Developing ECMWF's next-generation performance-portable atmospheric dynamical core

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In collaboration with:
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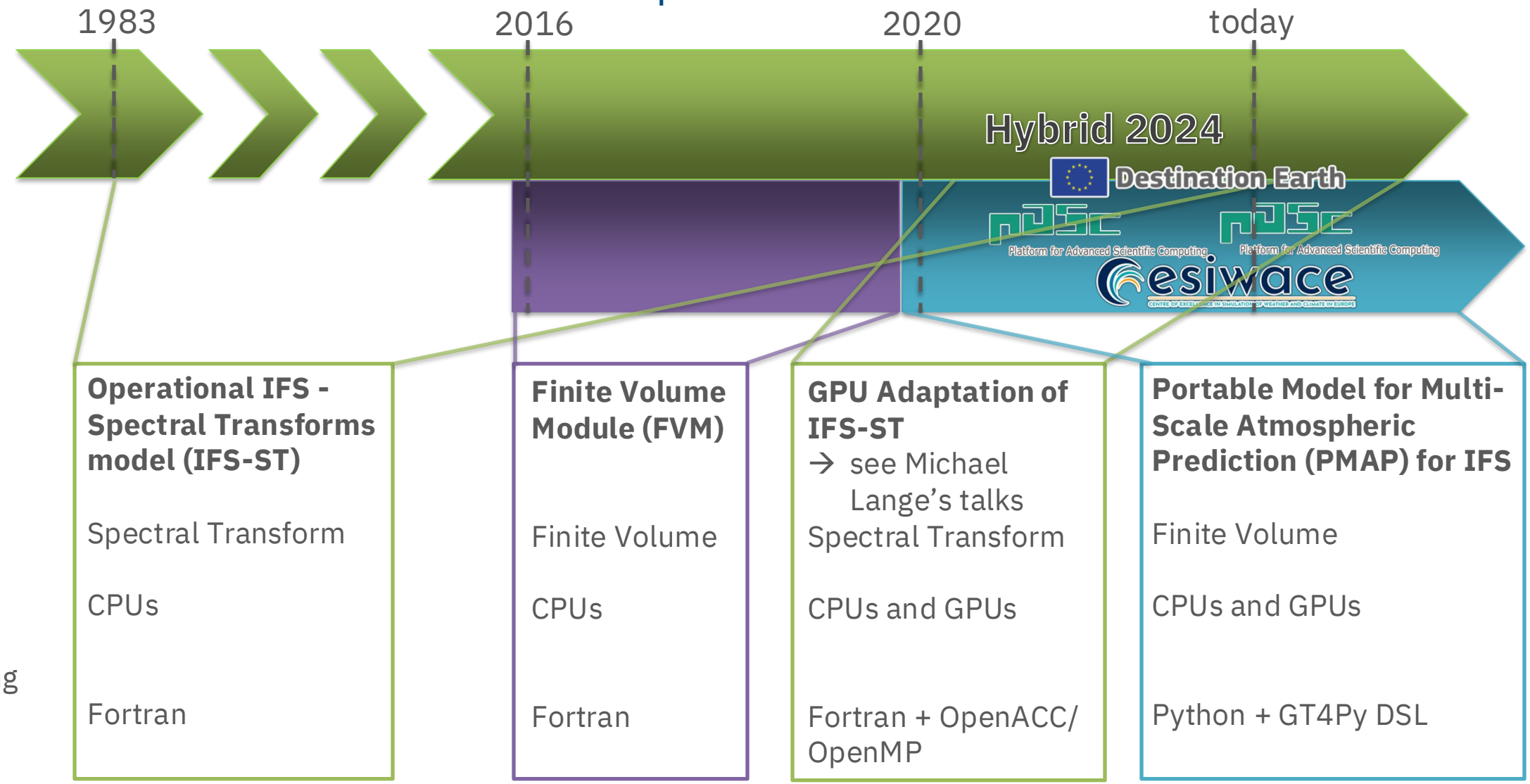
Numerical models and hardware adaptation at ECMWF



