Developing ECMWF's portable next-generation atmospheric dynamical core

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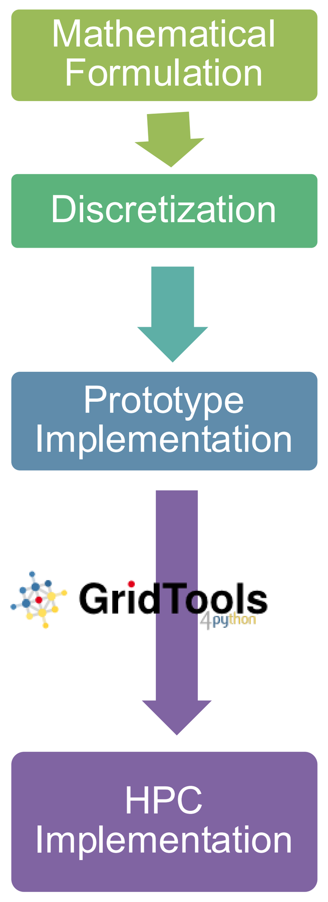
1. Future model development and coding practices

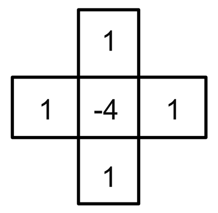
Separation of concerns:

- Domain scientists focus on numerical modelling
- Performance engineers implement hardware-specific optimizations



$$\Psi = \Delta_{x,y}\phi$$

$$\Psi(i,j) = \frac{1}{h^2}\{-4 * \phi(i,j) + \phi(i+1,j) + \phi(i-1,j) + \phi(i,j+1) + \phi(i,j-1)\}$$




```
@field_operator
def lap(inp: Field[[IDim, JDim], "float"], dx: float,
) -> Field[[IDim, JDim], "float"]:
    return -4.0 / dx**2 * inp + inp(IDim + 1) + inp(JDim + 1)
                                + inp(IDim - 1) + inp(JDim - 1)
```

```
struct _fun_1 {
  constexpr auto operator()() const {
    return [](auto const &__iasfop_4, auto const &inp) {
      return (((((gtfn::deref(__iasfop_4) * gtfn::deref(inp)) +
                 gtfn::deref(gtfn::shift(inp, _IDimOff, 1_c))) +
                gtfn::deref(gtfn::shift(inp, _JDimOff, 1_c))) +
               gtfn::deref(gtfn::shift(inp, _IDimOff, -1_c))) +
              gtfn::deref(gtfn::shift(inp, _JDimOff, -1_c)));
    };
  }
};
```

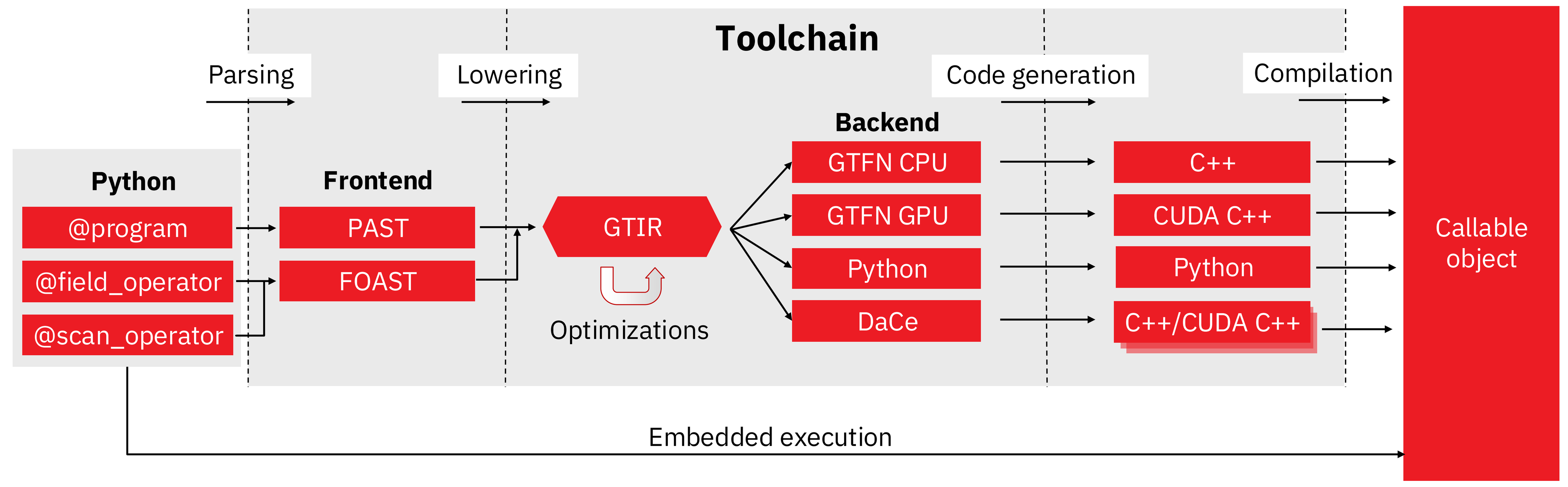
2. Portable Model for Multi-Scale Atmospheric Prediction (PMAP)

