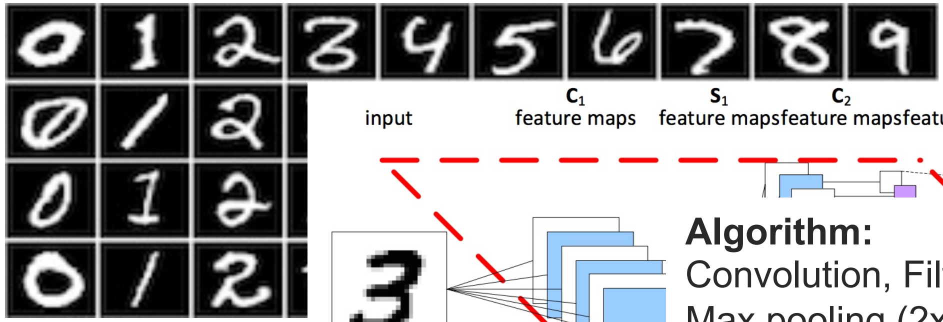
Enabling performance portability for FV3 / xSHIELD using a Python-based domain-specific language

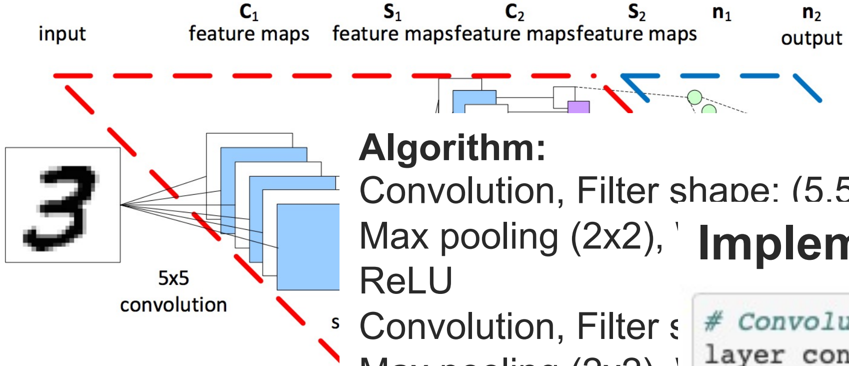
Oliver Fuhrer, Johann P. S. Dahm, Eddie C. Davis, Florian Deconinck, Oliver D. Elbert, Rhea C. George, Christopher Kung, Jeremy McGibbon, Andrew Pauling, Tobias F. Wicky, Elynn Wu

Partners: NOAA/GFDL and NASA/GMAO

September 3, 2021
ESCAPE-2 Dissemination Workshop

Machine Learning Scientist





Algorithm:
Convolution, Filter shape: (5,5,6), Stride=1, Padding='SAME'
Max pooling (2x2), '
ReLU
Convolution, Filter s
Max pooling (2x2), '
ReLU
Fully Connected La
ReLU
Fully Connected La
Softmax

Implementation (Python + Tensorflow):

```
# Convolutional Layer 1
layer_conv1, weights_conv1 = new_conv_layer(input=x_image, num_input_channels=1, fi
m_filters=6, name ="conv1")

# Pooling Layer 1
layer_pool1 = new_pool_layer(layer_conv1, name="pool1")

# RelU layer 1
layer_relu1 = new_relu_layer(layer_pool1, name="relu1")

# Convolutional Layer 2
layer_conv2, weights_conv2 = new_conv_layer(input=layer_relu1, num_input_channels=6
, num_filters=16, name= "conv2")

# Pooling Layer 2
layer_pool2 = new_pool_layer(layer_conv2, name="pool2")

# RelU layer 2
layer_relu2 = new_relu_layer(layer_pool2, name="relu2")

# Flatten Layer
num_features = layer_relu2.get_shape()[1:4].num_elements()
```

Climate Scientist

$$\vec{u}(\vec{x}) = \sum_{i=1}^{k} \lambda_i \phi_i(\vec{x}) \vec{n}_i$$

Implementation (Fortran + OpenACC):

```
!$ACC PARALLEL &
!$ACC PRESENT( iqidx_d, ..., ptr_vn_d, e_flx_avg_d, vn_d, vt_d, rbf_vec_coeff_e_d )
!$ACC LOOP GANG PRIVATE( i_startidx, i_endidx, jb )
    DO jb = i_startblk, i_endblk
      IF ( i_startblk == jb ) THEN; i_startidx = e_startidx; ELSE; i_startidx = 1; ENDIF
      IF ( i_endblk == jb ) THEN; i_endidx = e_endidx; ELSE; i_endidx = nproma; ENDIF
!$ACC LOOP VECTOR COLLAPSE(2)
     DO je = i_startidx, i_endidx
        DO jk = 1, nlev
          iqidx_1 = iqidx_d(je,jb,1)
          ! Average normal wind components
          ptr_vn_d(je,jk,jb) = e_flx_avg_d(je,1,jb)*vn_now_d(je,jk,jb)&
            + e_flx_avg_d(je,2,jb)*vn_now_d(iqidx_1,jk,iqblk_1) &
            :
          ! RBF reconstruction of tangential wind component
          vt_now_d(je,jk,jb) = rbf_vec_coeff_e_d(1,je,jb)  &
            * vn_now_d(iqidx_1,jk,iqblk_1) &
            :
        ENDDO
      ENDDO
    ENDDO
!$ACC END PARALLEL
```

