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Bundesamt für Meteorologie und Klimatologie MeteoSchweiz

Porting the MeteoSwiss weather forecast software to GPUs

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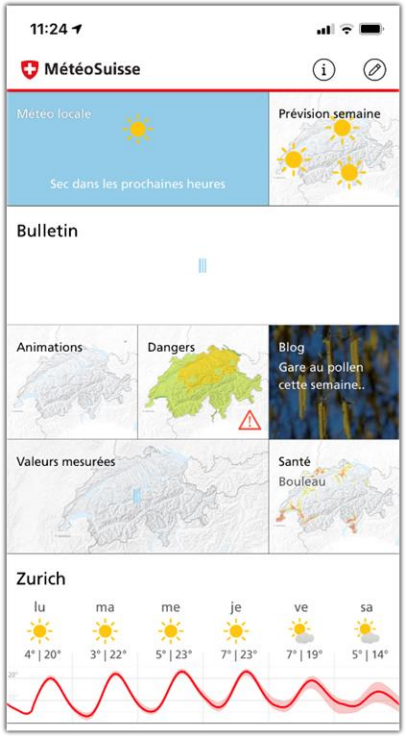
09.11.2022, CERN, Computer Accelerator Forum

MeteoSwiss

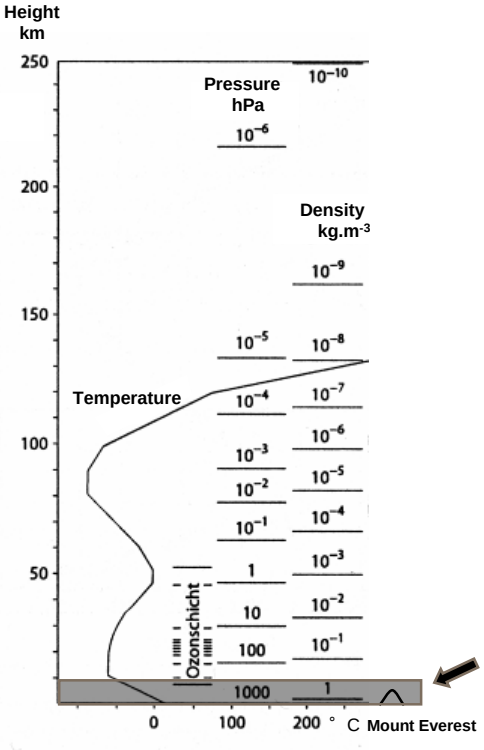
- Federal Office of Meteorology and Climatology
- Weather forecasting, warnings : population, authorities, Aviation ..
- Numerical Weather prediction
- Observation : station, radar, …
- Climatology
- Climate scenario and impact



MeteoSwiss App

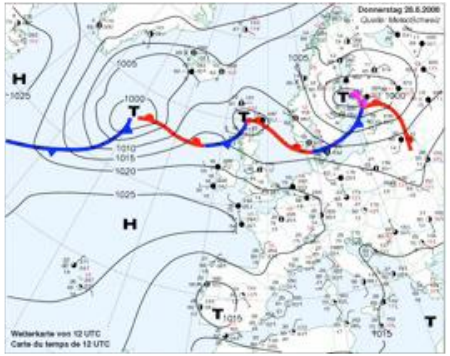
Numerical weather prediction: The atmosphere