- Two versions:
  - PMAP-GO: Global unstructured mesh
  - PMAP-LES: 3D structured grid for regional and large-eddy simulations
- Building on ECMWF's FVM (Smolarkiewicz et al. 2016; Kühnlein et al. 2019)
- Solves fully compressible equations with 3D semi-implicit time stepping and conservative finite-volume non-oscillatory advection
- Designed for performance portability on multiple platforms using the GT4Py domain-specific library to express stencil computations
- Supports CPUs and GPUs via distributed memory with the exascale-ready GHEX[1] library
- Executes entirely in either double or single precision

```
@field_operator
def advection_scheme_upwind(
  rho: Field[[Vertex], float],
  dt: float,
  vel: tuple[Field[[Vertex], float], Field[[Vertex], float]],
  vol: Field[[Vertex], float],
  dual_face_orientation: Field[[Vertex, V2EDim], float],
  dual_face_normal: tuple[Field[[Edge], float], Field[[Edge], float]],
  dual_face_length: Field[[Edge], float]
) -> Field[[Vertex], float]:
  flux = upwind_flux(rho, vel, dual_face_normal, dual_face_length)
  return rho - (dt / vol) *
     neighbor_sum(flux(V2E) * dual_face_orientation, axis=V2EDim)
```

3. GT4Py (GridTools for Python) [2]

- Python framework for weather and climate modelling, simplifying the development and maintenance of high-performance code for prototyping and production
- Separates model development from hardware architecture dependent optimizations
- The optimizing toolchain transforms high-level code into efficient, architecture-tuned implementations tailored to the chosen hardware architecture (e.g., optimized parallelization, memory layout, data flows)
- Has built-in integration to the DaCe (Data-Centric Parallel Computing [3]) library
- Two versions:
  - gt4py.cartesian: Established version supporting 3D structured (I, J, K) grids
  - gt4py.next: In development, additionally supporting horizontally unstructured grids



4. Grid and atlas4py

- Atlas (Deconinck et al. 2017): library for NWP and climate modelling
- atlas4py[4]: Python bindings for Atlas