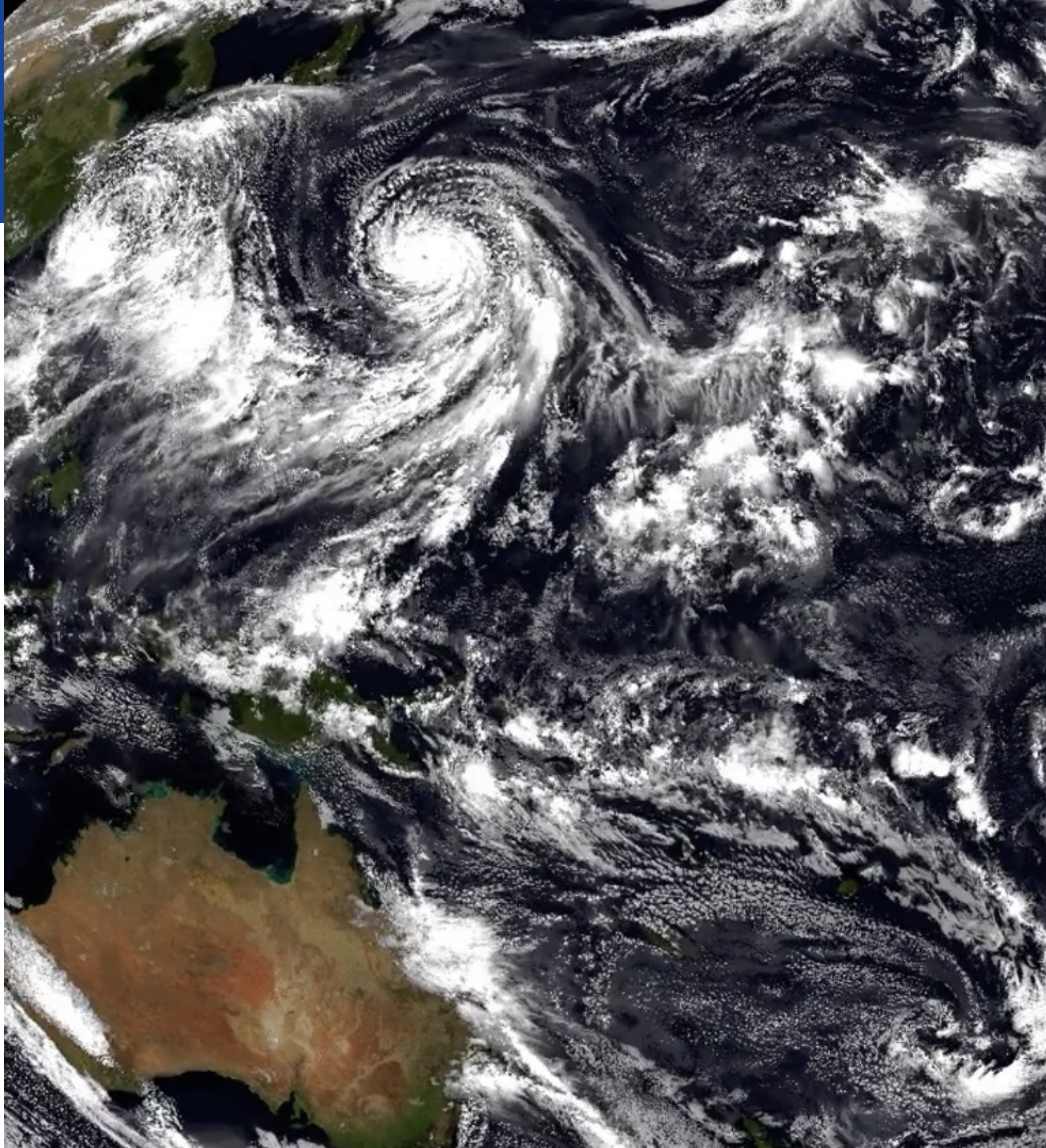
Goal

Build a global-storm resolving model in Python using an embedded domain-specific language that can run at scale on modern supercomputers

Started October 2019

Validation first, performance second

Focus on NVIDIA GPUs and x86 CPUs



But… Python is slow!

