Leibniz Supercomputing Centre
of the Bavarian Academy of Sciences and Humanities

Optimizing Astrophysical Simulations and Data Analysis codes on Intel Architectures

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LRZ machines

▲ CoolMUC-3 – KNL

64 cores/node, 16GB MCDRAM
Used in quadrant/cache mode

SKX – SuperMUC-NG ►

48 cores/node, 2GB/core RAM

6336 thin, 144 fat (768 GB/node)

I. Simulation codes (CFD + astro)

Optimizing code for Astrophysical Simulations

The FLASH[1] code

(Adaptive) Mesh code

CFD / MHD + Physics (+ Astro)

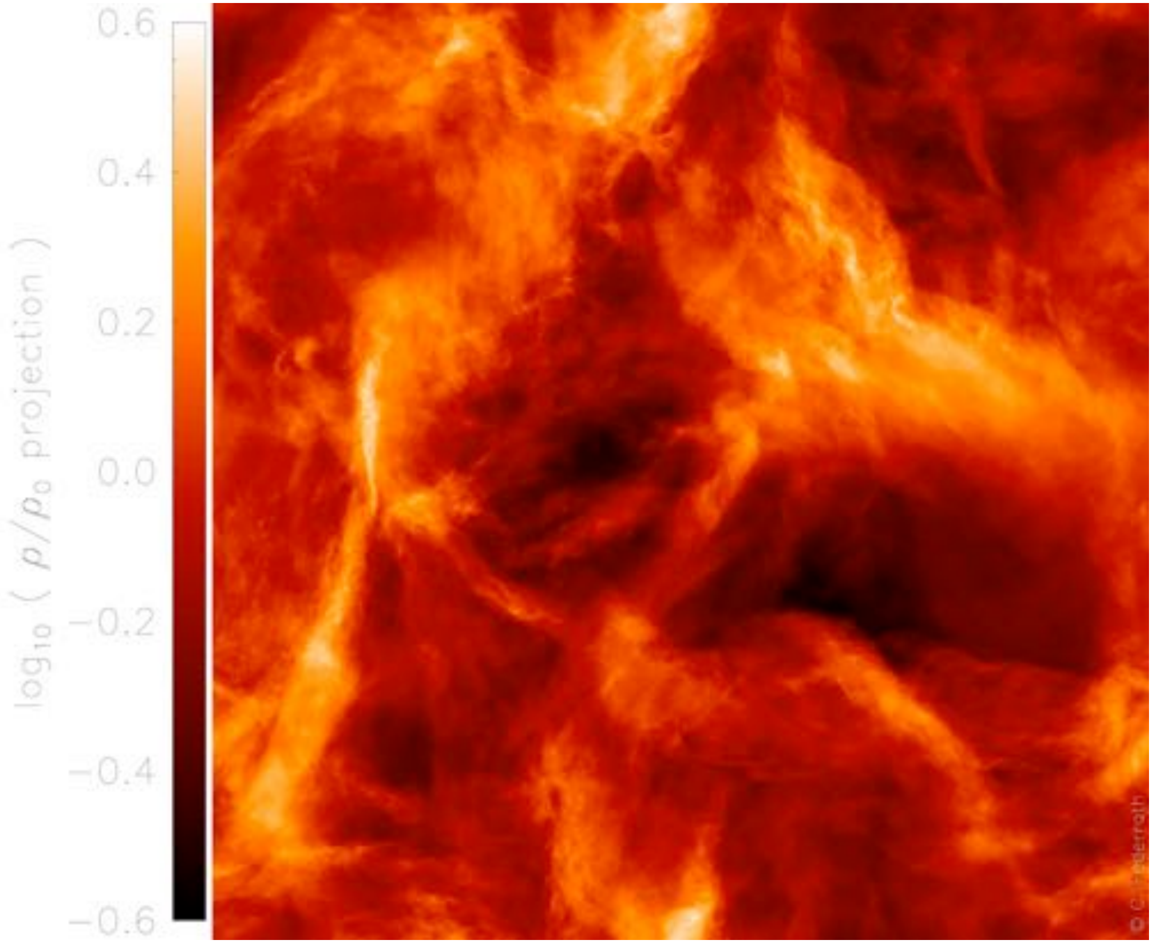
- nuclear + radiation (+ stars) +…
- here turbulence, shocks …

Optimizations by C. Federrath[2] with LRZ

Hybrid single/double-precision

Even in a difficult turbulent setup:

- improves MPI and memory usage
- further advantage with vectorization
- now extended to MHD