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

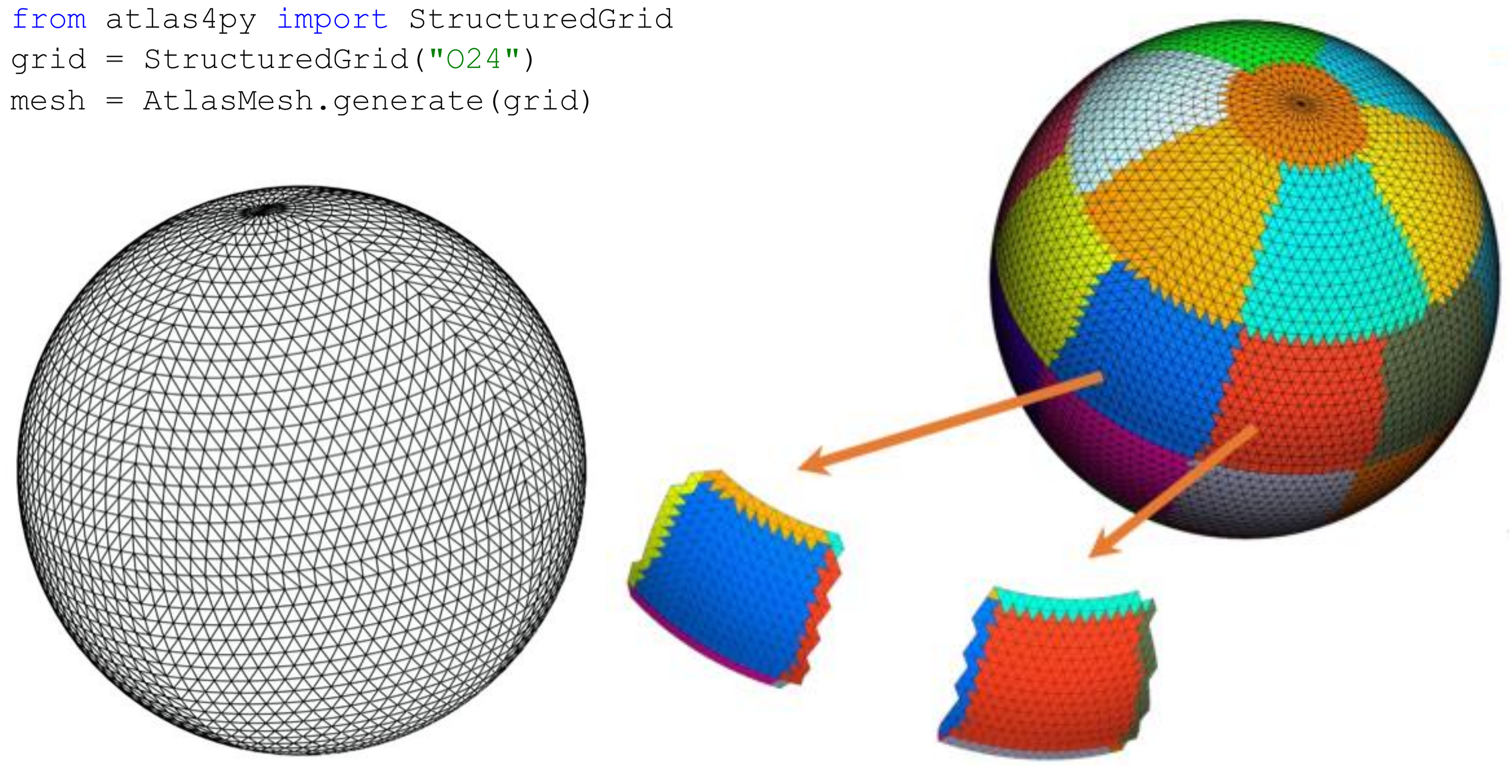


Figure: Octrahedral grid O24 and partition with halo layers.