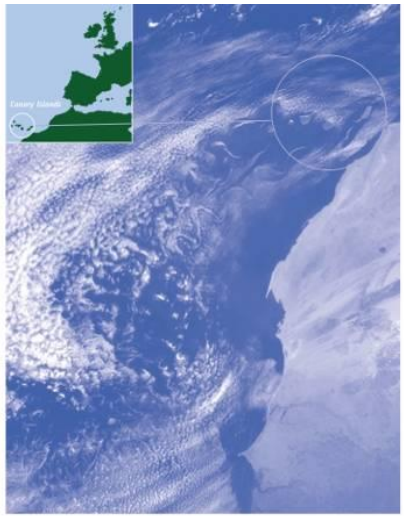
A thin gas layer around the earth



Troposphere:
in the order of 10km thickness
90% of air mass
99% of air humiduty

Numerical weather prediction: Multiscale





Meteosat-7 visible channel image, 10.00h UTC, 4 April 2001

source: meteoswiss

From 1 000 km to mm

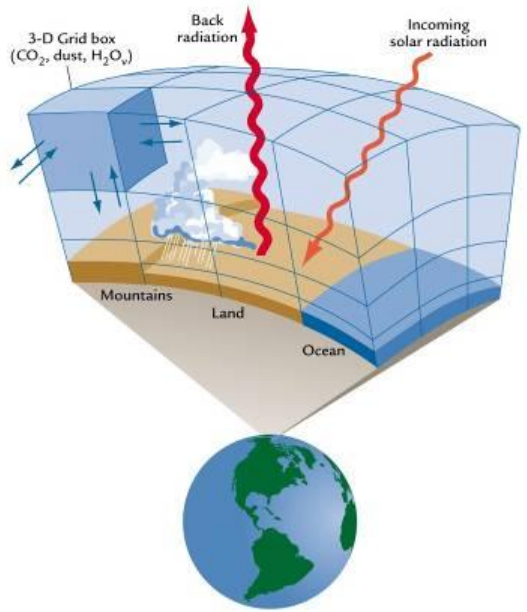
Numerical weather prediction: Atmospheric modelling

Fluid motion and thermodynamics processes
(Primitive equations : dynamics)

+

Subgrid scale processes
(physical parametrizations)

Discretised on a 3d grid



Atmospheric model (Ruddiman, 2001)

The governing equations

Momentum

$$\rho \frac{d\mathbf{v}}{dt} = -\nabla p + \rho \mathbf{g} - 2\boldsymbol{\Omega} \times (\rho \mathbf{v}) - \nabla \cdot \underline{\mathbf{t}}$$

