Ramba: High-performance Distributed Arrays in Python

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Overview

- First, a selective review of the history of numerical processing in Python along with computational trends that continue to drive innovation today.
- Second, a comparison of where Python stands versus the standard performance solution of C/MPI.
- Third, an introduction to our new distributed array system for Python called Ramba.

History of Python Numerical Processing

- Python created in 1991, with support for collections of numbers.
- Since then, data set sizes have grown and multicore/cloud revolutions have accelerated the desire for improved multithread/multinode performance.
- Different approaches to performance have been tried:
  - Library-based API with C implementation
    - Numeric package introduced in 1995 trying to improve performance of Python numerical processing.
    - NumPy package introduced in 2006 that supersedes *Numeric.*
  - JIT compilation
    - Numba introduced 2012 and auto-parallelization added in 2017.
  - Multiprocessing and distributed execution
    - Multiprocessing package.
    - Mpi4py introduced 2009.
    - Dask introduced 2015.
    - HeAT introduced 2020.

Python Numerics

- Python has interesting standard numeric support:
  - Arbitrarily large integers
  - Floating point is similar to IEEE
  - Standard arbitrary precision library
- Very convenient, powerful, but not a perfect match to underlying processor datatypes
- Numerical vectors, arrays, matrices based on List type
  - Internally an array implementation, but not typed – each element can be an arbitrary Python object
- Loop iteration over lists (or arrays) is quite slow

NumPy – Efficient numerical arrays

- Standard package
- Adds a typed array, internally represented like C or Fortran arrays
- Standard integer, floating point, complex data types
- De facto standard way of representing numerical arrays in Python – everyone uses / builds on this (e.g., PyTorch, OpenCV, etc.)

NumPy key features

- Vector-style operations on whole arrays, map operations, reductions
  - Avoid Python iteration loops
- Powerful indexing, slicing, view generation
  - Efficiently perform operations on parts of arrays, e.g. conditional on value, etc., while writing in vector style rather than explicit loop iteration
- Efficient internal implementation of arithmetic, matrix operations
  - Written using C or based on external libraries (e.g. Intel MKL as in the Intel Python distribution)

NumPy vs Python numerics

- Take a simple example:
  - Pure Python:

```
for i in range(len(A)):
    A[i] += B[i] + s*C[i]
```

  - NumPy vector-style:

```
A += B + s*C
```

- Some speed comparisons (64-bit floats, time in seconds)

	1M	10M	100M	1B
Python	0.178	1.78	17.9	Don't bother
NumPy	0.003	0.061	0.618	7.0

NumPy limitations

- Most operations are still single-threaded (few exceptions like matmul)
- Mapping functions still runs slow Python code
- Vector style avoids explicit loop iteration, but can hurt performance:
  - Each vector operation completes before starting next – multiple cache-inefficient traversals of large arrays
  - Large temporary arrays are materialized
- Fancy indexing, operations on views can greatly increase overheads

Just-in-Time Compilation with Numba

- Numba = NumPy + Mamba (one of the fastest snakes in the world)
- Most of Python not very amenable to compilation
  - Main problems: weak typing of function arguments, untyped container classes, arbitrary introspection and changing of classes, methods on the fly
  - However, most uses of NumPy have consistent typing, don't typically deal with Python objects

- Key idea: Selectively apply JIT compilation techniques to programmer-selected functions; Reduce to LLVM compiler, then generate and run native binary code

Numba example

- Same example as before:

```
@numba.njit
def my_func(A, B, C, s):
    for i in range(len(A)):
        A[i] += B[i] +s*C[i]
```

- We just need to add the decorator (@numba.njit) to mark functions that should be compiled
- Note: since this will be compiled, we don't need to worry about slow iteration in Python; we can write explicit loops, though vector-style code will work as well

Performance

- Function is transformed into “Dispatcher” object
- First call to will be very slow – dispatcher will compile the function based on argument types provided
- Subsequent calls will (with same types) will run cached binary

	1M	10M	100M	1B
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NumPy	0.003	0.061	0.618	7.0
Numba	0.0013	0.022	0.211	2.15