That depends on…

- Granularity
- Copy-free data-views

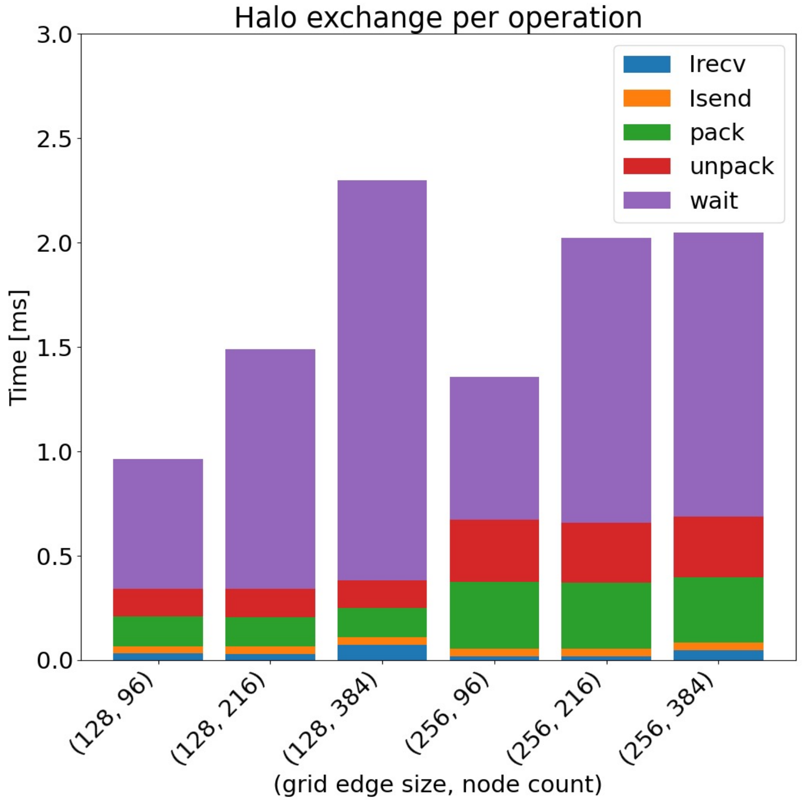
Example: Fully Python-wrapped version of NOAA's fv3gfs model is overhead-free.

McGibbon et al. 2020, GMD
https://doi.org/10.5194/gmd-14-4401-2021

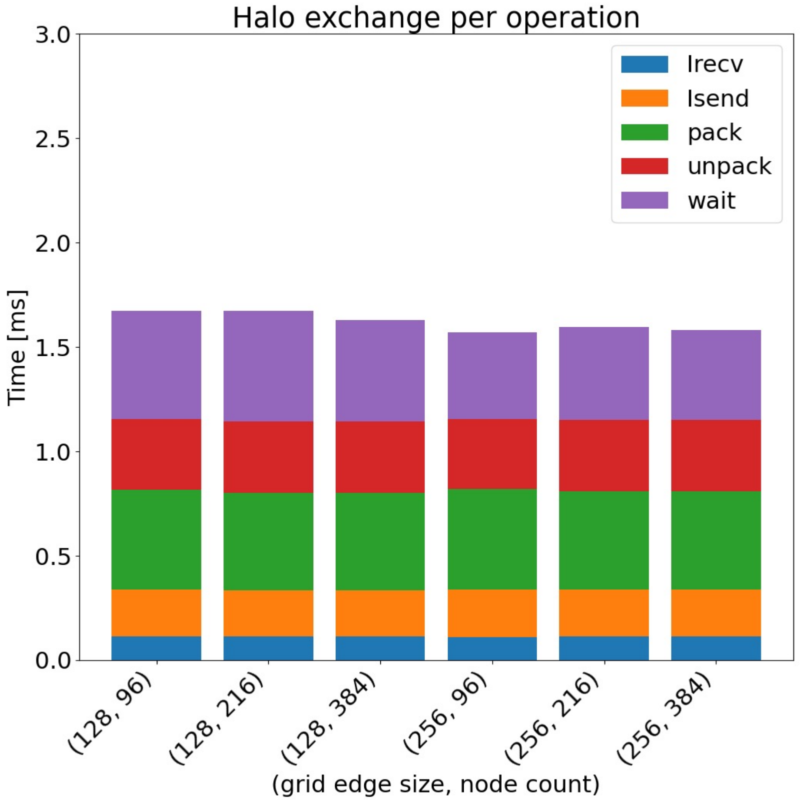
```
import fv3core
import fv3gfs.wrapper as wrapper
from fv3gfs.util import io
from mpi4py import MPI

comm = MPI.COMM_WORLD
rank = comm.Get_rank()

wrapper.initialize()

for step in range(wrapper.get_step_count()):
    wrapper.step_dynamics()
    wrapper.step_physics()
    if (io):
        state = wrapper.get_state()
        io.write_state(state, f"out_state_{rank}.nc")

wrapper.cleanup()
```

But… Python is not parallel!

Example: Halo-exchange of FV3 dynamical core on Piz Daint



Fortran (FMS/MPI)



Python (CuPy/mpi4pi)

But… Python is not HPC!

Driven by AI/ML, the fraction of HPC workloads written and tooling available in Python is rapidly increasing.

