Exploring Performance of GeoCAT data analysis routines on GPUs

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GeoCAT

Geoscience **C**ommunity **A**nalysis **T**oolkit (GeoCAT) is a toolkit used by the geoscience community to analyze and visualize data.

GeoCAT-comp program is one of the GeoCAT repositories, including previous NCL's non-WRF computational routines and other geoscientific analysis functions in Python.

GeoCAT-comp is built on **Pangeo** software ecosystem. The routines in GeoCAT-comp are either sequential or take advantage of **Dask for parallelization on the CPU.**

Data processing and data analysis is an embarrassingly parallel task and computationally intensive.

The project's focus is on porting GeoCAT-comp routines to GPUs.

GPU Programming in Python

CPU cores have a fast clock cycle but a limited number of cores. GPUs have hundreds of cores. By using GPUs in computations where a task can be divided into many subtasks, we can take advantage of **massive parallelization** and accelerate the code.

There are different CUDA-enabled packages in Python to help optimizing programs by GPUs, e.g., **Numba, Pycuda, and CuPy**. We investigated different approaches, and chose **CuPy**. CuPy is very similar to NumPy and it can be used as **a drop-in replacement** with NumPy.

With CuPy the programmer is not required to do memory management on both host and device or set and launch kernels manually.

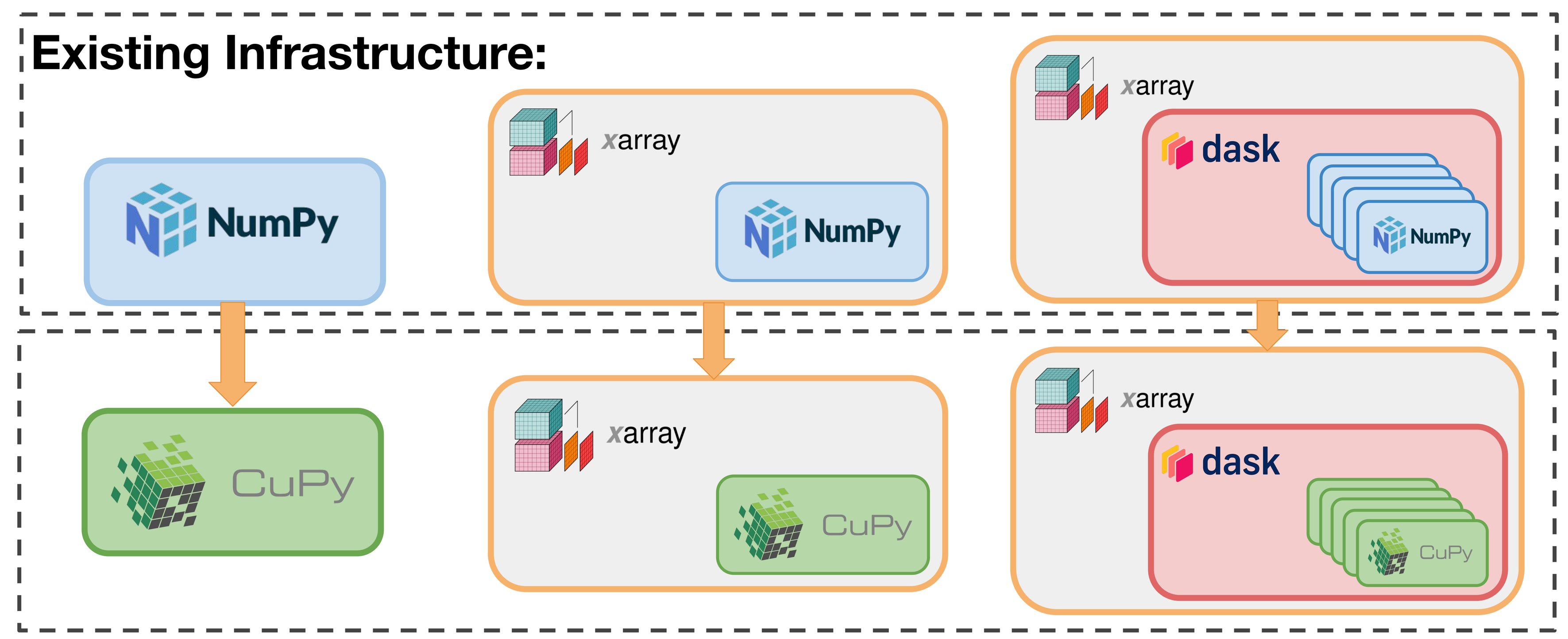
```
import cupy as cp
arr1 = cp.random.rand(10**2)
arr2 = cp.random.rand(10**2)
s = cp.add(arr1, arr2)
```

Xarray: Enables having labelled multi-dimensional arrays in Python.