Exploiting multicore CPUs

- Up to now, still used just a single core
- Numba has Parallel Accelerator component that parallelizes execution across cores
  - Parallel vector-style operations
  - Explicit parallel-for construct
- Parallel example:

```
@numba.njit(parallel=True)
def my_func(A, B, C, s):
    for i in numba.prange(len(A)):
        A[i] += B[i] +s*C[i]
```

Parallel Execution on Multiple Cores

- Gains from parallel execution:

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Python	0.178	1.78	17.9	Don’t bother
NumPy	0.003	0.061	0.618	7.0
Numba	0.0013	0.022	0.211	2.15
Numba-parallel	0.0003	0.006	0.046	0.43

- Only 4x improvement on a 20 core/40 thread machine?

  → This simple example is memory bandwidth bound

Numba limitations

- Works well for NumPy arrays, but does not work with Python objects
- No per-thread control / coordination
  - Only have an implicit barrier at end of parallel for sections
  - No thread-to-thread signaling primitives; can't make your own (no "volatile" variables)
  - No NUMA-awareness for multi-socket machines
- Tricky to differentiate compile-time and dynamic values
  - E.g., array dimension length, list length are dynamic; number of dimension, tuple size are compile-time values
- Limited to single node (can scale up, but not scale out)

Dask

- DaskArray implements the NumPy API on top of the Dask distributed (or multiprocessing) tasking system.
- Arrays are broken up into chunks.
- Operations are represented on these chunks in the task graph.
- Uses NumPy internally for operations on each chunk.
- Scales to large clusters
- https://examples.dask.org/array.html

HeAT

- Distributed NumPy-like arrays with MPI.
- SPMD programming model.
- Local arrays implemented with PyTorch tensors for CPU or GPU execution.
- https://github.com/helmholtz-analytics/heat

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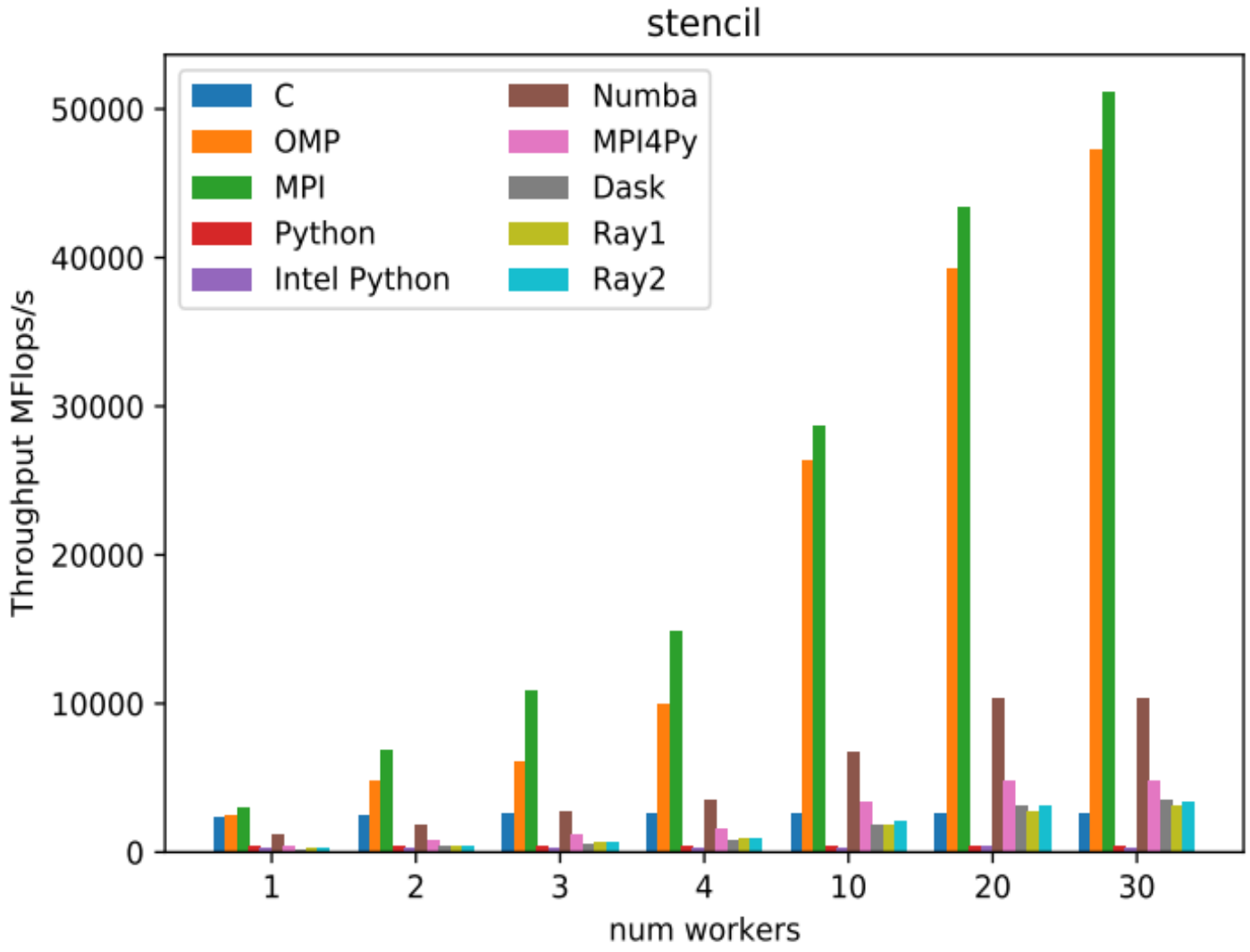
Python compared to C / MPI