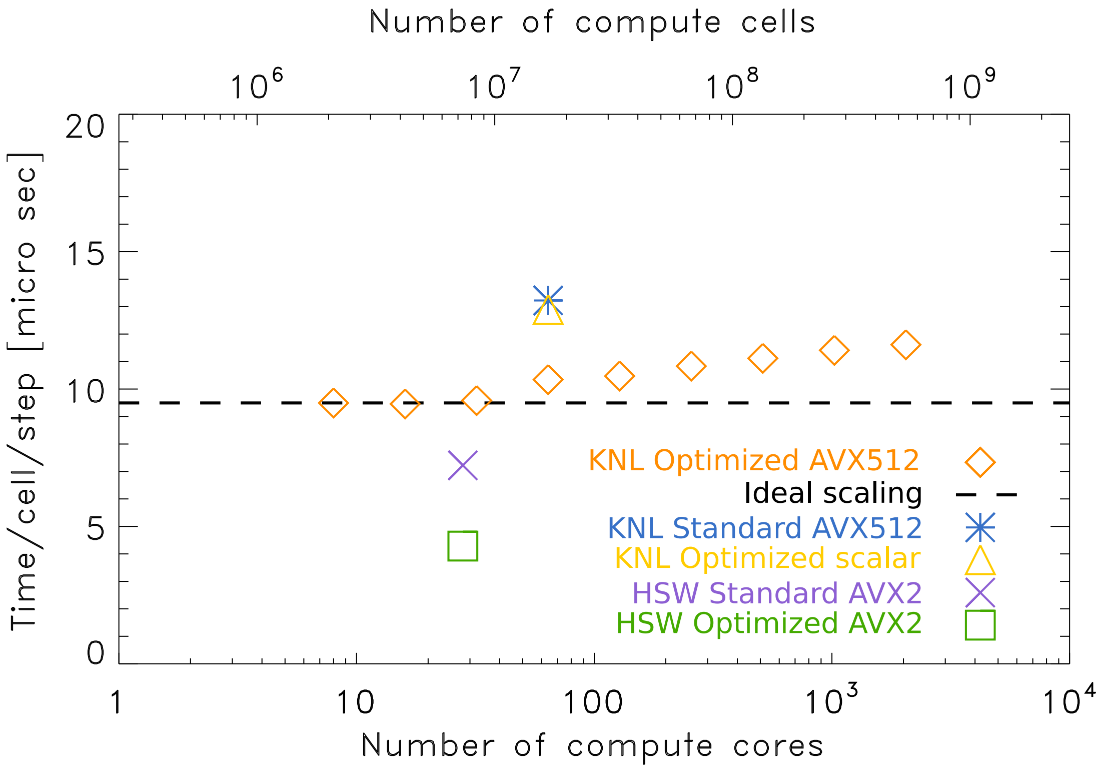


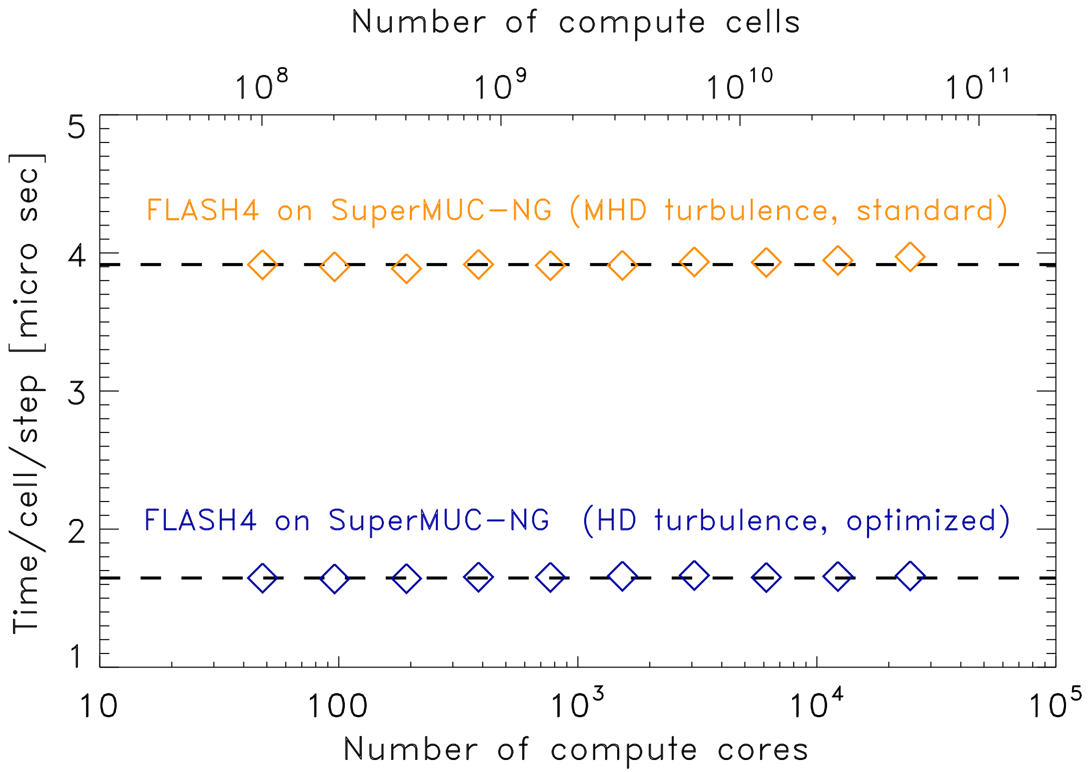
Credit: C. Federrath. Density and sonic-scale projections of a 10008^3 grids simulation, no MHD.