	Operational IFS - Spectral Transforms model (IFS-ST)	**Finite Volume Module (FVM)**	**GPU Adaptation of IFS-ST** → see Michael Lange's talks	**Portable Model for Multi-Scale Atmospheric Prediction (PMAP) for IFS**
Numerical scheme:	Spectral Transform	Finite Volume	Spectral Transform	Finite Volume
Hardware:	CPUs	CPUs	CPUs and GPUs	CPUs and GPUs
Programming language:	Fortran	Fortran	Fortran + OpenACC/ OpenMP	Python + GT4Py DSL

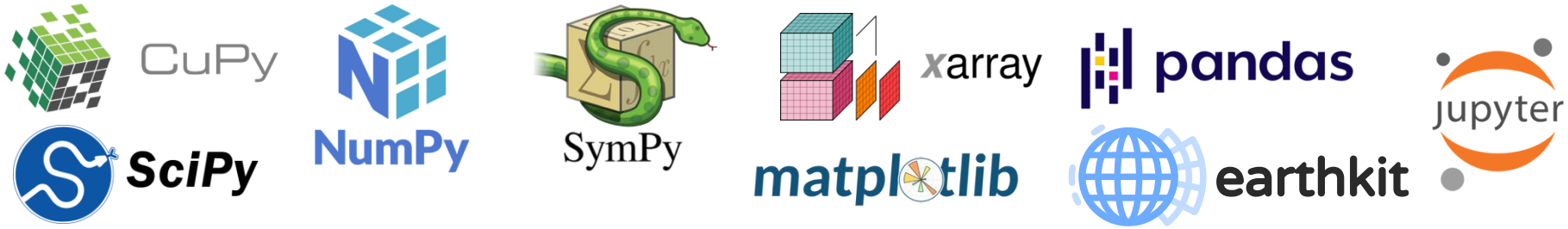
Portable Model for Multi-Scale Atmospheric Prediction (PMAP)

- Compact-stencil dynamical core in a high-level **Python-based** framework, designed to provide sustainable **performance-portability** leveraging **GT4Py** (GridTools for Python)
- **Joint effort** of
  - ECMWF (Core & ESiWACE3)
  - CSCS and
  - ETH Zurich (PASC-project)

  to port FVM to Python using the GT4Py domain specific library
- Solves the **non-hydrostatic fully-compressible equations** using **3D semi-implicit time-integration** and **finite-volume non-oscillatory advection**
- Model formulation supports **unstructured and structured grids, conservation, 3D diffusion and subgrid-scale turbulence, scalability, steep orography at sub-kilometer resolution**,…
- **Two configurations:**
  - **PMAP-LES**: **regional** model on quadrilateral grids with Large-Eddy Simulation capabilities
    → see Stefano Ubbiali's talk
  - **PMAP-GO**: **Global** dynamical core on the IFS **Octahedral** grid

Why GT4Py?

- **GT4Py** is embedded in the **Python** eco-system



- **Machine Learning** interoperability: **automatic differentiation** using JAX straight forward