- As seen in this graph, the performance gap between C/MPI and various Python alternatives is still quite large.
- This gap gets larger as we go from single-node (as in the graph) to multi-node systems.
- Programmer productivity in some of the Python distributed systems not that much better than C/MPI.



Why such a large gap?

- Some systems fail to efficiently utilize multiple cores or multiple nodes.
- Some systems still use slow Python code internally.
- Some systems fail to fuse consecutive operations, causing applications to become memory bound.
- Some systems divide work into chunks and then have large scheduling or data movement overheads.

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Ramba Idea

- Can we combine good single node efficiency with a Python distributed systems package to get efficient scale-up and scale-out while largely maintaining the programmer productivity of the NumPy API?
- Idea:
  - Combine Numba for its best-in-class Python single-node efficiency…
  - …with Ray or MPI4Py for distribution.

Ramba Programming Methodology

- Introduce a distributed array data structure
  - Looks like a NumPy array, but is sharded across a set of nodes
- Preserve NumPy-like operations, API:
  - Basic per-element arithmetic operations
  - Simple reductions
  - Array slicing / views [but limited fancy indexing or strided view support]

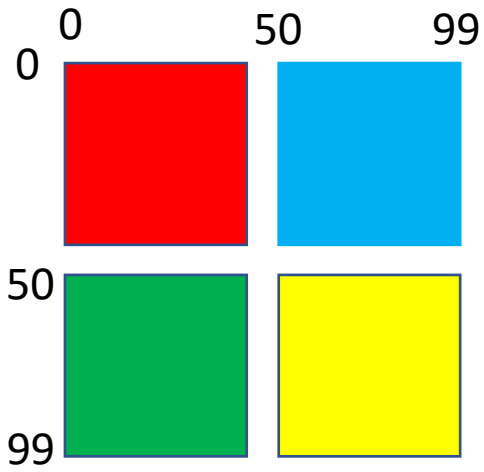
- Now, can write NumPy vector-style code, and have it execute in a distributed context
- Also, provide “skeletons” that represent common computation and communication patterns (e.g., map, reduce, cumulative)

How Ramba works

- Ramba starts a set of actors on each node – these are the Ramba remote workers
- Ramba array class (“ndarray”) provides a set of methods that mimic the NumPy API
  - Ndarray construction triggers an array shard to be constructed on each remote worker; shards are NumPy arrays
  - Ndarray operations, e.g., __add__(), trigger corresponding local NumPy operations on the remote worker shards
  - Indexing/slicing an Ndarray triggers construction of a new Ndarray object, which refers to (portions of) the original shards; Thus, provide in-place views like in NumPy
- Operations on remote workers use Numba-JIT functions where possible