Dask: Flexible open-source Python library for parallel computing.

Implementation

- The project's focus in on porting CPU parallelized routines, i.e., **meteorology.py and crop.py.**
- Arrays and multidimensional arrays in the GeoCAT routine are either **NumPy** or **Xarray.** Some routines used **Dask** for parallelizing Xarray arrays on the CPU.



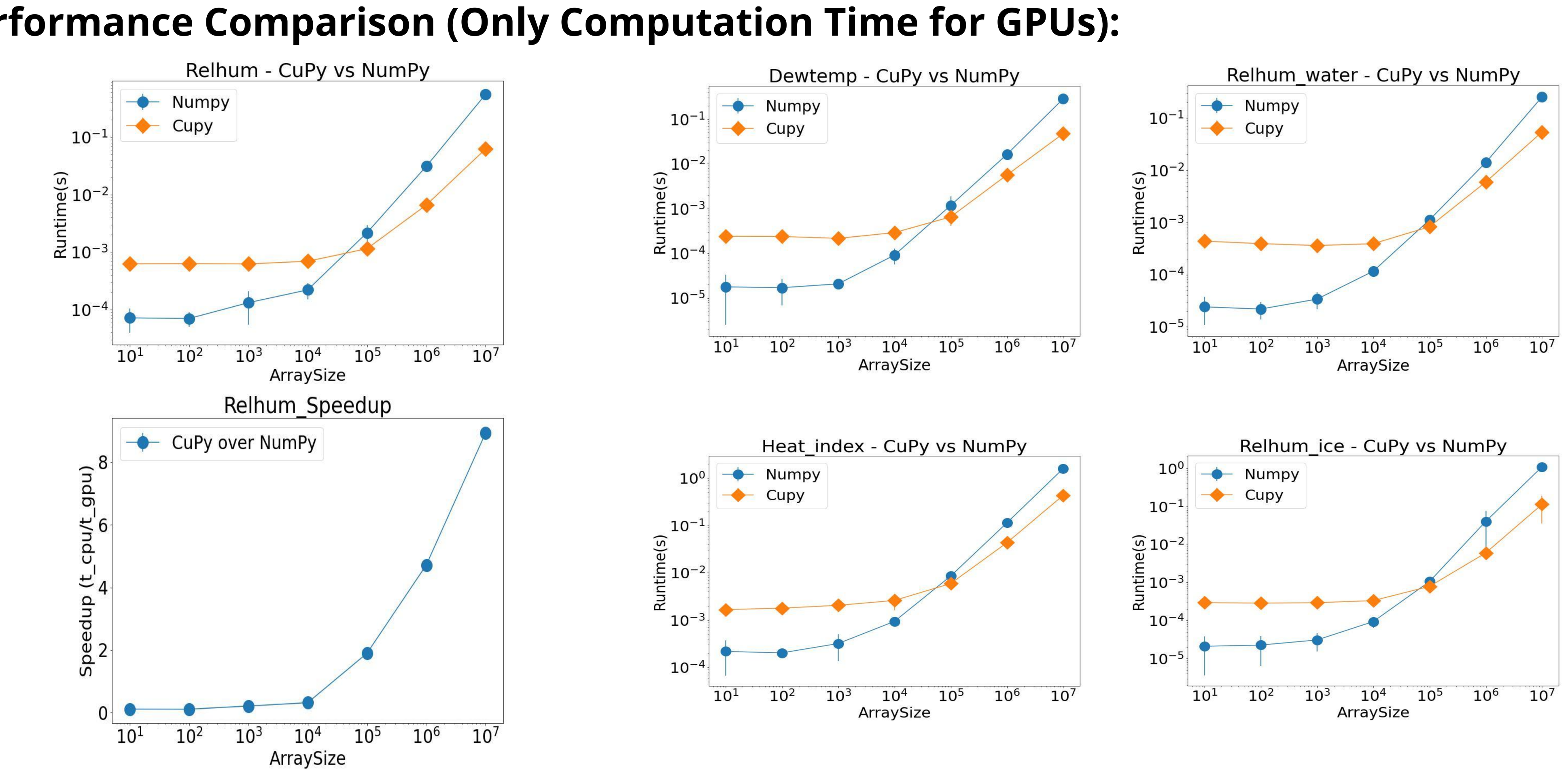

```
g_array = cupy.asarray(c_array)
```

```
g_array = xarray.DataArray(cupy.asarray(c_array.data))
```