[1] Fryxell et al. 2000

[2] Federrath et al. 2016 „The world's largest turbulence simulations" + Federrath et al. 20XX – submitted to Nature Astronomy

The FLASH code: weak scaling tests





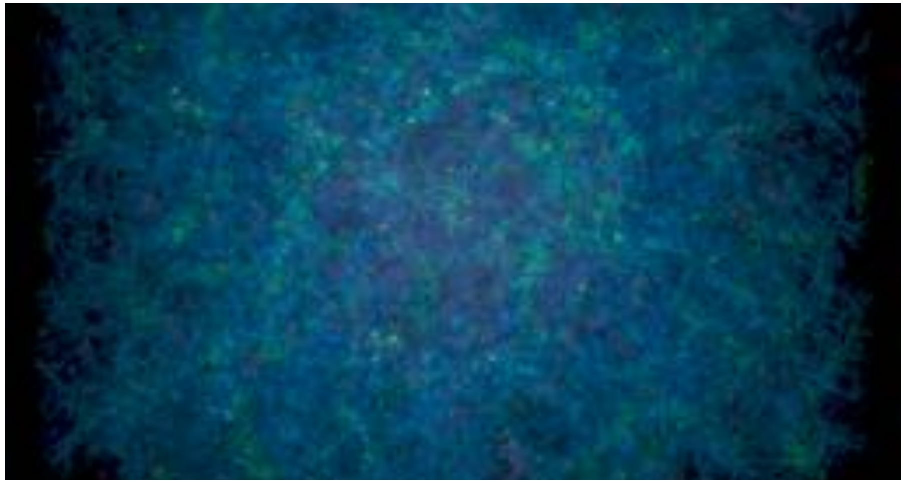
Optimization work on previous architectures shines on both KNL and SKX!