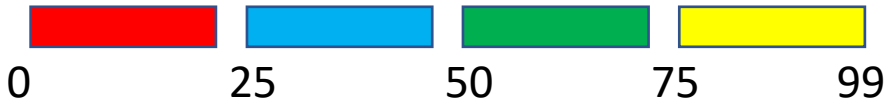
Ramba examples

- A=ramba.zeros((100,100))



Create 50x50 array on each worker; init to 0

- B=ramba.ones(100)



Create array size 25 on each worker; init to 1

- B[20:60] += 4

Temporary ndarray refers to parts of arrays on subset of workers; execute in-place add of 4

Lazy Evaluation

- Ndarray operations do not immediately trigger execution on remote workers
- Instead, the operations are added to a graph of pending operations (i.e., a DAG)
- Main thread continues to additional operations which may also be added to the DAG
- Accessing individual element of an array or I/O operations cause Ramba to determine which operations in the DAG must be run to generate the needed output
- Subsets of those operations which do the same amount of work per neighbor and have no data dependence conflicts are fused together, for cache efficiency, and Numba-JIT-compiled for native code performance
- Ramba does pattern matching on the operations in the DAG to replace a series of inefficient operations with a more efficient one

Lazy Evaluation Example

- A = B + s*C
- Ramba lazy ops:
  - All are fused into single loop
  - Temp arrays not materialized
  - Single call to workers, single traversal of arrays
  - Generated Code:

- Standard Controller-Worker:
  - Do s*C, store in tmp1
  - Do B+tmp1, store in tmp2
  - Do A+=tmp2
  - 3 separate remote worker fan outs
  - Extra storage for temporaries

```
@numba.njit(parallel=True)
def ramba_deferred_ops_func_6079497222952596368(ramba_tmp_var_00002,ramba_tmp_var_00004,ramba_tmp_var_00005,ramba_tmp_var_00001):
    for index in numba.pndindex(ramba_tmp_var_00002.shape):
        ramba_tmp_var_00000 = ramba_tmp_var_00001 * ramba_tmp_var_00002[index]
        ramba_tmp_var_00003 = ramba_tmp_var_00004[index] + ramba_tmp_var_00000
        ramba_tmp_var_00005[index] += ramba_tmp_var_00003
```

Lazy Partitioning

- Part of lazy evaluation is that partitioning (i.e., sharding) decisions are also delayed.
- Ramba has mechanism for operations to describe partitioning constraints on their input arrays that enable performant execution, for example:
  - Some input should not be partitioned along a certain axis.
  - Two or more input arrays should have the same partitioning along a given axis.
- At DAG execution time, Ramba determines the partitioning of the arrays to be created such that they satisfy these constraints, if possible.
- Ramba's automatic partitioning can be overloaded with a programmer specified partitioning at array creation time.

