Porting IDL programs into Python for GPU-Accelerated In-situ Analysis

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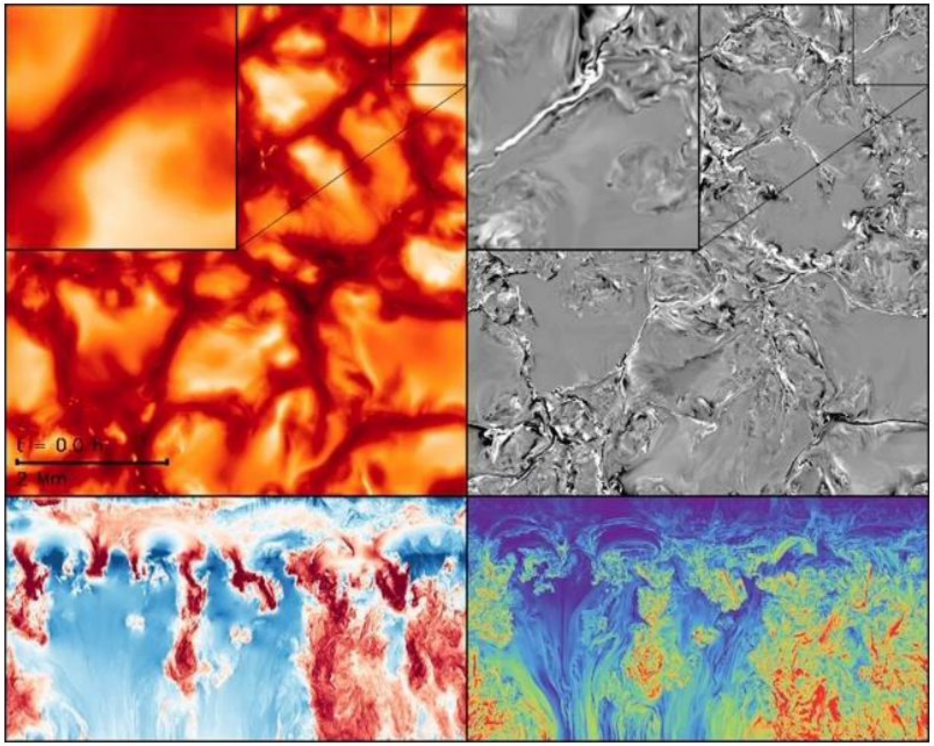
Background

- MURaM is the primary solar model used for simulations of the upper convection zone, photosphere and corona.
- 100x acceleration is needed to keep up the simulation with the real time data from telescope.
- MURaM have been ported to use scalable GPUs to achieve this!
- As computation is optimized, I/O and post processing becomes the next major bottleneck.