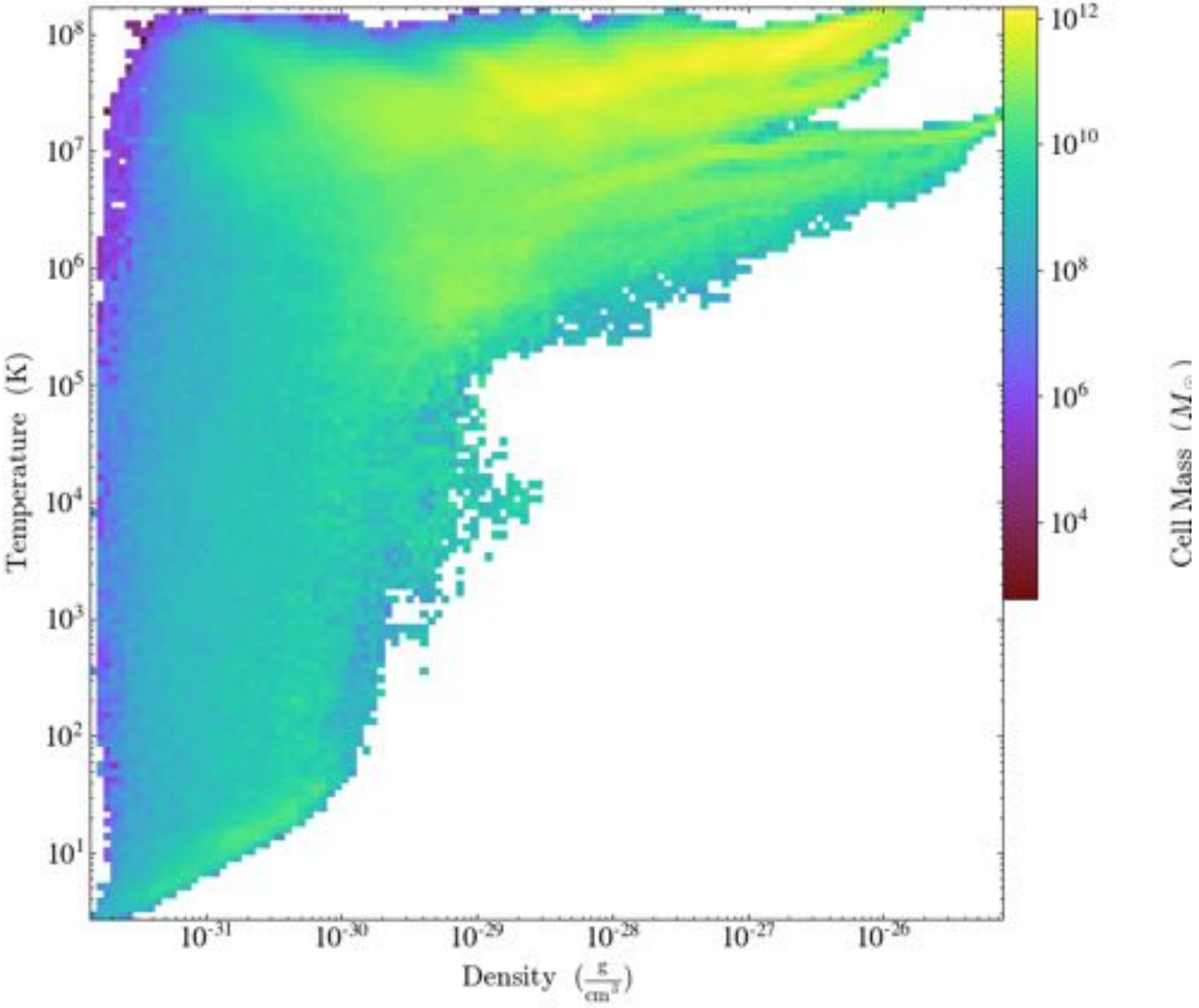
II. yt: Intel VS Anaconda python on SKX

yt: data analysis python package

submbitted to Intel PUM, Issue #38

- Python-based: numpy, scipy, mpi4py, …
- Integration with professional tools:
  RT, X-ray, mock observations, …
- Cross-code, general-purpose
- Sample tasks: 2D phase plot ►
  ▼ Volume rendering





Scripted, and parallel via mpi4py

yt: tasks with synthax

submitted to Intel PUM, Issue #38

Preamble

```
import yt, mpi4py
yt.enable_parallelism()
ds = yt.load("RD0028/RedshiftOutput0028") # Opening file header only
sp = ds.sphere("c", (10.,"Mpc"))          # Central 10 Megaparsec sphere
```

Derived

```
j  = sp.quantities.angular_momentum_vector(use_gas=True, use_particles=True)
```

Phase

```
pp = yt.PhasePlot(sp, "density", "temperature", ["cell_mass"], weight_field=None)
pp.save()
```

Volume

```
im, sc = yt.volume_render(ds, ('gas', 'density'), fname='volume.png')
```

X-ray: Preamble

```
import soxs, pyxsim
soxs.soxs_cfg.set("soxs", "response_path", "./soxs_responses" )
redshift  = 0.05
src_model = pyxsim.ThermalSourceModel("apec", 0.05, 11.0, 10000, Zmet=0.3)
exp_time  = (100., "ks")
area      = (2000.0, "cm**2")
sp        = ds.sphere("c", (50.,"Mpc")) # Enlarge to 50 Megaparsec
```

X-ray: Photons

```
# Computation 1/2: Montecarlo radiative transfer
photons  = pyxsim.PhotonList.from_data_source(sp, redshift, area, exp_time, src_model)
```

X-ray: Events

```
# Computation 2/2: Photons produce events into simulated detector
events_z = photons.project_photons("z", (45.,30.), absorb_model="tbabs", nH=0.04)
```