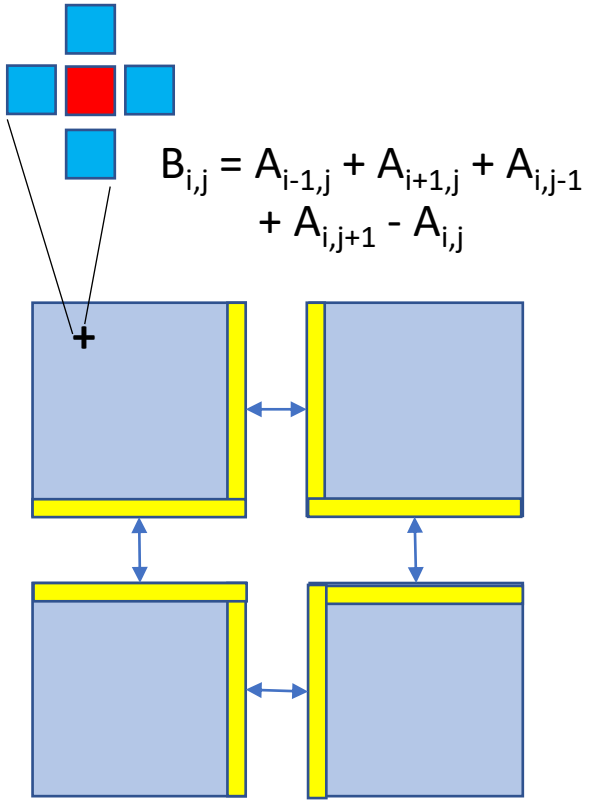
Controller-Worker vs. SPMD model

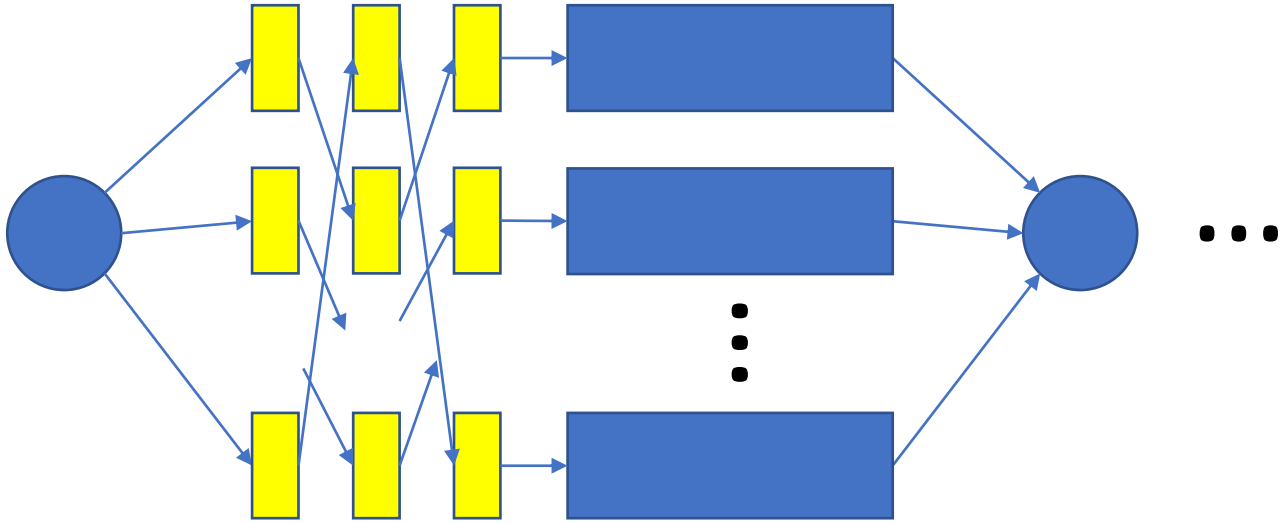
- Ramba by default uses the Controller-Worker model
  - Main Python thread is the controller
  - Each ndarray operation adds to the DAG
  - Fusion during lazy evaluation reduces the Fan-out, Fan-in for remote execution of operations

- Single Program, Multiple Data (SPMD) model
  - Ramba will soon support SPMD natively.
  - Dominant model for HPC; Native model for MPI programs
  - Program binary executes on each node, running on its own shard of data
  - Each runs independently until explicit synchronization or communications
  - Can be much more efficient / performant than Controller-Worker

More Complex Example: stencil

- Apply stencil operation on large 2D arrays
- Value computed at $A_{i,j}$ depends on neighbor values
- Canonical distributed implementation:
  - Shard in two dimensions, share boundary data
  - Iterations of communication, computation phases



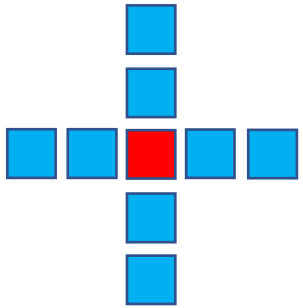


Stencil Example Code

- Write code like we have one big local array (NumPy vector-style)

