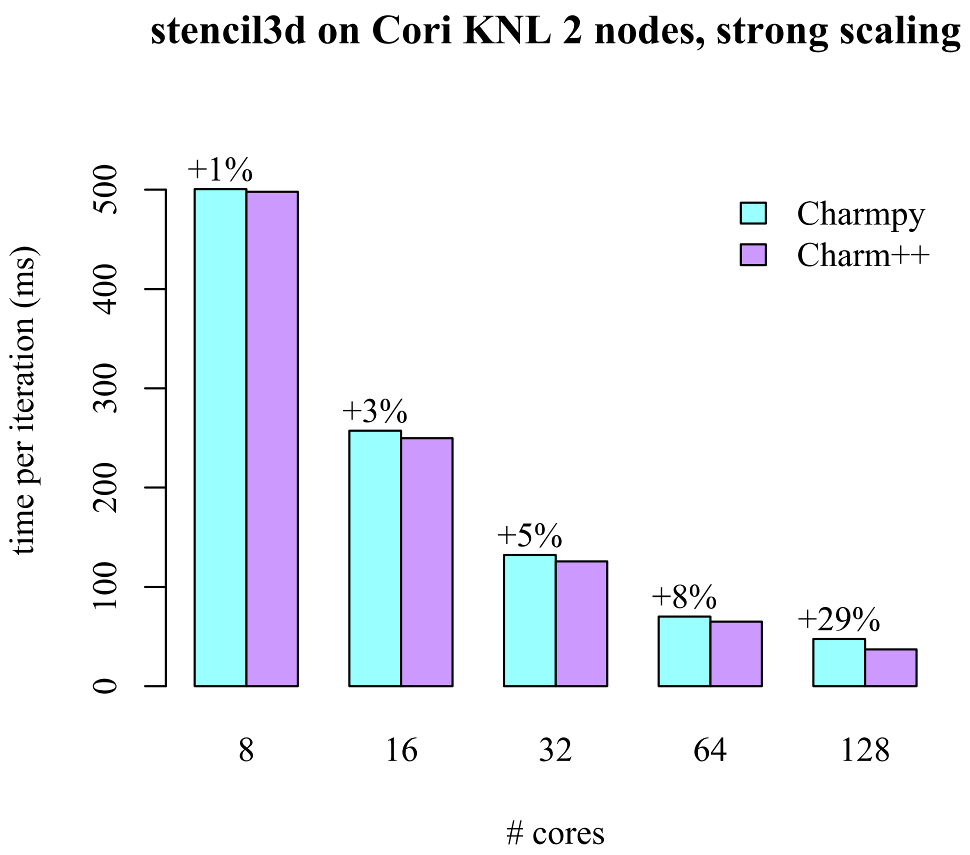
```
def work(self, x, y, z):
    A = numpy.arange(100)
    self.contribute(A, Reducer.sum, obj.collectResults)
```

- Easy to define custom reducer functions. Example:
  - `def mysum(contributions): return sum(contributions)`
  - `self.contribute(A, Reducer.mysum, obj.collectResult)`