X-ray: Printout

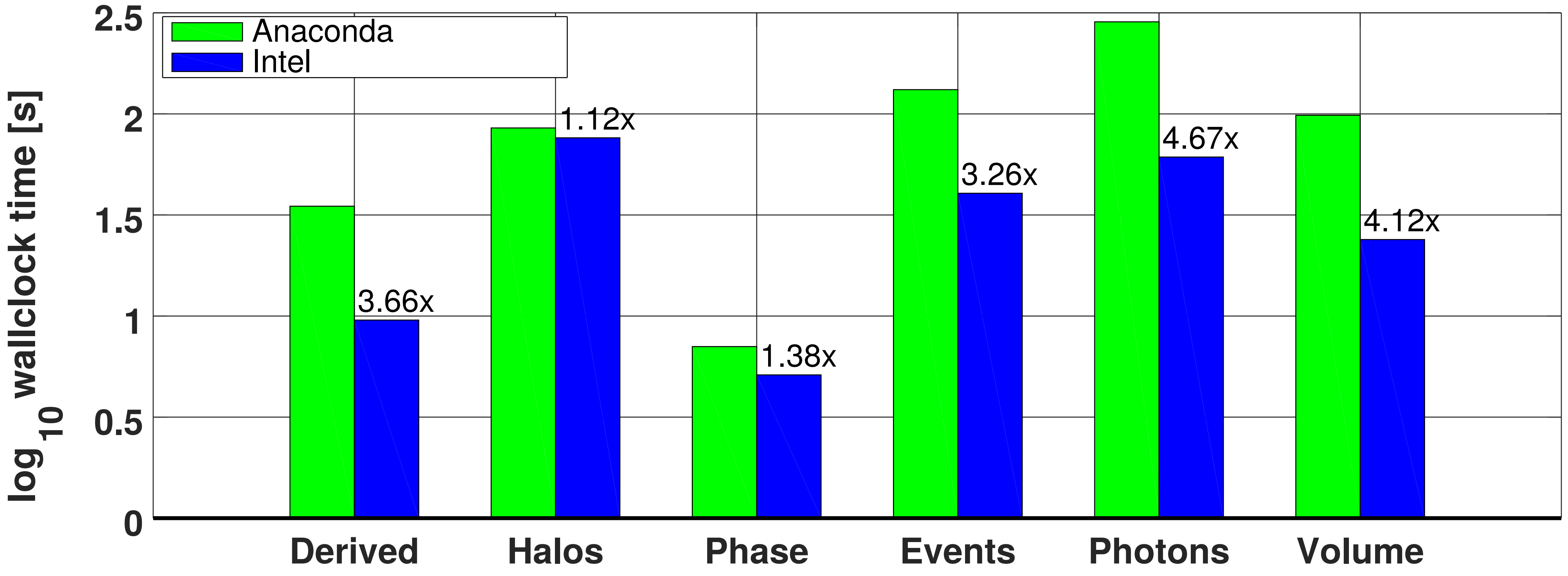
```
events_z.write_simput_file("RD0028", overwrite=True) # Warning: very large fits file!
soxs.instrument_simulator("RD0028_simput.fits", "evt.fits", (100.0, "ks"), "acisi_cy0", [45.,30.],overwrite=True)
soxs.write_image("evt.fits", "img.fits", emin=0.5, emax=11.0, overwrite=True)
exit()
```

Intel vs Anaconda python

yt: performance

(lower is better)