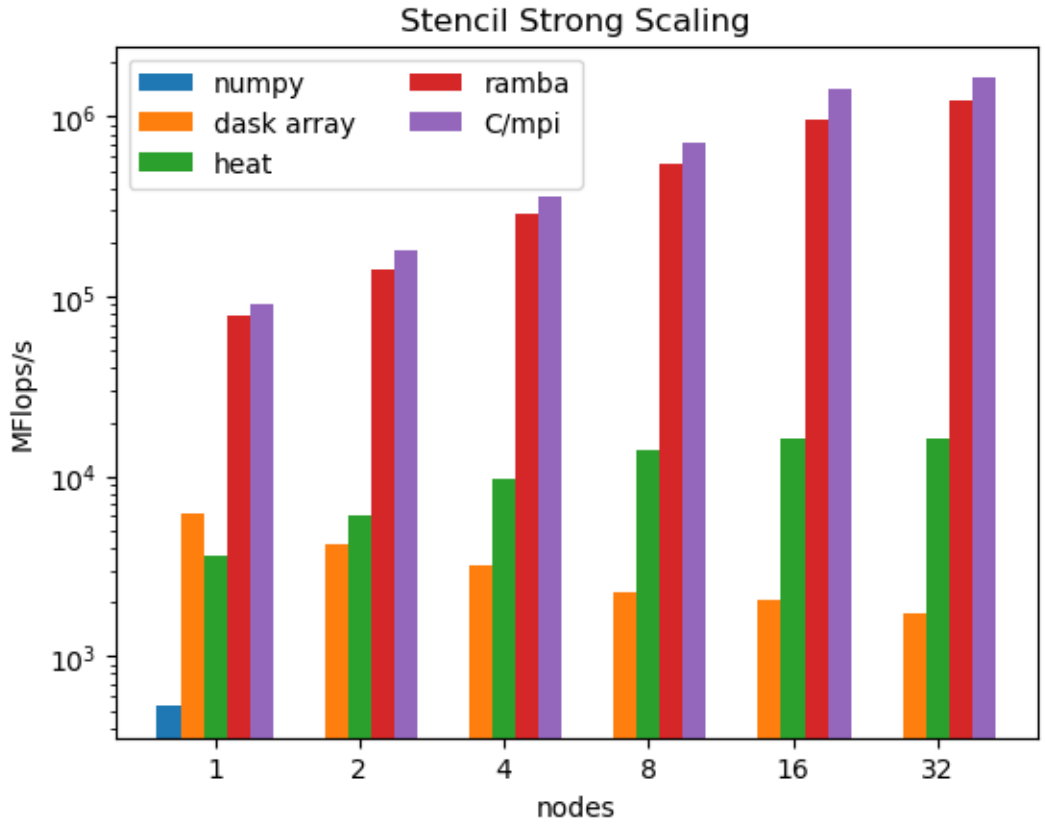
```
B[2:n-2,2:n-2] += W[2,2] * A[2:n-2,2:n-2] \
        + W[2,0] * A[2:n-2,0:n-4] \
        + W[2,1] * A[2:n-2,1:n-3] \
        + W[2,3] * A[2:n-2,3:n-1] \
        + W[2,4] * A[2:n-2,4:n-0] \
        + W[0,2] * A[0:n-4,2:n-2] \
        + W[1,2] * A[1:n-3,2:n-2] \
        + W[3,2] * A[3:n-1,2:n-2] \
        + W[4,2] * A[4:n-0,2:n-2]
```