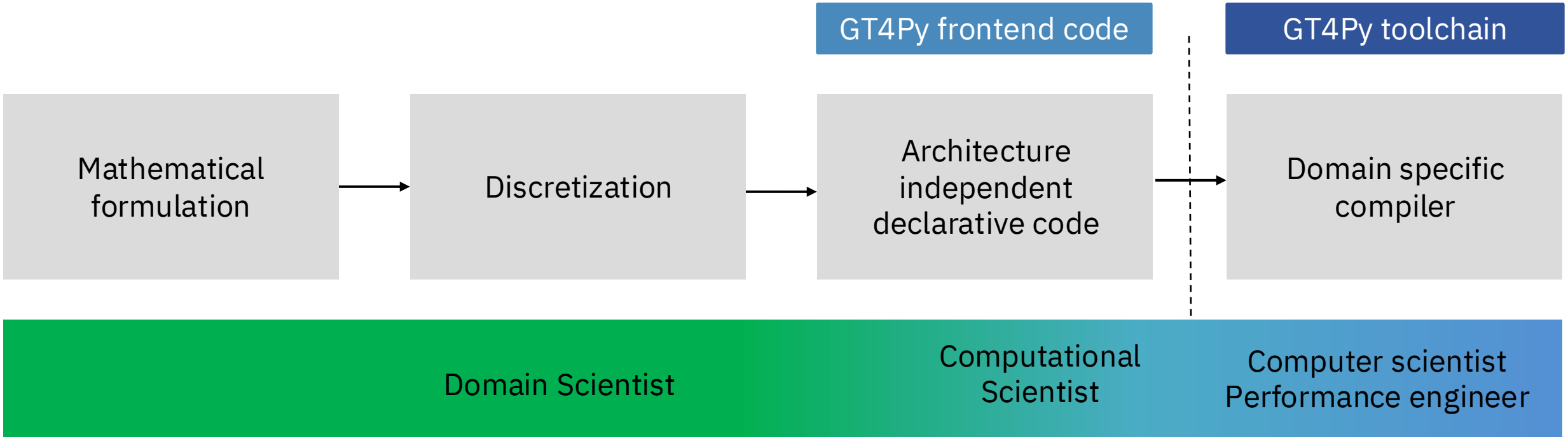
- **Portability**:
    - Example: **Porting to AMD GPUs**: ecosystem supported on AMD → model runs **without any code changes** after providing the software stack

Further NWP models using GT4Py:

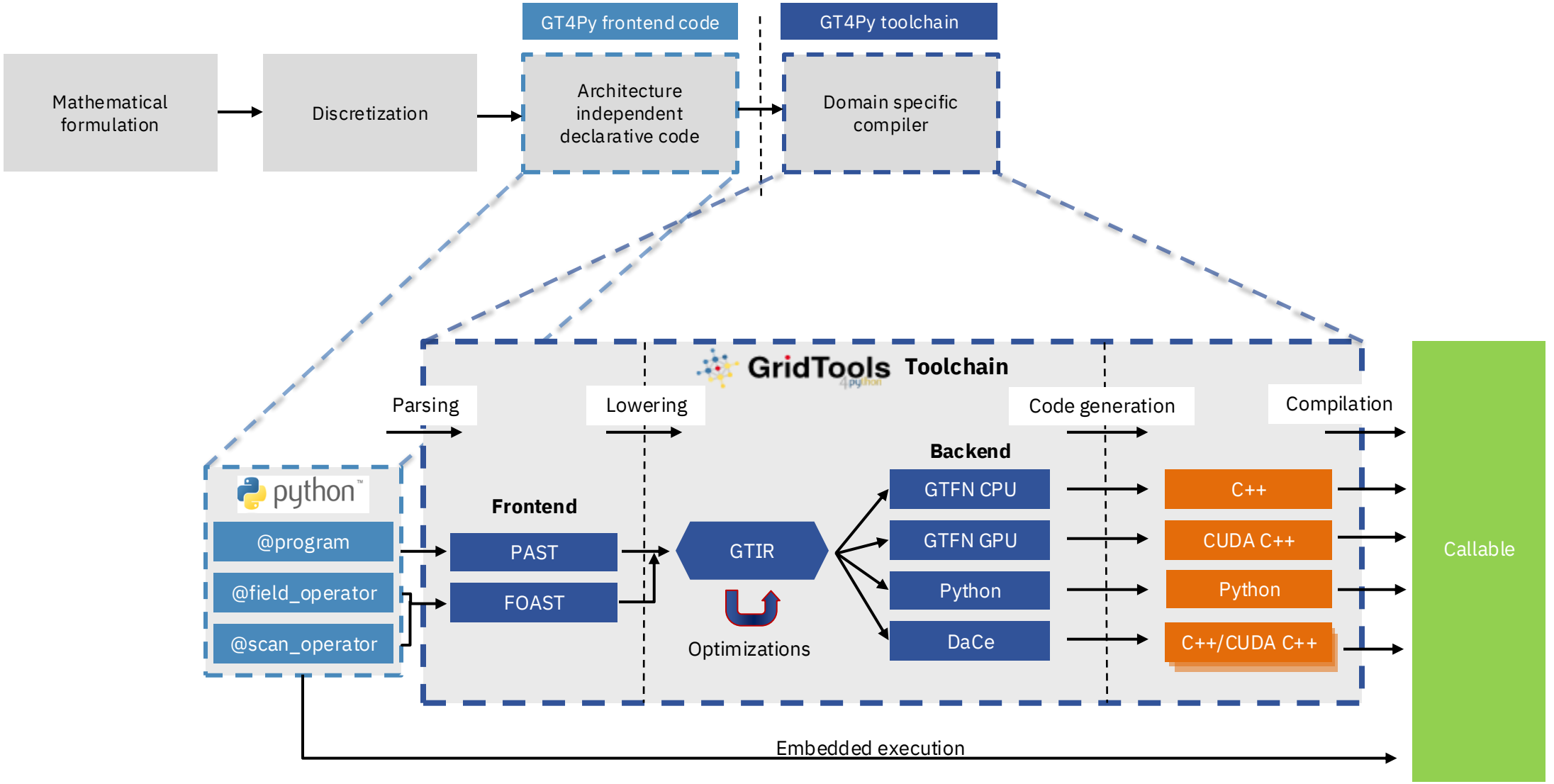
- **ICON** atmospheric model dynamics and physics ported to GT4Py (next) by MeteoSwiss, EXCLAIM project at ETH Zurich and CSCS → see Daniel Hupp's and Magdalena Luz's talk
- **Pace** is a GT4Py (cartesian) implementation of the FV3GFS / SHiELD atmospheric model of NOAA/GFDL by Allen Institute for AI (AI2)