Mass

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v}$$

Heat

$$\rho c_v \frac{dT}{dt} = -p \nabla \cdot \mathbf{v} + Q_h + Q_m$$

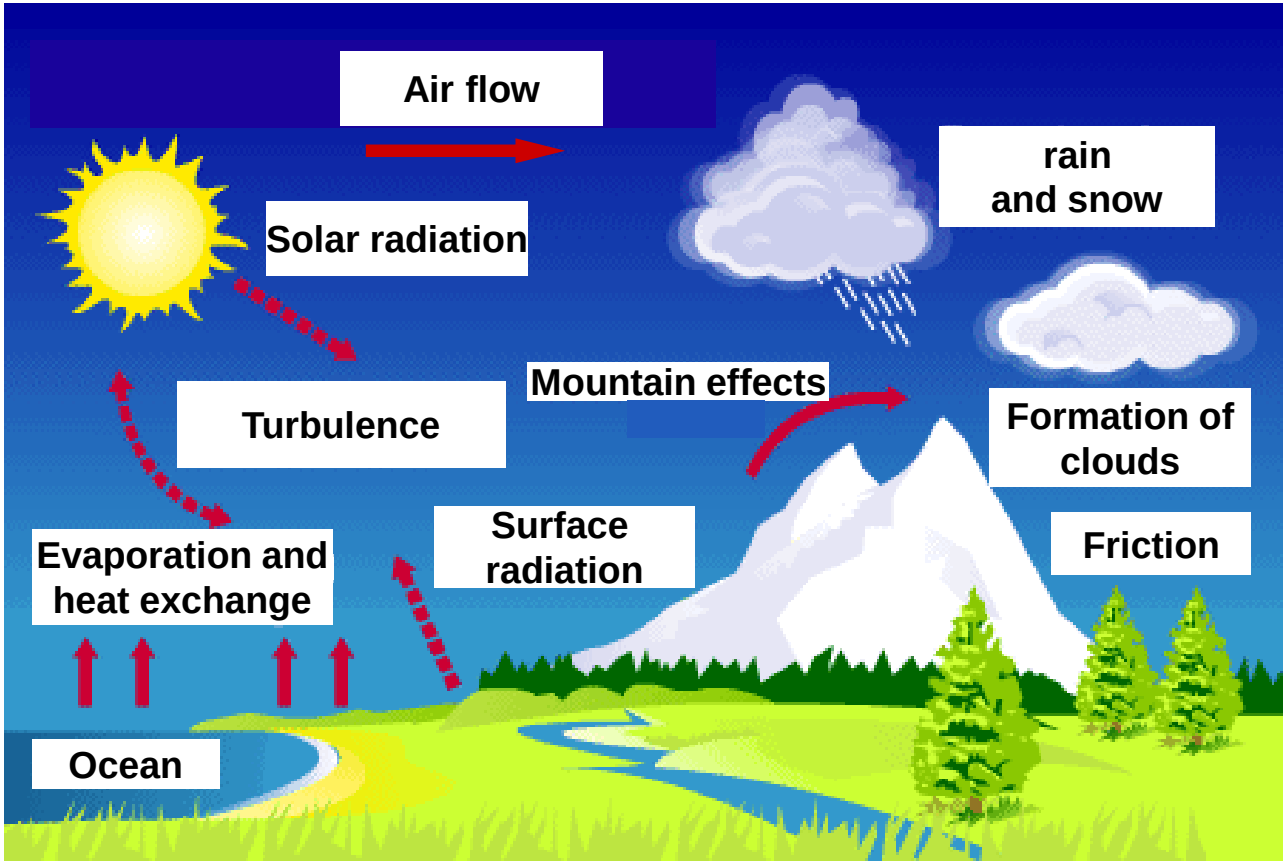
Vapor/Liquid/ solid water

$$\rho \frac{dq^x}{dt} = -\nabla \cdot \mathbf{J}^x + I^x$$

pressure

$$p = \rho R_d (1 + \alpha) T.$$

Atmospheric processes parametrizations

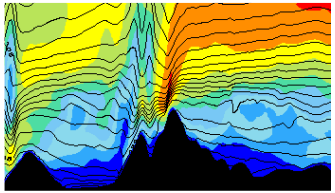


What do we need for numerical weather prediction ?

Atmospheric model = Dynamic + Parametrization

Discretization on a finite grid:

→ Numerical model



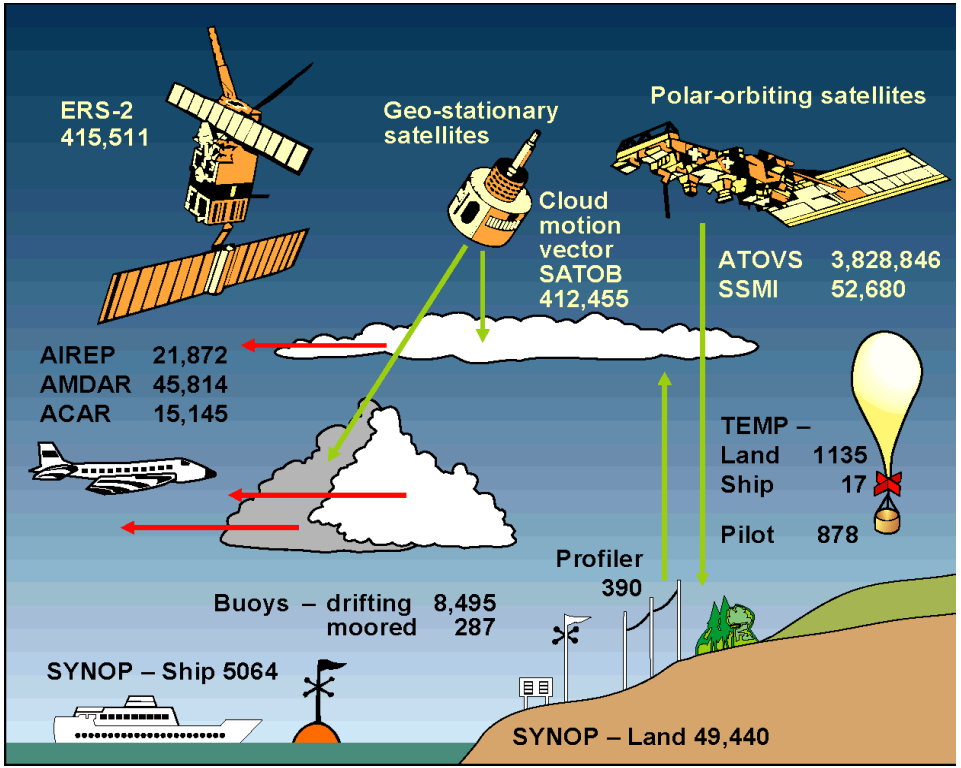
Knowledge of the initial state of the atmosphere