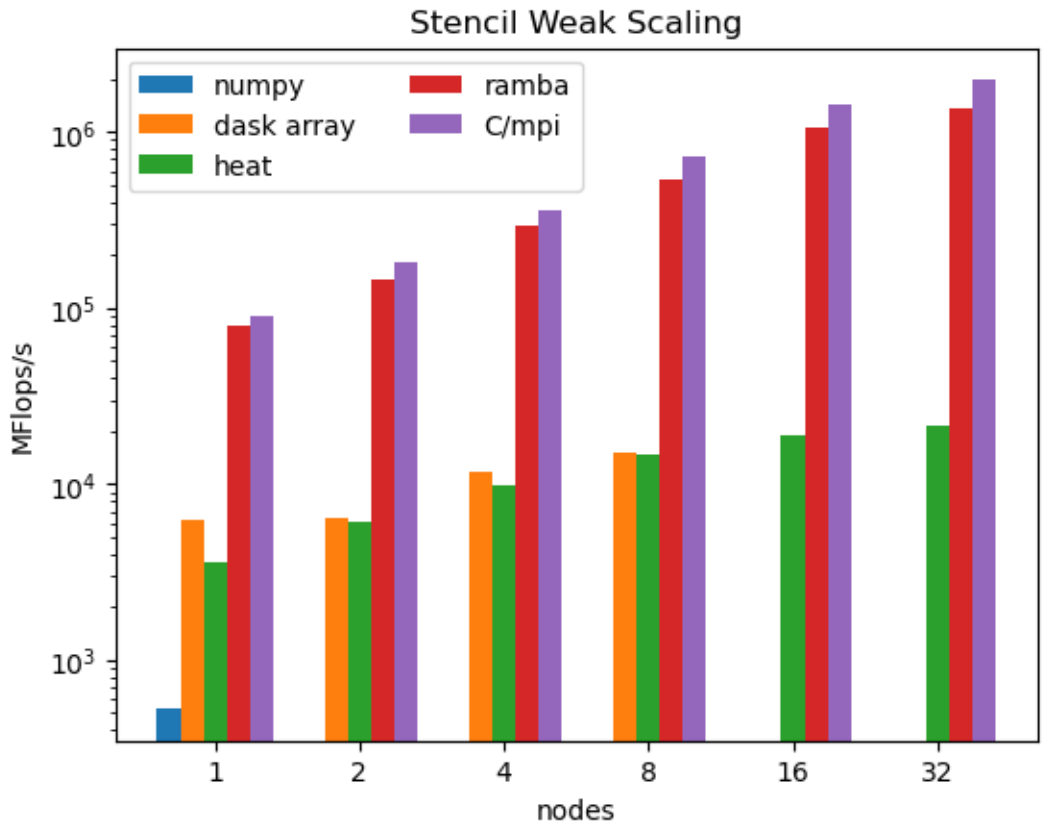
Star-2 stencil



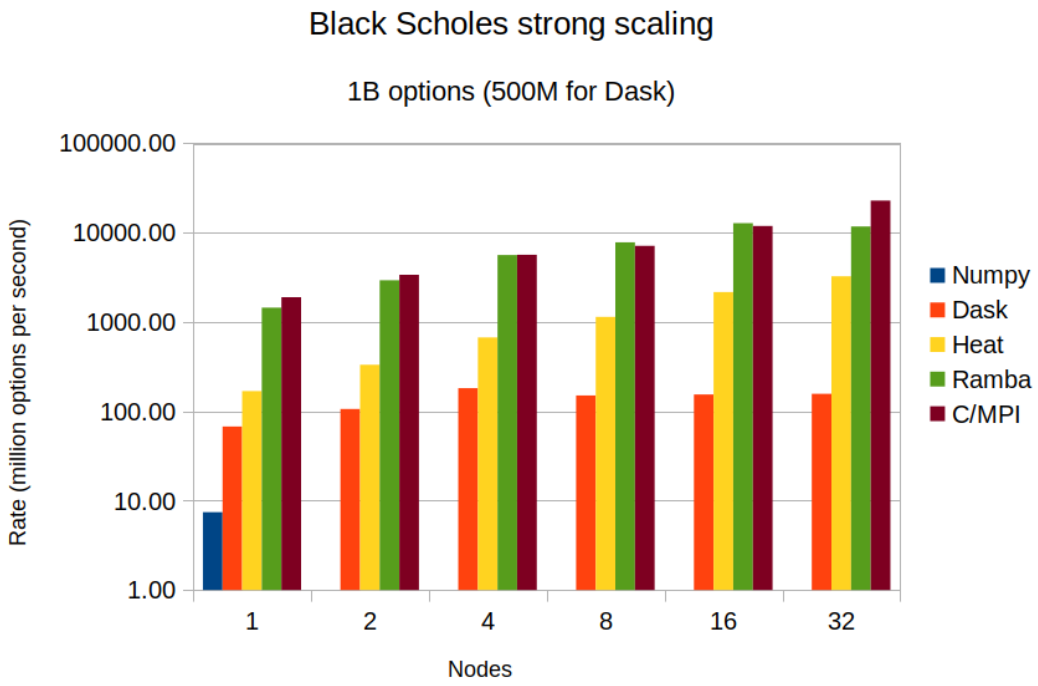
- All operations fuse into single function
- Shifted slices incur communications – all automated