Separation of concerns

- **Domain scientists** write **high-level code** specifying the algorithm and the mathematical operations
- **GT4Py optimizing toolchain** transforms high-level code into **efficient, architecture-tuned** implementations



GT4Py toolchain



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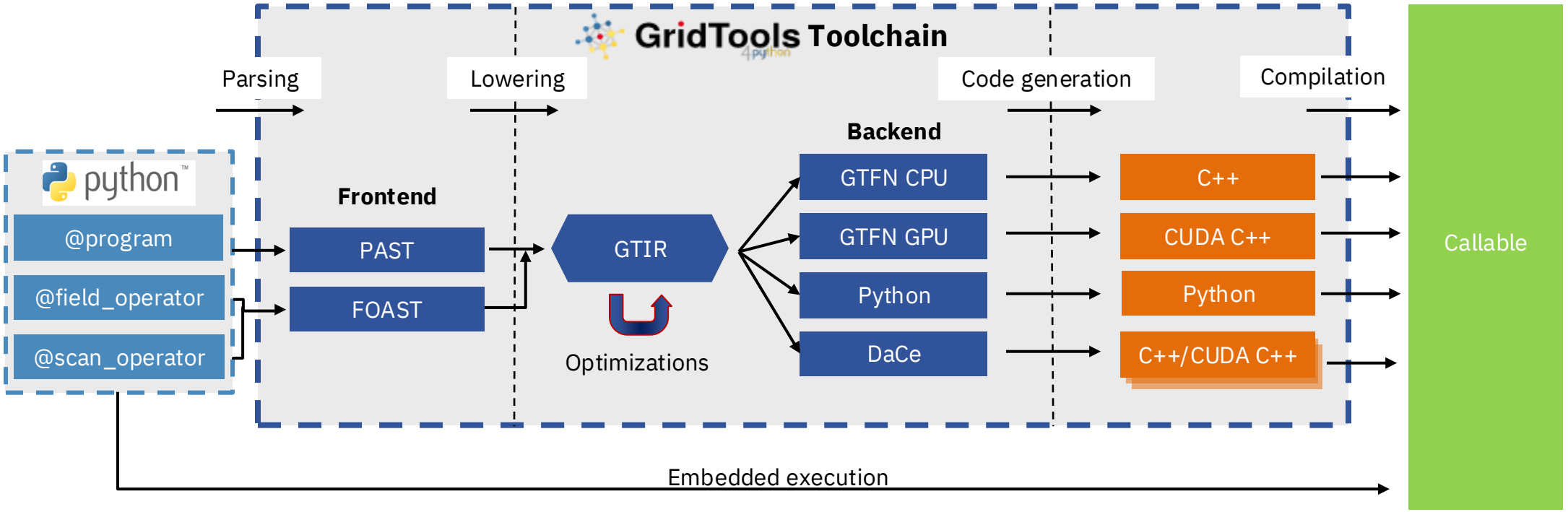
GT4Py toolchain