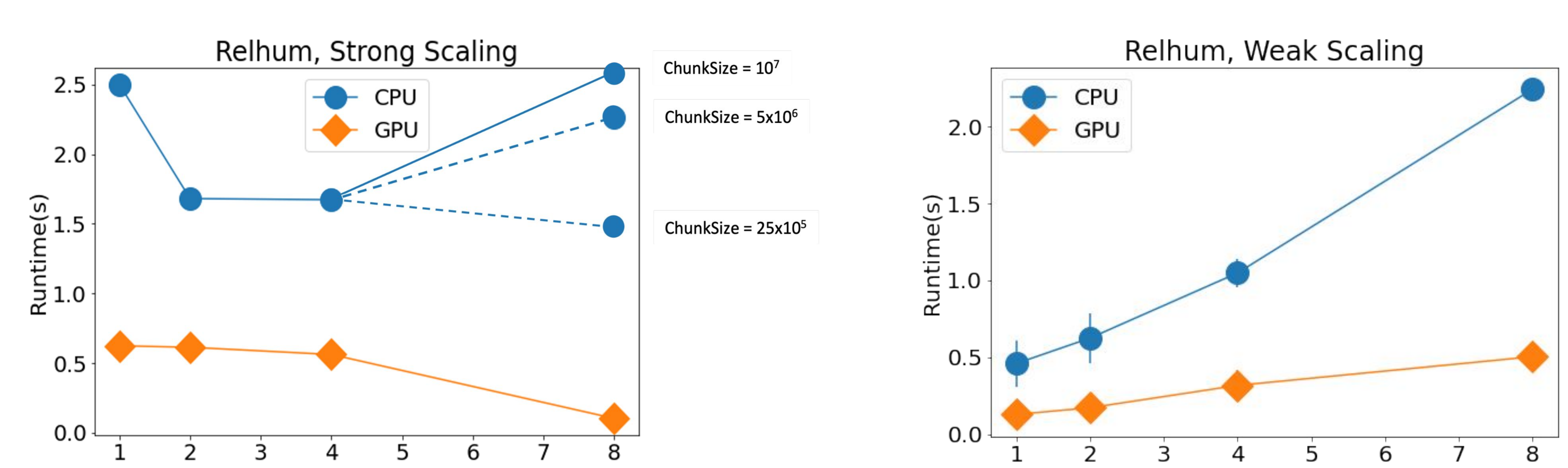
```
g_array = xarray.DataArray(c_array.data.map_blocks(cupy.asarray))
```

Performance Results

Performance Comparison (Only Computation Time for GPUs):



Scalability: Strong and Weak Scaling



Experimental Setup

GPU nodes:
2 18-core 2.3-GHz Intel Xeon Gold 6140 (Skylake) processors per node
8 NVIDIA Tesla V100 32GB SXM2 GPUs with NVLink

CPU nodes:
Dual-socket nodes, 18 cores per socket
2.3-GHz Intel Xeon E5-2697V4 (Broadwell) processors
16 flops per clock

Challenges

- Adapting Xarray and Dask with CuPy
- Inability to get performance improvements with some GPU tasks, e.g., Search functions: xarray.where().
- Numba JIT compiler auto-parallelizes NumPy arrays on CPU, but it is not adapted to CuPy arrays
- Correct way for benchmarking and gathering data:
  - Setting the correct chunksize

Conclusion and Future Work

- Explored ways to port GeoCAT-comp to run on GPUs, as recent supercomputers are shifting to include GPU accelerators as the major resource.
- Ported CPU parallelized routines to GPU.
- Validated output results with the precision of 10^{-7}.

Future Work:

→ Port all the routines.
→ Push to production.
→ Investigate writing kernel functions with CuPy's user-defined kernel capabilities or Numba and PyCuda.

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Ported Branch: **GeoCAT Github:**

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