→ observations

The process of bringing observations to the numerical model is referred to as data assimilation

Observing the atmosphere

Initial state:
model+observation

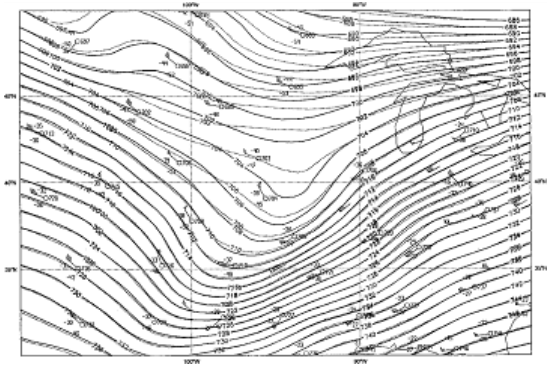


@ECMWF 2001

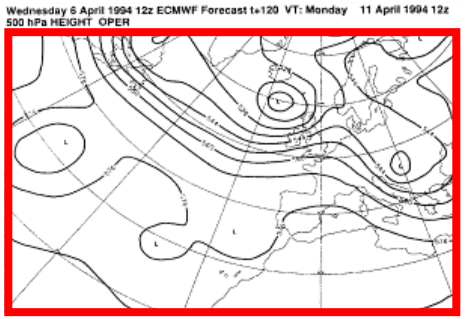
Chaos theory and predictability

The atmospheric system is a chaotic system:
i.e. high sensitivity to initial condition

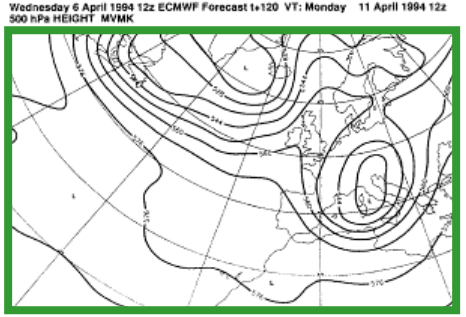
Initial conditions (dotted lines)



Initial conditions (full lines)