- **Code generation** optimized **for** a **specific architecture**, leveraging **knowledge** of the **typical computation patterns in the domain**
- **Backend selects implementation strategy** (parallelism, memory layout, etc.)
- Has built-in integration to the **DaCe** (Data-Centric Parallel Computing) library
- **Backends** can be **added** to provide efficient implementations **for new platforms**



GT4Py simple illustration: advection-diffusion equation

$$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x} + D\frac{\partial^2 u}{\partial x^2}$$

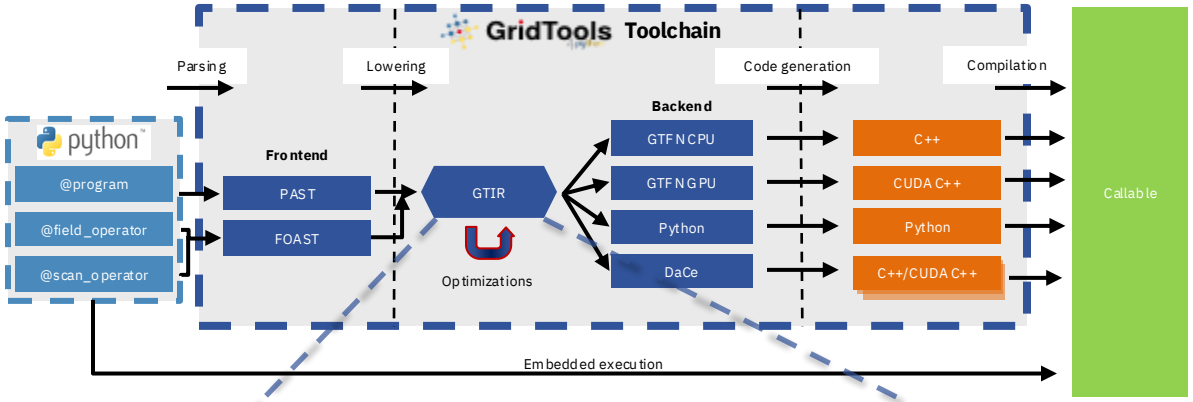
Discretization with first order space derivatives ($\Delta x = 1$) and forward Euler in time:

$$u_i^{n+1} = u_i^n - a\,\Delta t \cdot (u_i^n - u_{i-1}^n) + D\,\Delta t \cdot (u_{i+1}^n - 2u_i^n + u_{i-1}^n)$$

$a, D \in \{0, 1\}$ used to dis-/enable advection and diffusion

```
@gtx.field_operator(
    static_params=["enable_advection",
                   "enable_diffusion"])
def solve_advection_diffusion(
        u: gtx.Field[[I], float],
        dt: float,
        enable_advection: bool,
        enable_diffusion: bool,
):
    u_new = u
    if enable_advection:
        u_new = u_new - dt * (u - u(I - 1))
    if enable_diffusion:
        u_new = u_new +
          dt * (u(I + 1) - 2.0 * u + u(I - 1))
    return u_new
```

GT4Py optimization pass: constant folding (excerpt)




```
if_(True, true_branch, false_branch)
```

```
if (
    cpm.is_call_to(node, "if_")
    and isinstance(node.args[0], itir.Literal)
):
    if new_node.args[0].value == "True":
        return node.args[1]
    else:
        return node.args[2]
```