5. PMAP-GO results

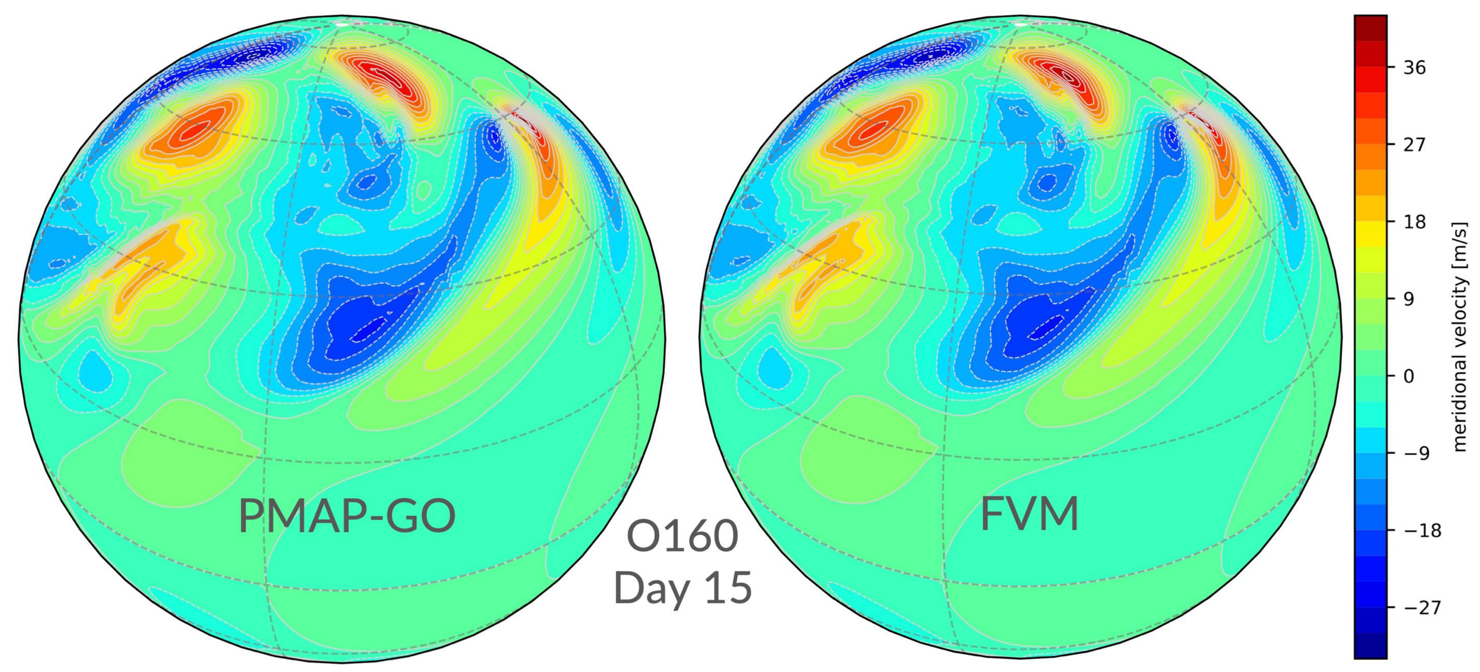


Figure: DCMIP-2016 baroclinic wave benchmark with PMAP-GO (GT4Py) and FVM (Fortran) on the same O160 grid: meridional wind (m/s, shaded) on day 15 at an altitude of 2km.

6. First performance results

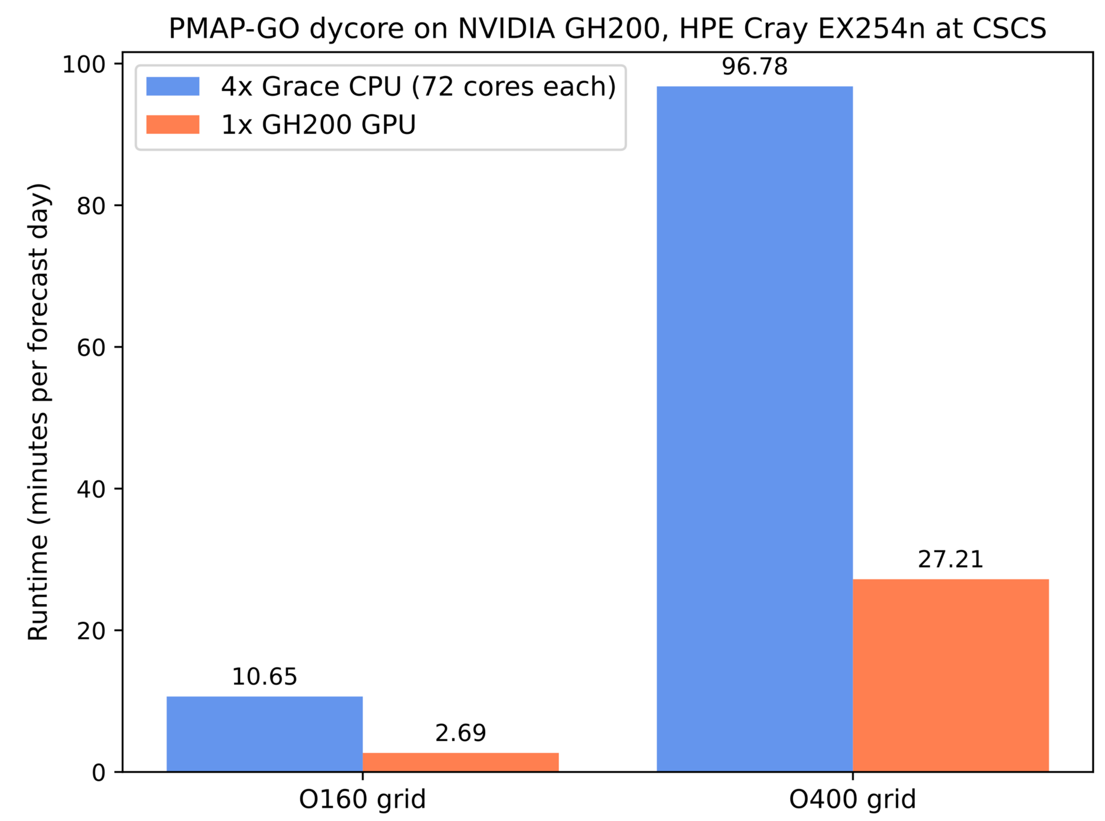


Figure: PMAP-GO CPU and GPU runs on the NVIDIA Grace Hopper superchip.

References and footnotes

Deconinck et al. (2017). Atlas : A library for numerical weather prediction and climate modelling. Computer Physics Communications. 220.

Kühnlein et al. (2019). FVM 1.0: A nonhydrostatic finite-volume dynamical core for the IFS. Geoscientific Model Development, 12(2).

Smolarkiewicz et al. (2016). A finite-volume module for simulating global all-scale atmospheric flows. Journal of Computational Physics, 314.

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

[2] GT4Py: https://github.com/GridTools/gt4py

[3] DaCe: https://github.com/spcl/dace

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

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