Train GPT-3

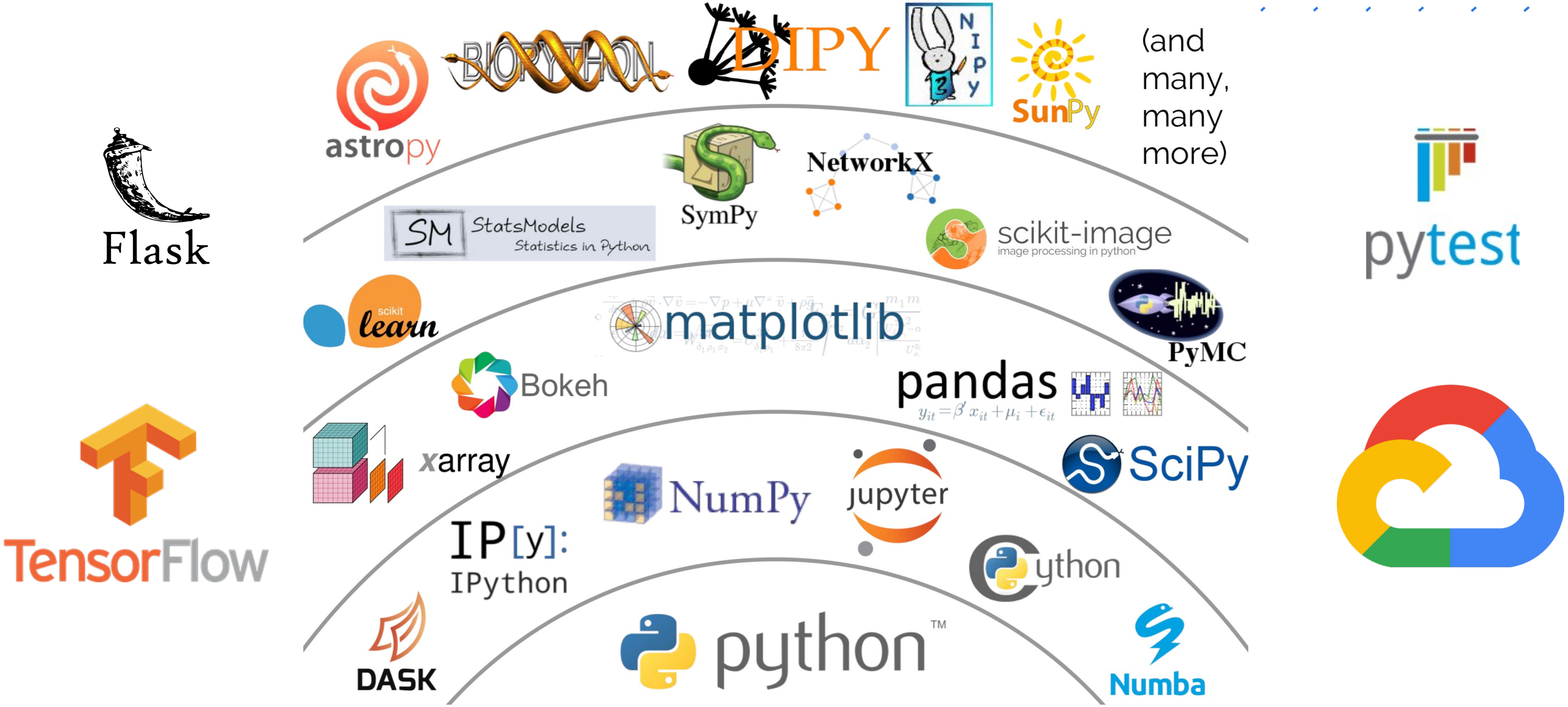
175 billion parameters

PyTorch

1km Global Storm Resolving Model

5 year integration

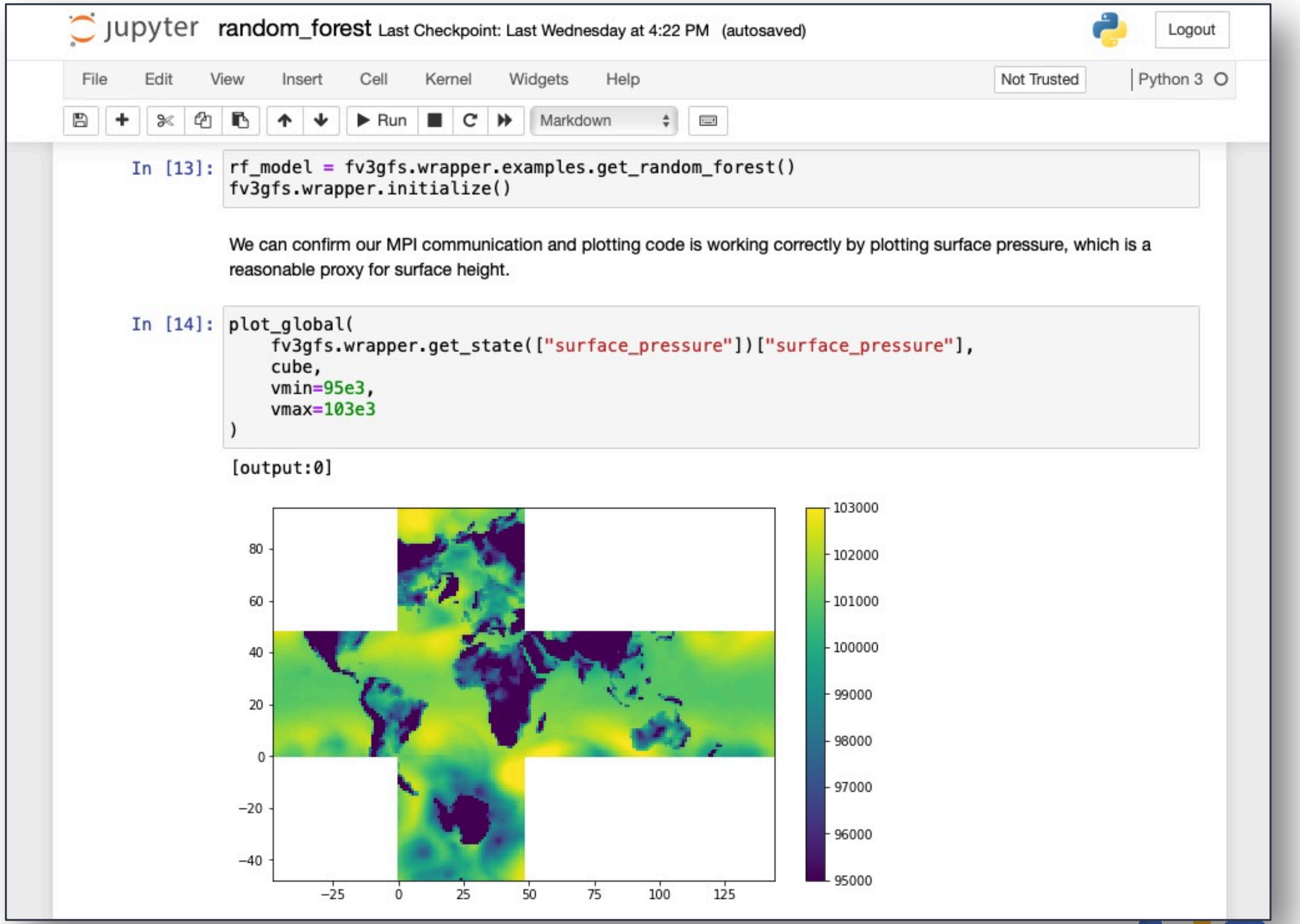
And… Python Ecosystem



Credit: Jake VanderPlas, "The Unexpected Effectiveness of Python in Science", PyCon 2017

And... Developing in Python

- Python enables interactive development
- Easy to integrate with machine learning, analysis code, online diagnostics
- Same code runs at scale or on a laptop