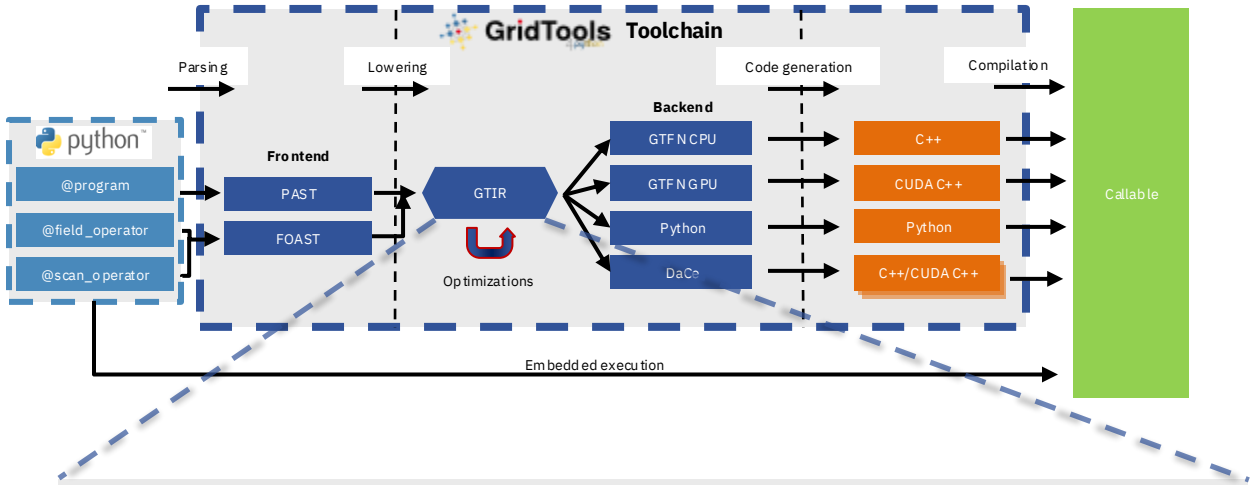
```
true_branch
```

- Thanks to our **functional** intermediate representation (**IR**) **no side effects** need to be considered in all passes
- **Further optimizations**:
  - Temporary fusion
  - Function inlining
  - Common subexpression elimination
  - …

GT4Py toolchain example

- Possible to specify **static parameters**, which are just-in-time- or pre-compiled

```
@gtx.field_operator(
    static_params=["enable_advection",
                   "enable_diffusion"])
def solve_advection_diffusion(
        u: gtx.Field[[I], float],
        dt: float,
        enable_advection: bool,
        enable_diffusion: bool,
):
    u_new = u
    if enable_advection:
        u_new = u_new - dt * (u - u(I - 1))
    if enable_diffusion:
        u_new = u_new +
            dt * (u(I + 1) - 2.0 * u + u(I - 1))
    return u_new
```

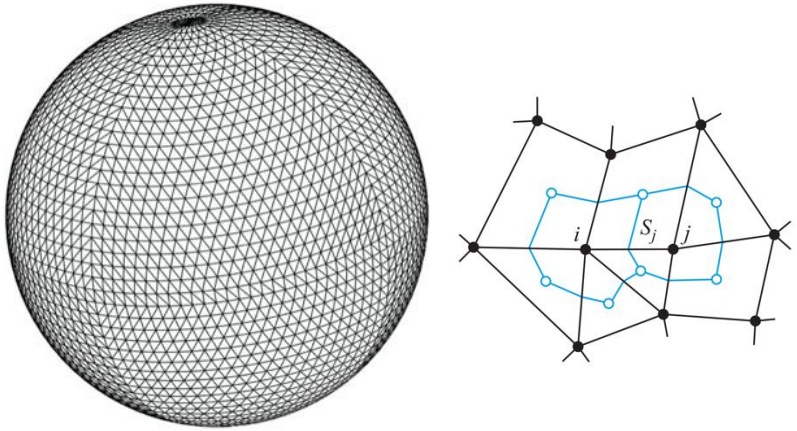



```
if_(enable_advection, true_branch, false_branch)
                          ↓
if_(False, true_branch, false_branch)
```