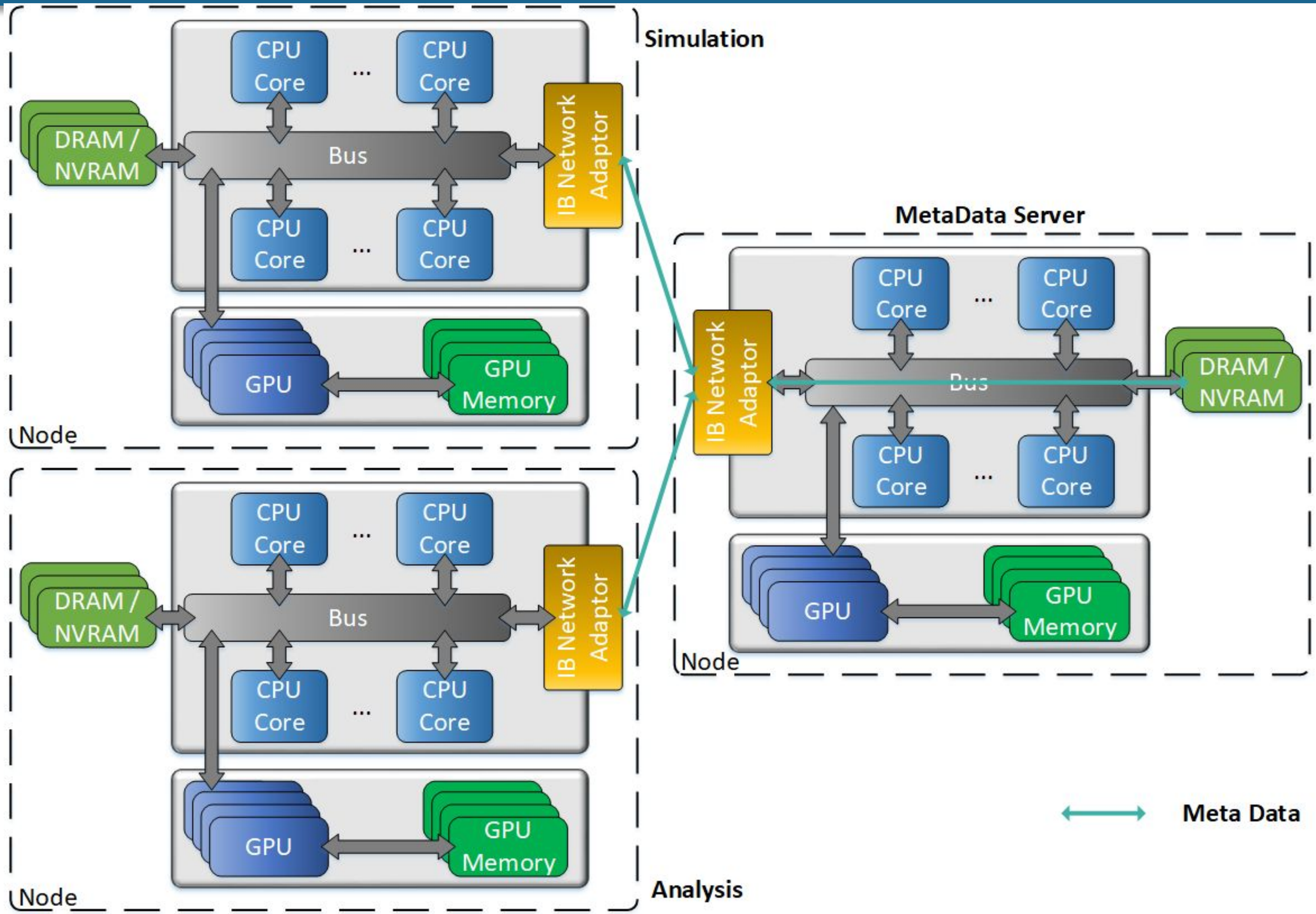
MURaM simulation of solar granulation

- Thus, both converting this workflow to an in-situ approach and a staging-based IO subsystem for this in-situ workflow are critical problems need to be addressed.

Motivation

- One bottleneck is post processing analysis
- A way to reduce the bottleneck is to parallelize data analysis
- Current analysis programs are in IDL
- IDL is proprietary has a small community (astrophysics researchers)
- Python is a better choice for analysis: open source, large library selection, can be optimized for different hardware