- Easy to maintain and use extensive unit tests

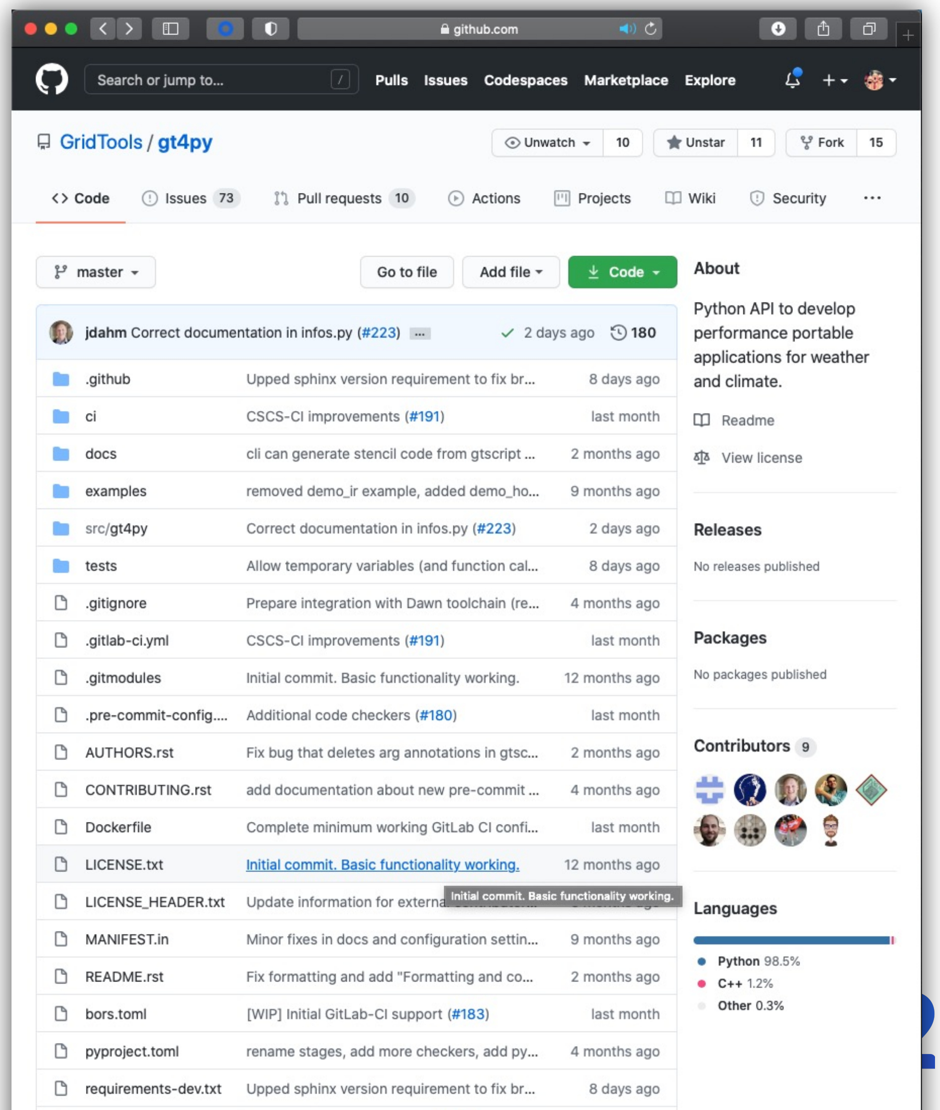


The FV3GFS / xSHIELD Model

- FV3 dynamical core integrated into UFS, GEOS, CESM, GFDL models
- xSHIELD = FV3 + GFS physics for global storm-resolving simulations (DYAMOND)
- Cubed-sphere grid balances uniform resolution and simple code
- Horizontal finite volume dynamics
- Vertical Lagrangian dynamics with remapping
- Highly optimized for x86 CPU architectures