PMAP-GO details

- **Global dynamical core** using GT4Py.next
- Local **low-volume communication** footprint
- Using **height-based terrain-following vertical coordinates**
- Supports **semi-implicit integration with adaptive time step**
- Executes entirely in either **double or single precision**
- Supports **CPUs** and **GPUs** via different GT4Py backends
- Uses median-dual FV mesh built around the nodes of the **octahedral reduced Gaussian grid**
- Grid generation with ECMWF's Atlas[1] library and **atlas4py**[2] Python bindings

```
from atlas4py import StructuredGrid
grid = StructuredGrid("O24")
mesh = AtlasMesh.generate(grid)
```



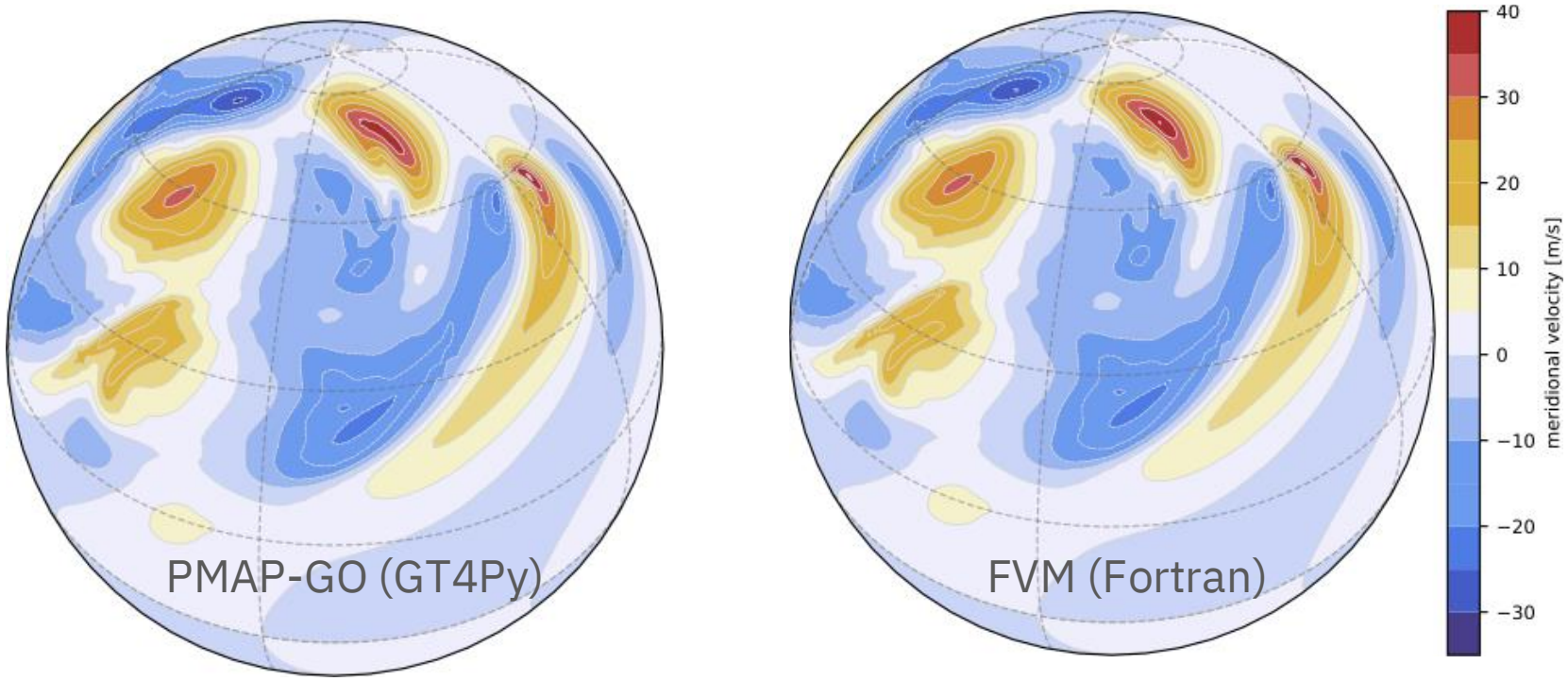
Octahedral grid O24 (left) and schematic of the median-dual mesh (right).