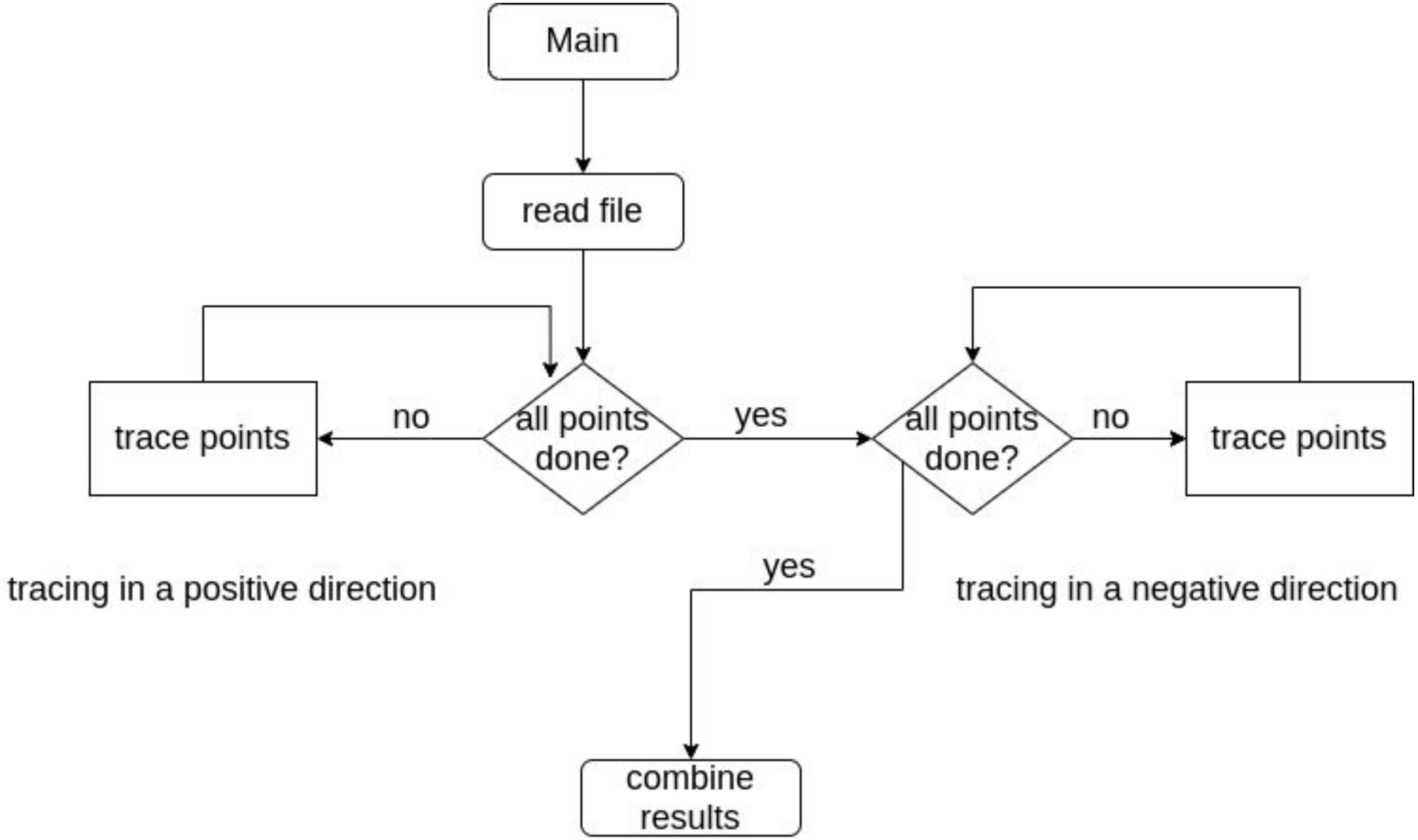
Bigger Picture



Goals

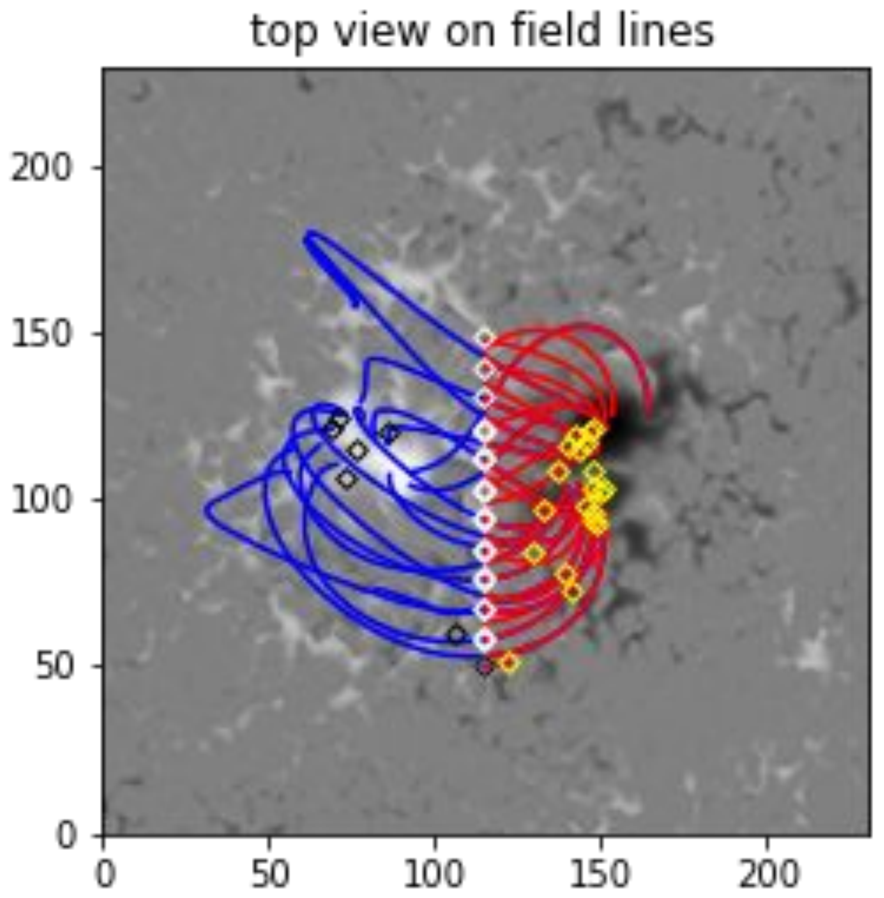
- Port analysis IDL programs into Python
- Optimize Python code (better data structures, efficient libraries, etc.)
- Parallelize Python code for both CPUs and GPUs
- Integrate Python analysis scripts with the larger workflow
- If time permits, look into automating IDL to Python conversion