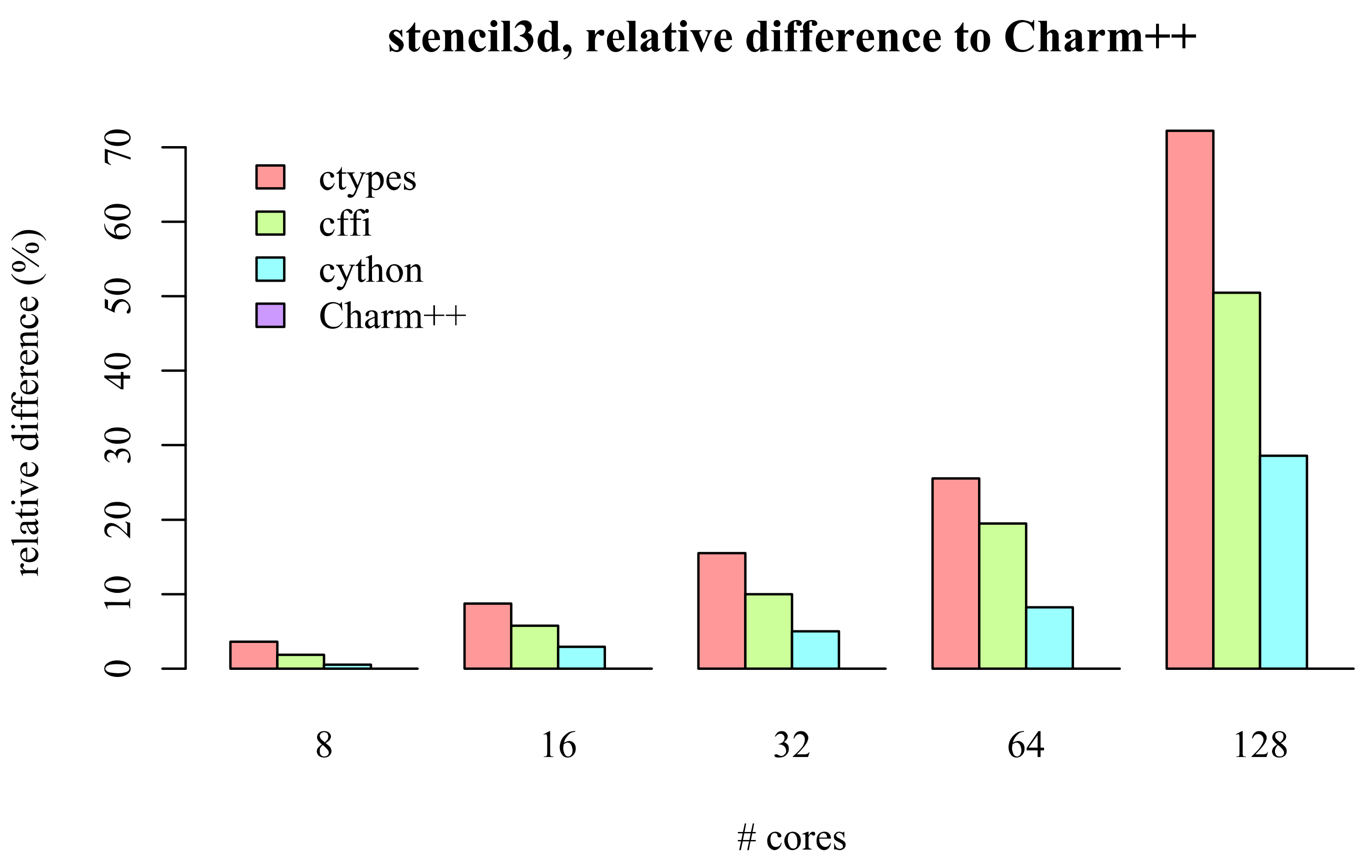
Benchmark using stencil3d

- In `examples/stencil3d`, ported from Charm++
- Stencil code, 3D array decomposed into chares
- Full Python application, array/math sections JIT compiled with Numba
- Cori KNL 2 nodes, strong scaling from 8 to 128 cores