submitted to Intel PUM, Issue #38



Intel vs Anaconda python

yt: detailed scaling

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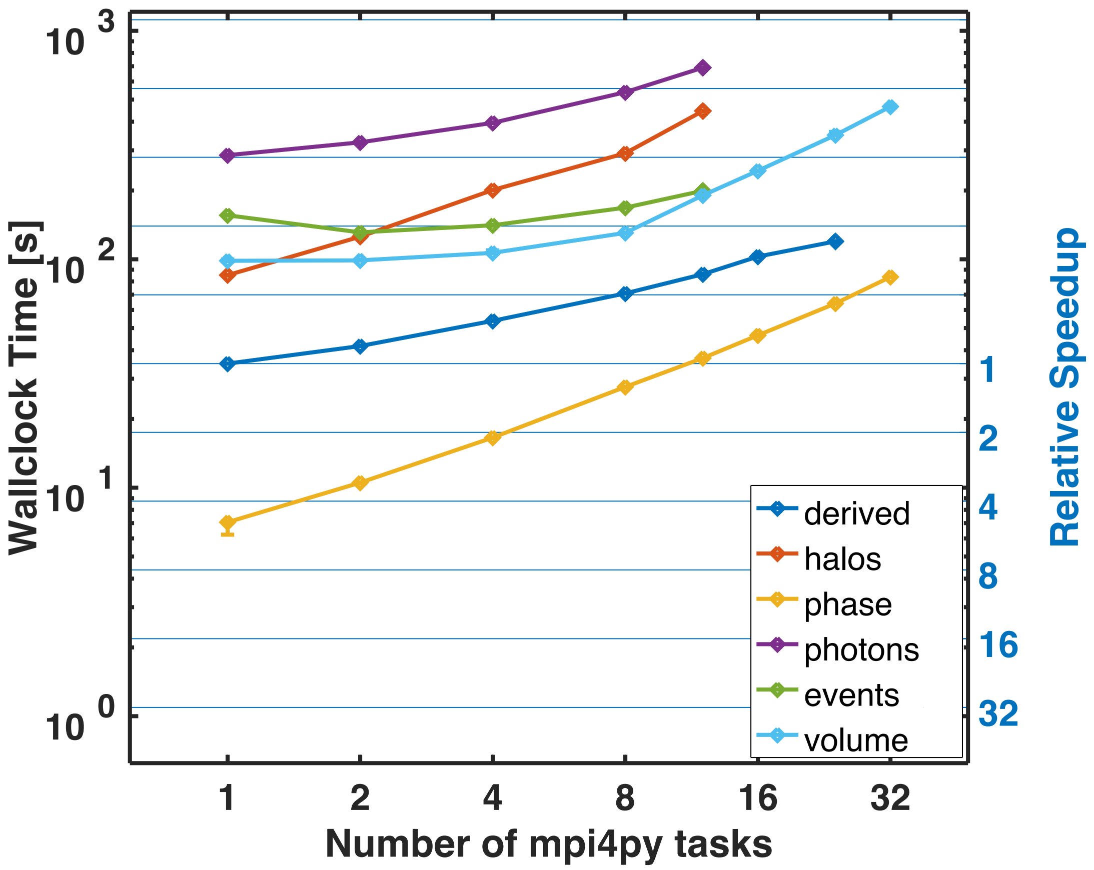
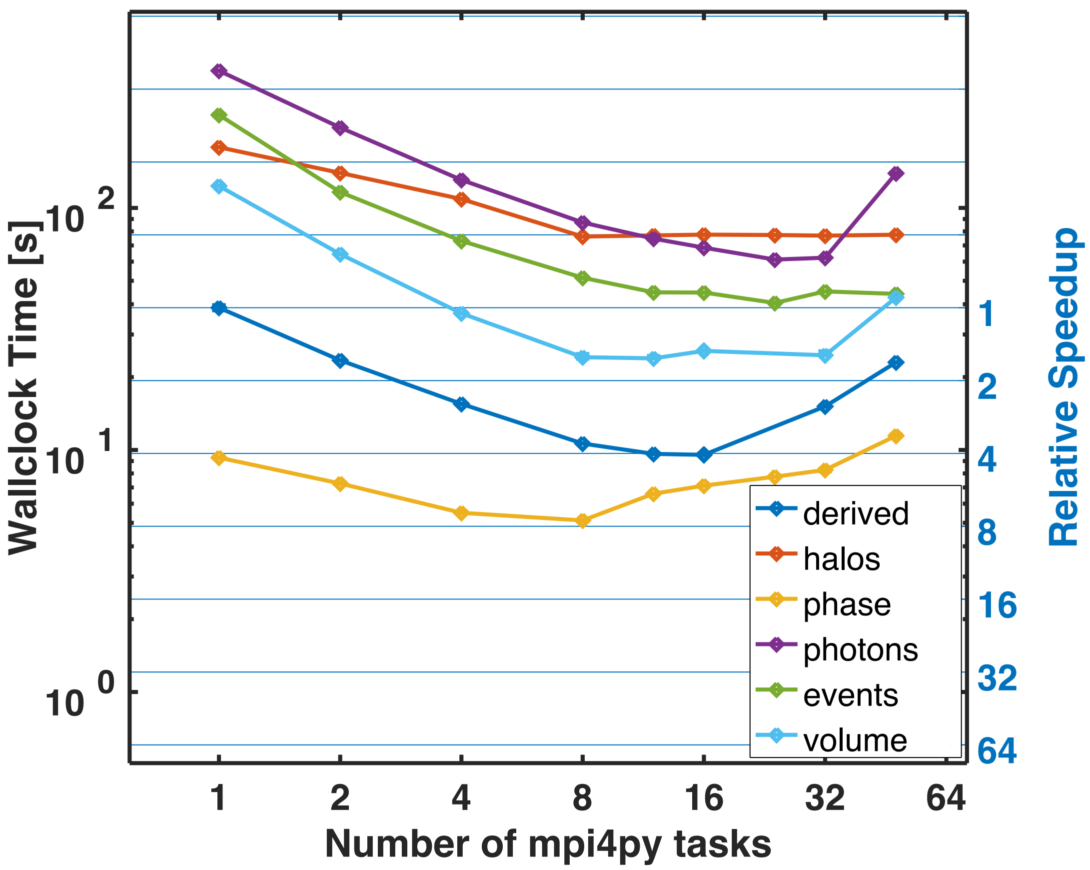