Algorithm

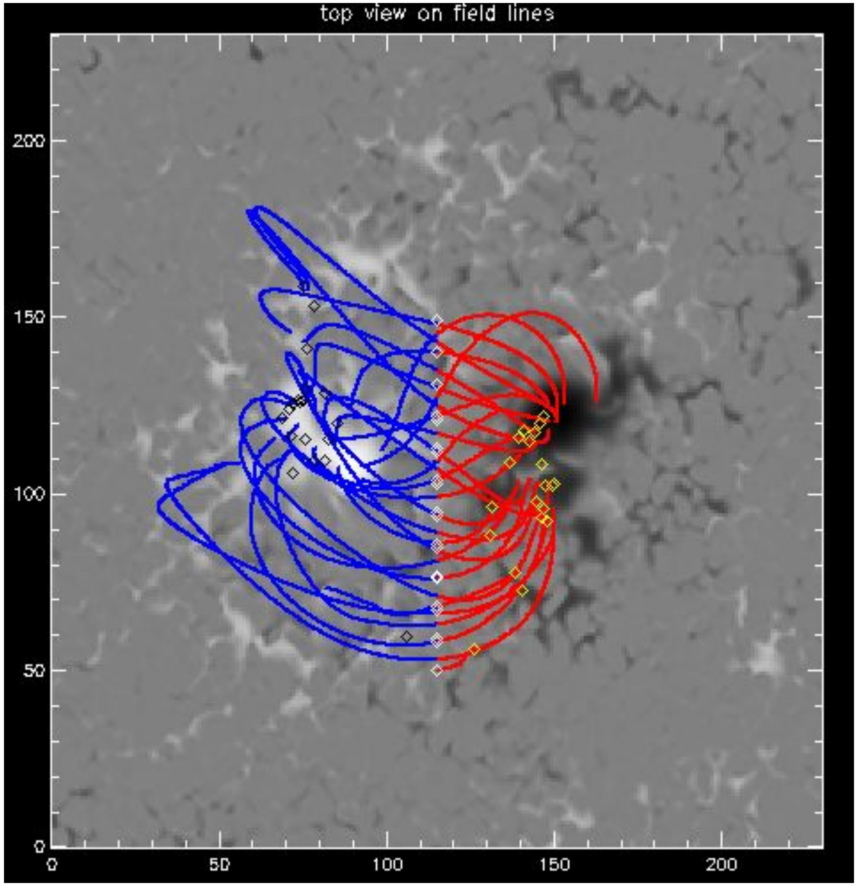

Main
read file
trace points
no
all points done?
yes
all points done?
no
trace points
yes
tracing in a positive direction
tracing in a negative direction
combine results