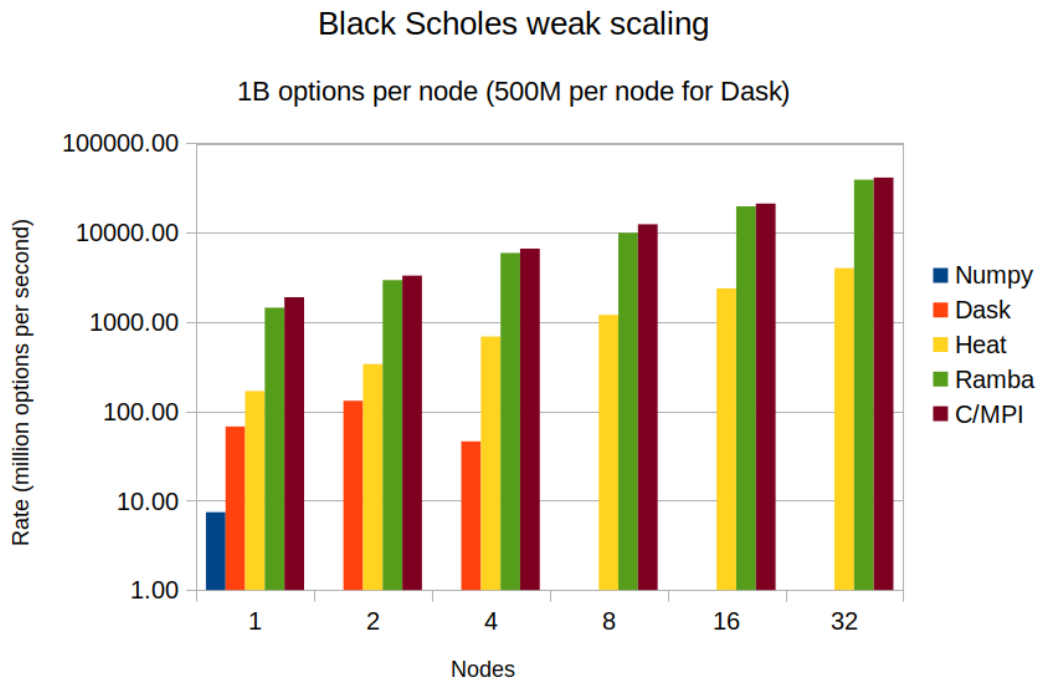
Stencil Performance





Blackscholes Performance





Ramba Skeletons

- Ramba skeletons capture computation and communication patterns.
- Skeletons take one or more functions as input that are applied to points in an index space or define how to combine sub-results from different Ramba workers.
- The skeletons also take at least one array argument but up to any number of additional arrays or scalars.
- Supported patterns: map, reduce, stencil, cumulative, “spmd”.
- Function passed to spmd skeleton can request the portion of an input array that is resident on the current Ramba worker.
- Skeletons may also be part of the DAG of operations and the functions to execute the skeleton on each worker are Numba-compiled.

Ramba Groupby

- Ramba supports groupby functionality similar to xarray.
- A grouped array, named RambaGroupby, is formed by invoking the ndarray.groupby() method.
- This method takes the dimension to group on and a 1D array equal in length to the size of that dimension and whose contents map that point in that dimension to a group number.
- RambaGroupby supports mean, sum, prod, min, max, var, std as well as the usual numeric binary operations, add, sub, mul, etc.
- Implemented using map and reduce skeletons.

Challenges and Limitations

- NumPy API is very large – only a fraction covered now
- Optimal distribution varies with algorithm/operation; hard to guess in advance the best approach
- Some operations (e.g., reshape) not practical in distributed case
- Explicit looping through arrays will be horribly slow
- System only “sees” sequence of array operations, not actual source; hard to reason about intent, scope of variables, etc.
- Keeping overheads down is hard – communications, calculating which remotes need to exchange data, compiling deferred operations, etc. all add to overheads

Ramba Availability

- Available publicaly on Git Hub:
  https://github.com/Python-for-HPC/ramba
- Open Source, BSD-style license
- Please try it and contribute!

References

- Ray – https://ray.io/
- Numba – https://numba.pydata.org/
- Ramba – https://github.com/Python-for-HPC/ramba
- Parallel Research Kernels – https://github.com/ParRes/Kernels
- Dask – https://dask.org/
- NumS – https://github.com/nums-project/nums