GT4Py

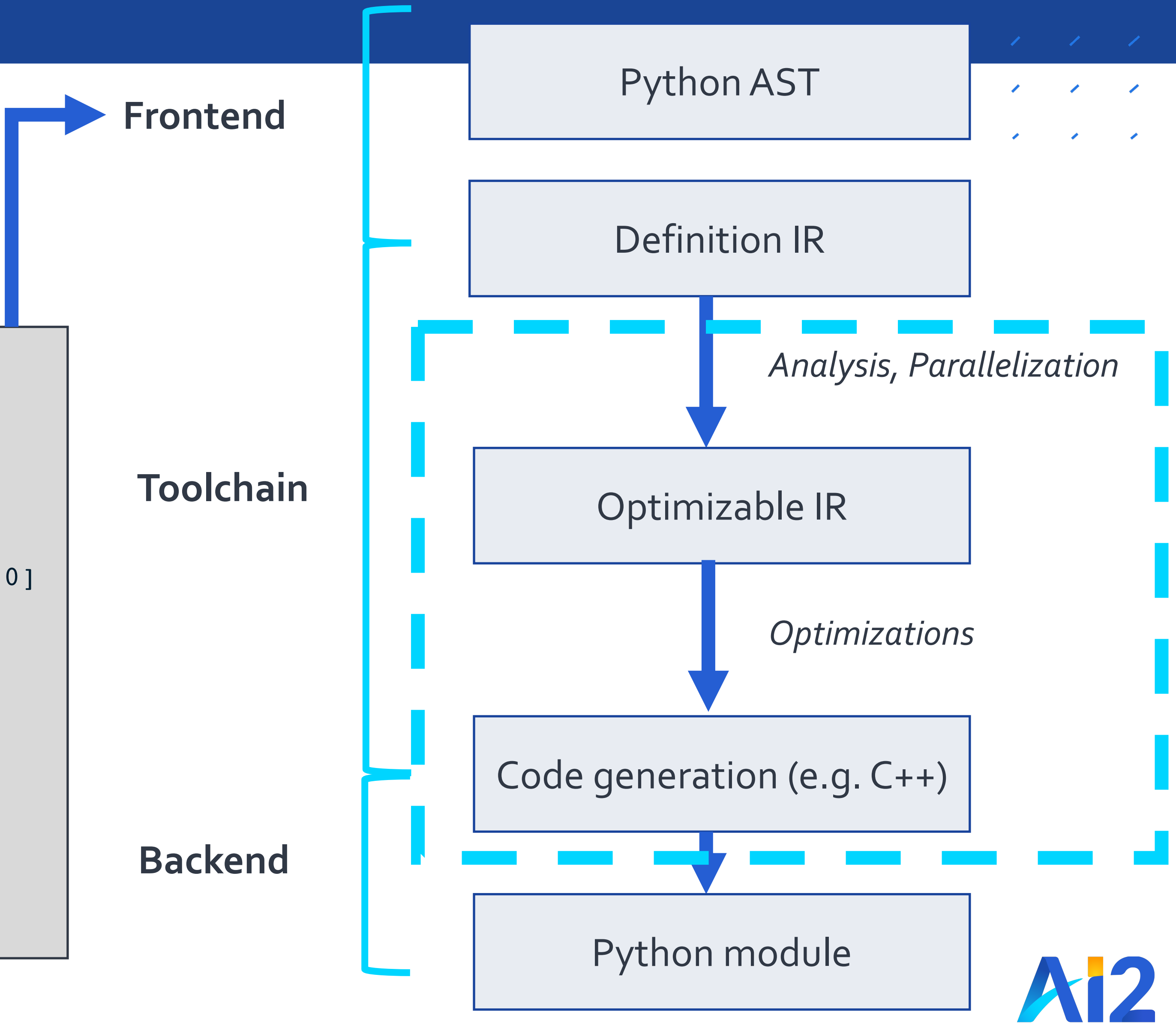
- Open-source, open-development project
  https://github.com/GridTools/gt4py
- Joint development with ETH Zurich/CSCS and MeteoSwiss
- Part of the GridTools ecosystem of tools and libraries for weather and climate
- GT4Py is embedded in Python
- Emphasis on tight integration with scientific Python stack
- Multiple backends: **Python** (NumPy), **CPU** (C++/OpenMP), **GPU** (CUDA), …



GT4Py Pipeline

Application (DSL Code)