Top View

Python

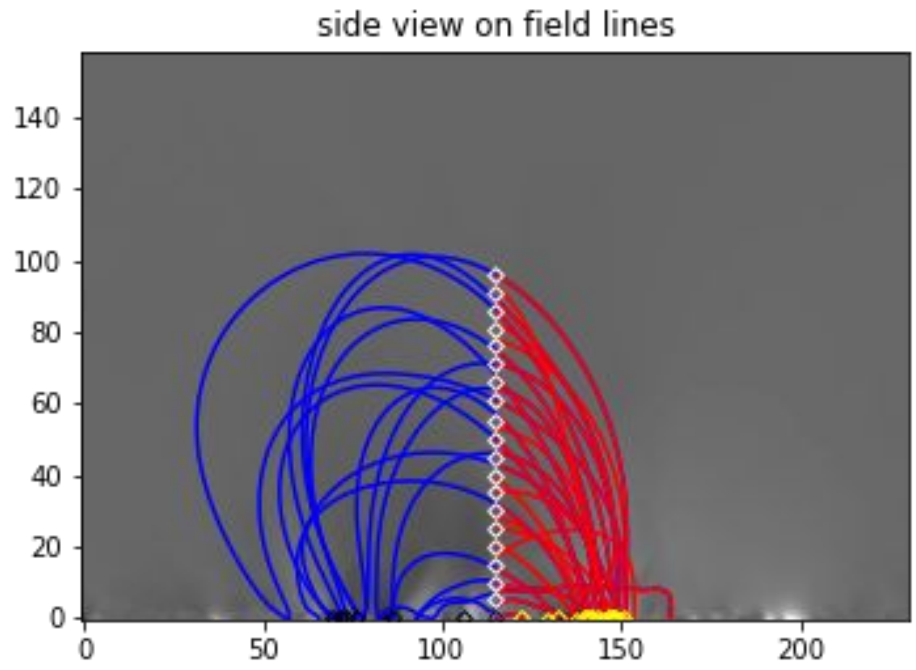


IDL

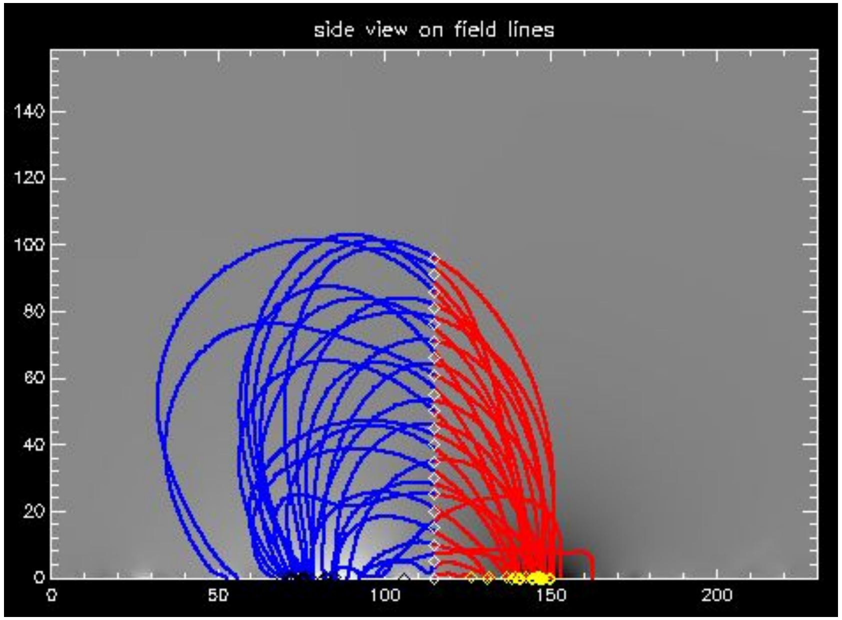


Side View

Python

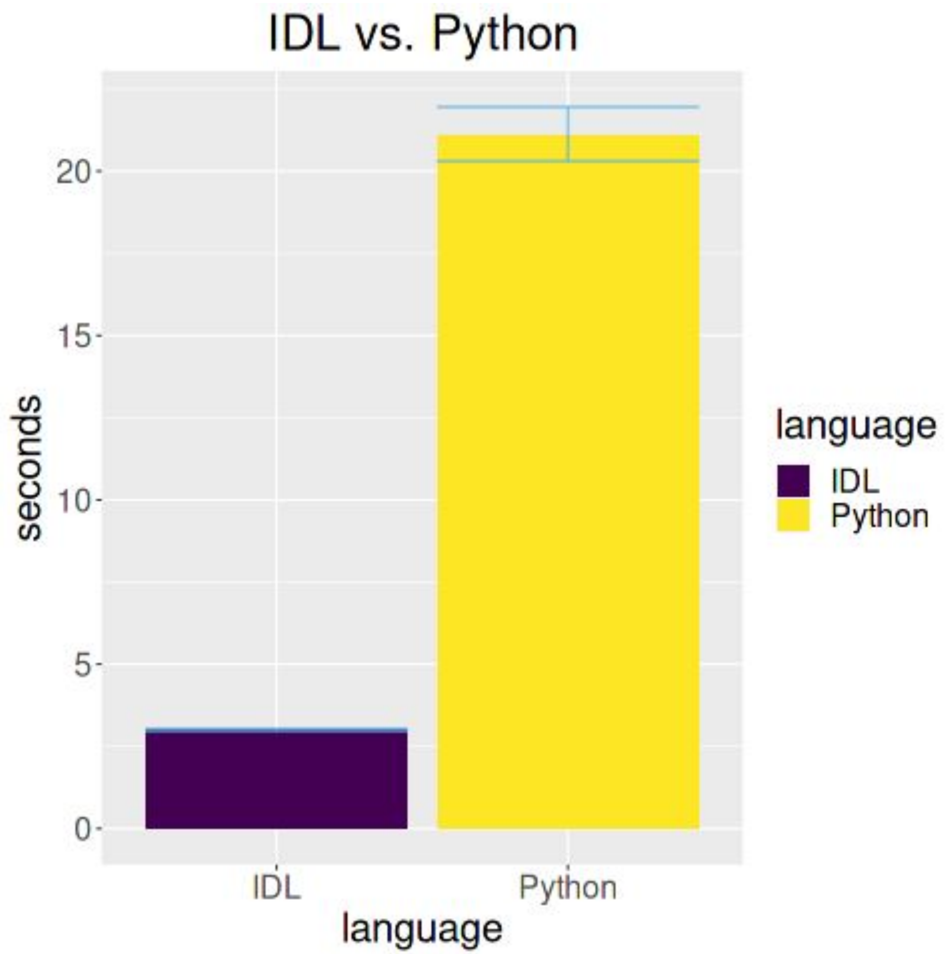


IDL



More about my experience + comparison of the two languages:
https://wiki.ucar.edu/display/~dpulatov/Comparison+of+IDL+and+Python

Benchmarking



Code Profiling

Python:

```
#1: 6.189 _evaluate_linear  scipy/interpolate/interpolate.py:2534 call tree depth: 4
#2: 5.111 [self]   call tree depth: 5
#3: 4.326 _find_indices  scipy/interpolate/interpolate.py:2554 call tree depth: 4
```

IDL:

Module	Type	Count	Only(s)	Avg.(s)	Time(s)	Avg.(s)	LinesRun	Total
DBLARR	(S)	3	1.190213	0.396738	1.190213	0.396738	0	0
FINDGEN	(S)	2	0.000021	0.000010	0.000021	0.000010	0	0
FLTARR	(S)	1	0.000071	0.000071	0.000071	0.000071	0	0
HELP	(S)	1	0.000046	0.000046	0.000046	0.000046	0	0
INTERPOLATE	(S)	4488	1.003250	0.000224	1.003250	0.000224	0	0

Libraries

Numpy

- Numerical computation library for Python
- Fast array operations written in C

Xarray

- Extends Numpy with labels
- Intuitive data access thanks to metadata
- Tailored to work with NetCDF format

Zarr/NetCDF

- Xarray allows easy read/write with Zarr/NetCDF formats
- Implemented a variable reader for MURaM that saves data into Zarr
- Zarr is format for storing compressed, chunked arrays

xarray.Dataset

▸ Dimensions: (x: 288, y: 144, z: 576)

▸ Coordinates: (0)

▾ Data variables:

vx	(z, x, y)	float32	3.898e+03 519.4 ... -1.061e+06