[1] Atlas: W. Deconinck et al. “Atlas : A library for numerical weather prediction and climate modelling”. In: Computer Physics Communications 220 (2017) DOI: 10.1016/j.cpc.2017.07.006

[2] atlas4py: https://github.com/GridTools/atlas4py

PMAP-GO simulations

- PMAP reproduces FVM and at the same time provides a fully portable future-proof model in Python



DCMIP-2016 baroclinic wave benchmark with left: PMAP-GO (GT4Py) and right: FVM (Fortran) on the same O160 grid: meridional wind (m/s, shaded) on day 15 at an altitude of 2km.

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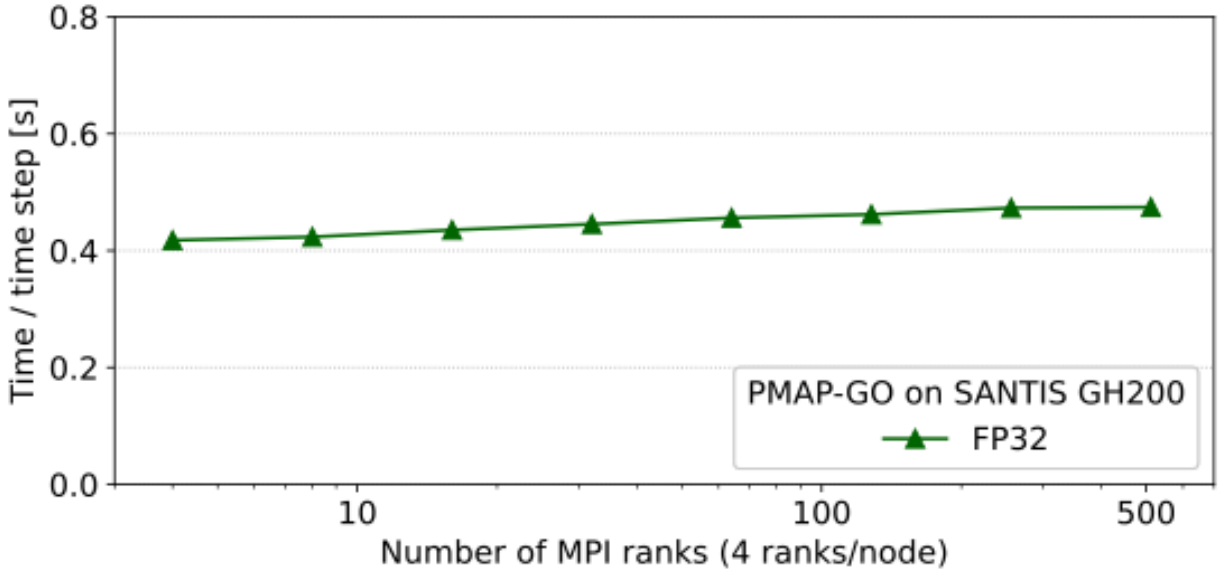
PMAP-GO scaling results

- **Weak scalability** of the **dynamical core**
- **Distributed memory implementation** using the exascale-ready library **GHEX**[1]
- Significant **optimizations** are still **ongoing**



DCMIP-2016 baroclinic wave benchmark: early weak scaling results on the CSCS Alps-Santis cluster (Grace Hopper GH200 GPUs).
Computational grids: O640 (for 4 ranks) to O7240 (for 512 ranks)

[1]GHEX: https://github.com/ghex- org/GHEX

GridTools 4python

https://github.com/GridTools/gt4py

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Thank you for listening!