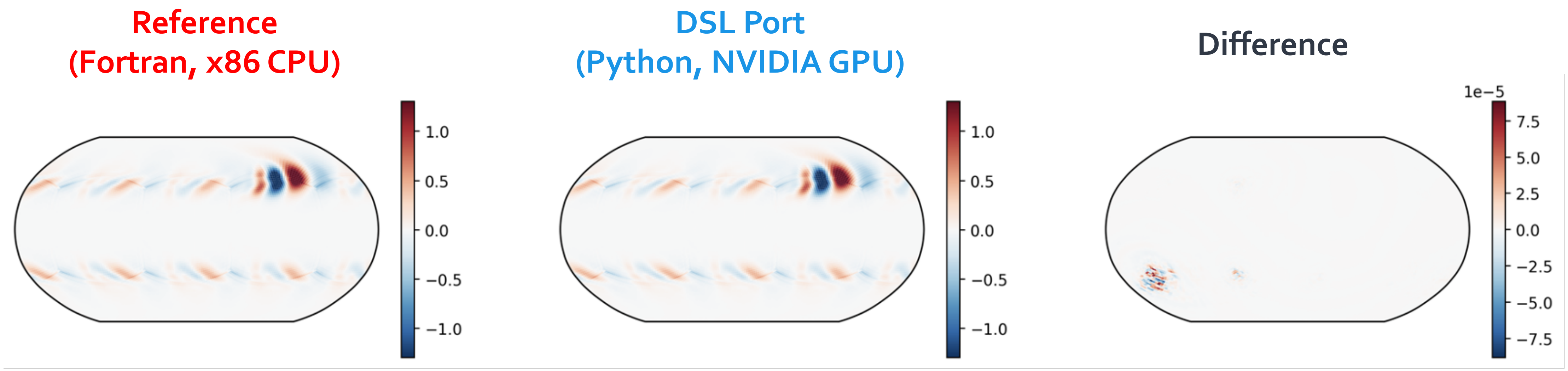
```python
import numpy as np
from gt4py.gtscript import Field, PARALLEL,
computation, interval

def laplacian(field):
    return - 4. * field[ 0, 0, 0] + field[-1, 0, 0]
        + field[1, 0, 0] + field[0, -1, 0]
        + field[0, 1, 0]

def laplap_stencil(in_field: Field[np.float64],
out_field: Field[np.float64]):
    with computation(PARALLEL), interval(...):
        tmp = laplacian(in_field)
        out_field = laplacian(tmp)
```



FV3core: DSL port of FV3

Check it out on GitHub!
https://github.com/VulcanClimateModeling/fv3core

Baroclinic instability testcase (Jablonowski and Williamson 2006)
6 day surface temperature anomaly [K]



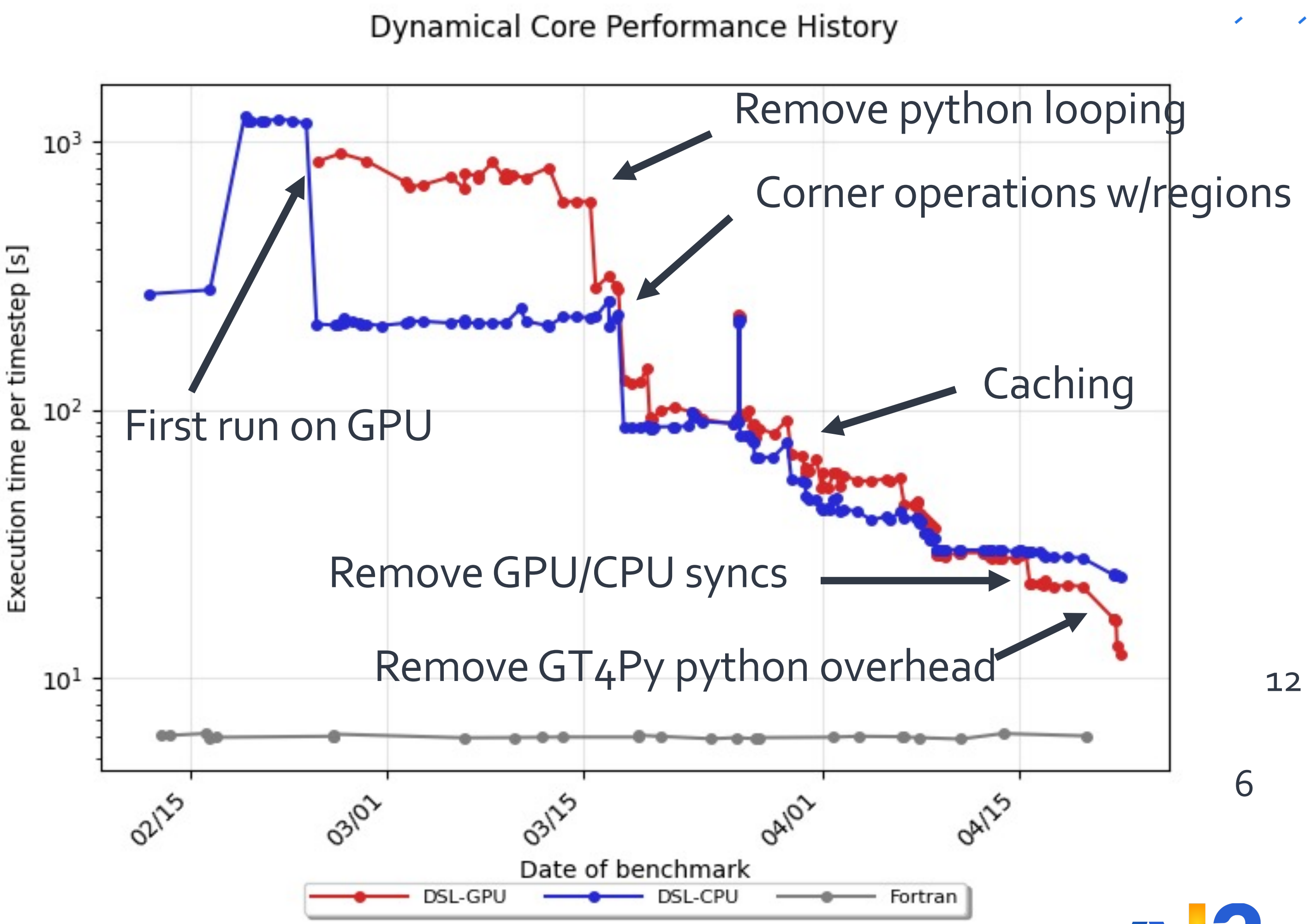
Performance: FV3core

Making it fast…

10 weeks of improvements

- Remove python code
- Use new GT4py features to merge stencils
- Cache temporary objects
- Asynchronous execution model