shape :	(576, 288, 144)		
by	(z, x, y)	float32	-412.6 -320.7 ... -0.6506 -0.4422
bx	(z, x, y)	float32	-352.5 -126.0 214.5 ... 13.29 13.28
bz	(z, x, y)	float32	-623.5 -419.3 ... 2.681 2.735
rho	(z, x, y)	float32	0.0004166 0.0004166 ... 1.654e-16
vy	(z, x, y)	float32	537.7 307.7 ... -4.539e+05

▾ Attributes:

description : MURaM files converted into zarr format

Parallelism in Python

Dask

- Library for parallel computing
- Integrates well with Numpy and Xarray

Cupy

- Array library for GPU computing
- Almost drop-in replacement for Numpy

Numba

- Just-in-time compiler for Python
- Translates Python to machine code

Cython

- Static compiler
- Makes writing C extensions easy

Exploring Parallelism

There are two potential routines to parallelize: tracing and interpolation. Both were explored during this stage.

Libraries	Results
Dask	Algorithm too complex for Dask to parallelize
Cupy	Limited support for Scipy functions in our implementation
Numba	No parallelization due to mixing of data types
Cython	No parallelization due to GIL in CPython

Future Work

- Reimplement interpolation in C++ with native support for parallelism instead of Python

- idlwrap library provides IDL-like interface for Python
  Not complete, possible avenues for improvement

- Using/extending IDL to Python translators
  pyIDL, Pike, i2py
  None are complete, all projects are abandoned

Acknowledgement

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Questions?