III. Deeper into yt: parallelism beyond mpi4py on KNL

yt and HPC: beyond mpi4py

OpenMP Enabling HPC since 1997

- native support through mpi4py, just set OMP_NUM_THREADS
- pure or hybrid

Cython

- optimising static compiler for both Python and itself.
- Get efficient C code from python…
- ... but one must go that extra mile to rewrite and compile your code!
- No tutorials from yt! Users must learn from Cython tutorials and apply to yt functions.

yt scripted synthax

```
$ mpiexec -np 8 python volume.py
```

volume.py

```
import yt, mpi4py
yt.enable_parallelism()
ds = yt.load("RD0028/RedshiftOutput0028")
im, sc = yt.volume_render(ds,  ('gas', 'density'), fname='volume.png')
exit()
```

Cython compiled synthax

```
$ python setup.py build_ext --inplace
$ mpiexec -np 8 python launch.py
```

setup.py

```
from setuptools import setup
from Cython.Build import cythonize
setup(name = 'Volume_app', ext_modules = cythonize("*.pyx"))
```

launch.py

```
import myvolume, yt
ds = yt.load('RD0028/RedshiftOutput0028')
myvolume.do_volume(ds)
exit()
```

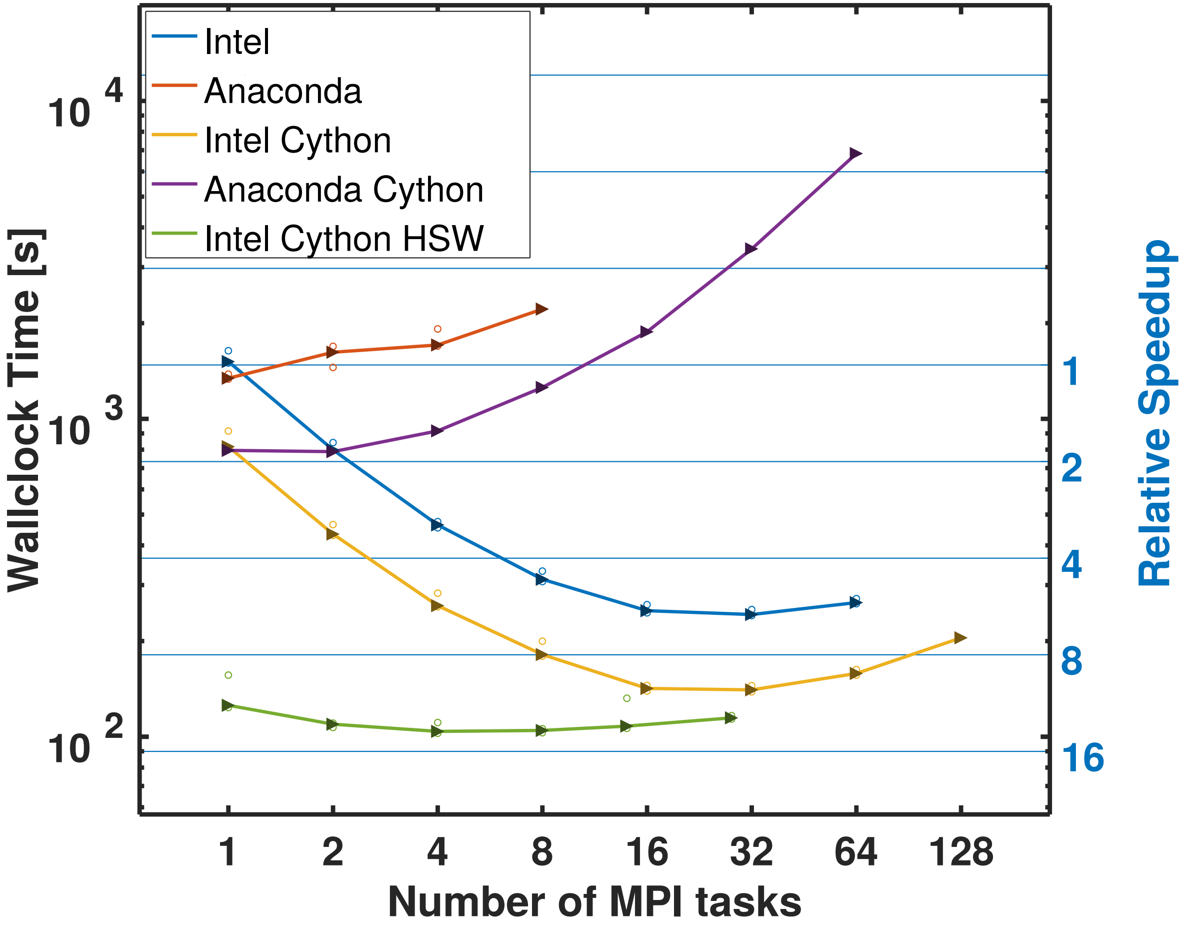
myvolume.pyx

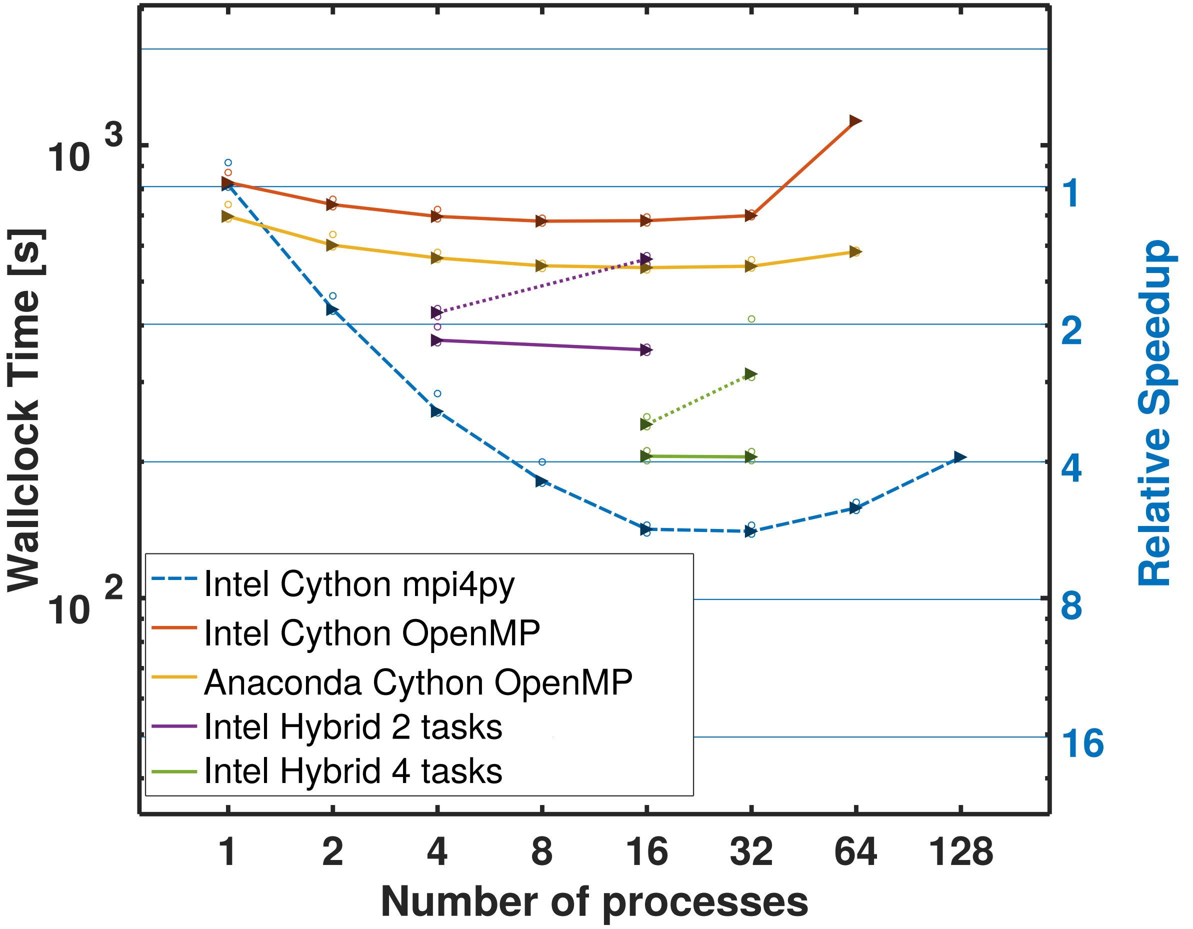
```
def do_volume(ds):
    import yt
    im, sc = yt.volume_render(ds, 'density', fname='rendering.png')
```

Intel → scalability out-of-the-box Cyhton→ work harder for performance OpenMP → ???

Scaling behaviour with Cython and OpenMP

submitted to FGCS, in review





Also: automatic process pinning best option (dotted lines). Hard to get anything from hyperthreading.

Summary

Simulation Codes

- Code optimization on previous Intel architecture shines on KNL and SKX
- Treasure the lesson of the KNL!

yt and data analysis

- post-processing with HPC techniques is possible (and fun!)
- using Intel python is a must, and works out-of-the-box
- further optimization requires changing workflow

For the near future…

- Involve yt developers in Intel python discussion
- Investigate where and why yt scaling breaks
  - Characterization with Intel Advisor