Currently 2.8x slower on CPU and 1.6x faster on GPU as compared to Fortran reference



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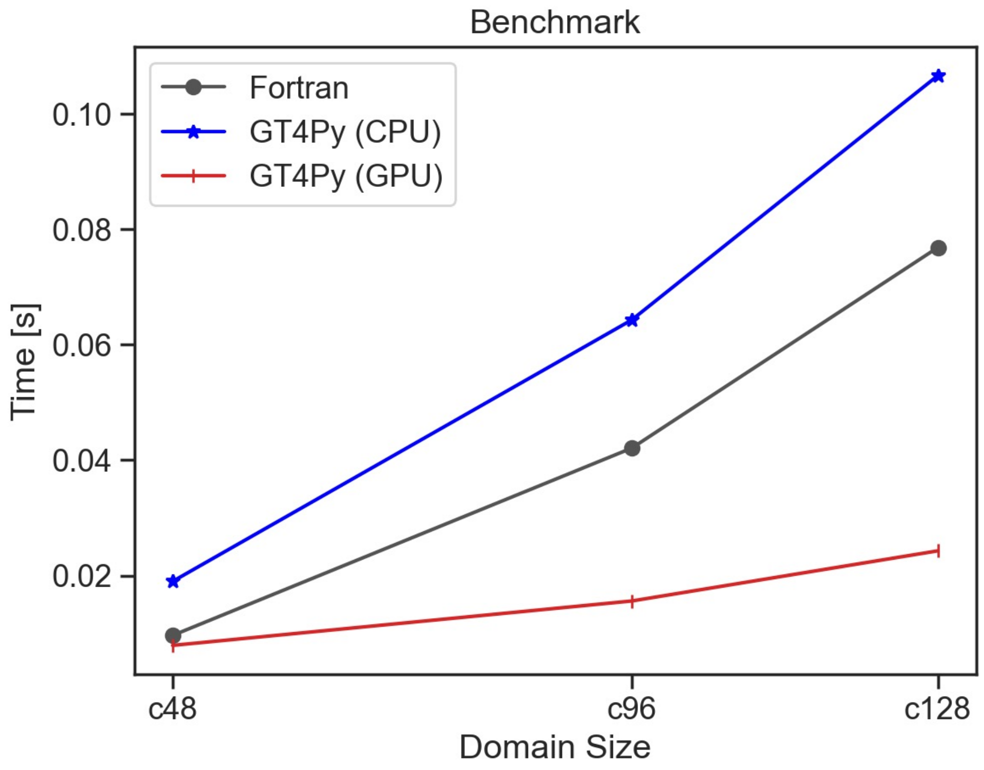
Physical Parameterizations

	Microphysics	PBL &Turbulence	Sea-Ice	Shallow Convection	LSM	Radiation
Authors	 Mikael	 Chris	 Vera  Nadja  Nicolai	 Mikael  Chenwei  Langwen	 Safira	 Andrew
Scheme	GFDL Cloud Microphysics Scheme	GFS scale-aware EDMF PBL and Free Atmospheric Turbulence Scheme	GFS Sea Ice Scheme	GFS SAS-based Mass-Flux Scheme for Shallow convection (sa-MF)	GFS Noah Land Surface Model	GFS RRTMG
Status	Ported	Ported	Ported	Ported	Ported	In progress

Performance: Microphysics



Domain size: 128 x 128 x 79

	Runtime [s]	Speedup
Fortran	0.077	REF
GT4Py (CPU)	0.107	0.72
GT4Py (GPU)	0.024	3.2

System: Piz Daint, CSCS
CPU: Intel Xeon E2690 v3 @ 2.6 GHz, 12 core
GPU: NVIDIA Tesla P100

Further optimization of DSL toolchain needed to speed up runtime

Next Steps

Model

- Finish port of radiation scheme
- Integrate physical parameterizations with dynamical core
- Refactor code to make use of new DSL features

DSL Toolchain

- Finish migration to new backends
- Extend with new features to eliminate more Python code
- Improve performance of x86 CPU and NVIDIA GPU backends

Summary & Outlook

Python/DSL-based weather and climate models can be fast and portable.
Huge push from AI/ML continually improving ecosystem for HPC applications.

They enable exciting new possibilities

- Optimizations that would not be desirable / feasible without the high level of abstraction (collaboration with CSCS/ETH)
- Integration with ML learning and emulation workflows (in house)
- Automatic differentiation (on-going collaboration with Google Research)
- Integration with other toolchains (collaboration with SPCL/ETH and DaCe)

Thank you!