stencil3d results on Cori KNL



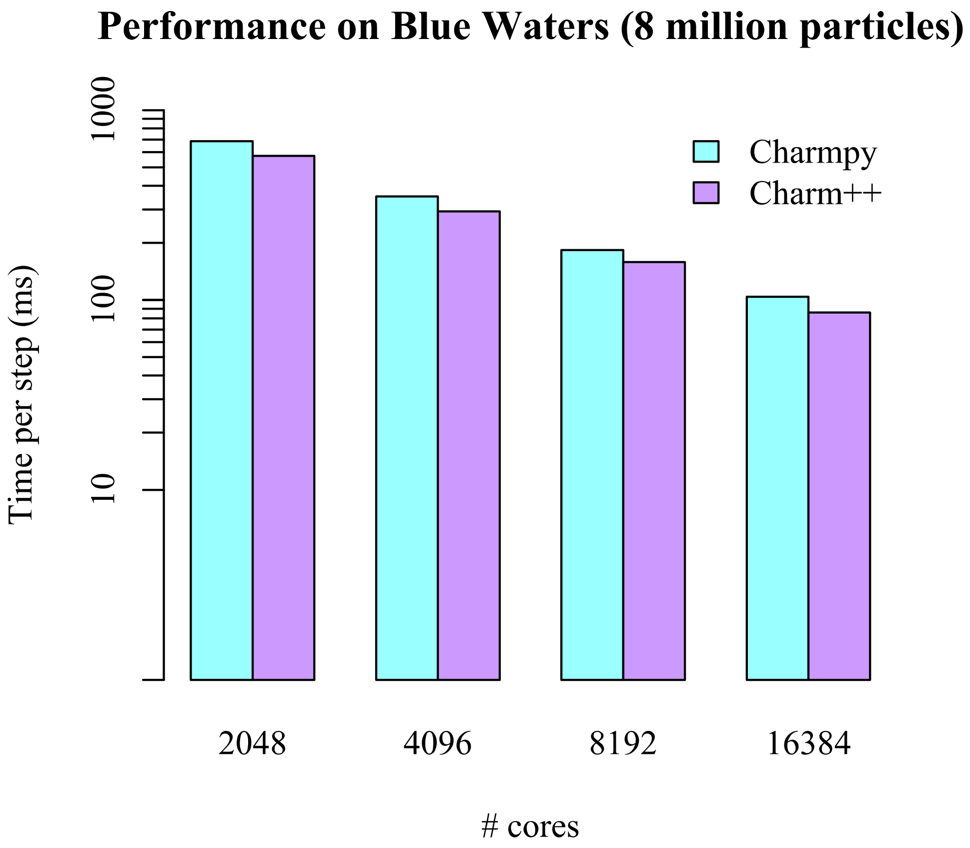
Evolution of performance



Benchmark using LeanMD

- MD mini-app for Charm++ (http://charmplusplus.org/miniApps/#leanmd)
  - Simulates the behavior of atoms based on the Lennard-Jones potential
  - Computation mimics the short-range non-bonded force calculation in NAMD
  - 3D space consisting of atoms decomposed into cells
  - In each iteration, force calculations done for all pairs of atoms within the cutoff distance
- Ported to Charmpy, full Python application. Physics code and other numerical code JIT compiled with Numba

LeanMD results on Blue Waters



Avg difference is 19%

(results not based on latest Charmpy version)

Serialization (aka pickling)

- Most Python types, including custom types, can be pickled
- Can customize pickling with `__getstate__` and `__setstate__` methods
- pickle module implemented in C, recent versions are pretty fast (for built-in types)
  - Pickling custom objects not recommended in critical path
- Charmpy bypasses pickling for certain types like numpy arrays

Shared memory parallelism

- In the Python interpreter, **NO**
  - CPython (most common Python implementation) still can't run multiple threads *concurrently*
- Outside the interpreter, **YES**
  - Numpy internally runs compiled code, can use multiple threads (Intel Python + numpy seems to be very good at this)
  - Access external OpenMP code from Python
  - Numba parallel loops

Summary

- Easy way to write parallel programs based on Charm++ model
- Good runtime performance
  - Critical sections of Charmpy runtime in C with Cython
  - Most of the runtime is C++
- High performance using NumPy, Numba, Cython, interacting with native code
- Easy access to Python libraries, like SciPy and PyData stacks

Thank you!

- More resources:
- Documentation and tutorial at http://charmpy.readthedocs.io
- Examples in project repo: https://github.com/UIUC-PPL/charmpy