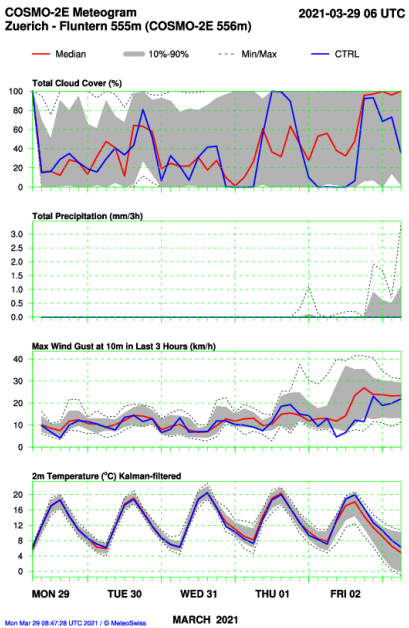
Operational 120 h forecast

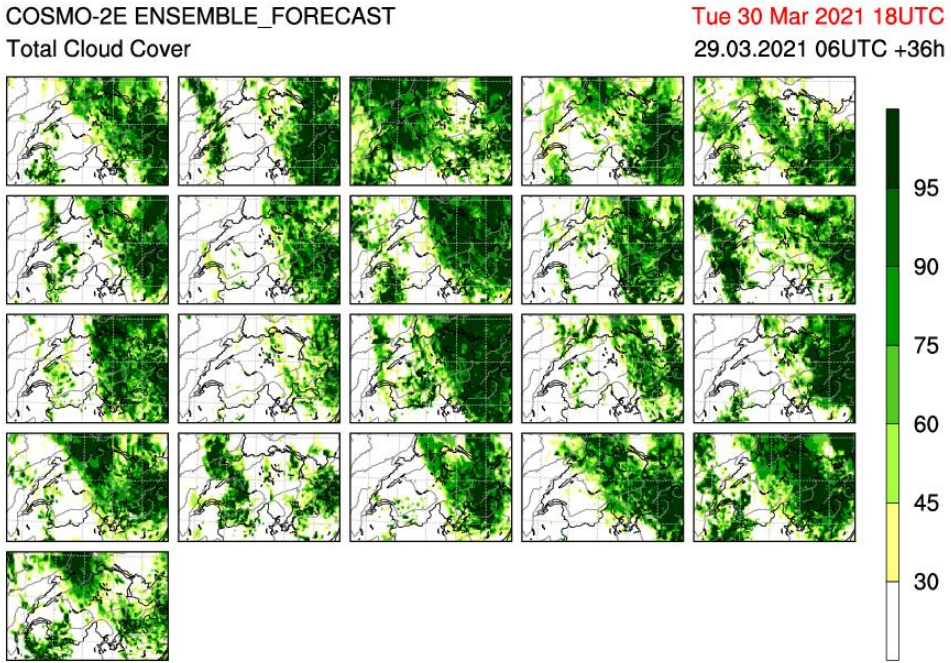


Modified forecast

Ensemble prediction

- Run multiple simulations with different initial condition and with perturbations





High Perormance Computing (HPC)

- NWP is a time critical problem
- Large computing requirement, grid, ensembles …
- Need to adapt to latest advances in computer architecture
- Usually runs on dedicated HPC systems

Cray XC-30 Hybrid Piz Daint at CSCS (5,272 GPUs)

GPU computing at MeteoSwiss

- GPU : Graphical Processing Units
- Most of the fastest supercomputers (Top500) are based on accelerator/many-core technologies
- Moore’s law is ending, what do we do ? => Increase on chip parallelism
- Take advantage of the high computational capacity and energy efficiency of GPUs
- MeteoSwiss was the first National Weather Service to use GPUs for production in 2016

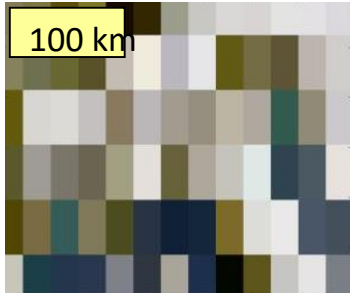
GPU

CPU

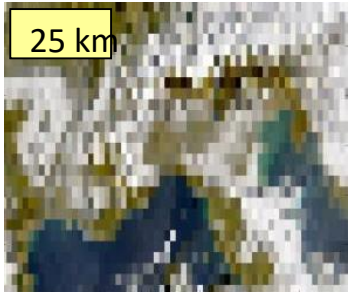
MeteoSwiss Cray CS-Storm
Hybrid GPU system at CSCS

What can we do with more computing power ?

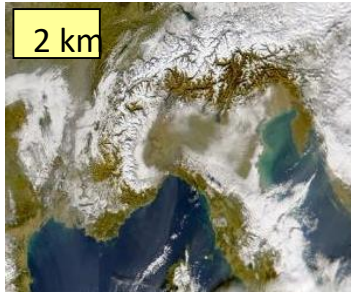
- Improve model representation and physical processes



Global climate model



Global weather model



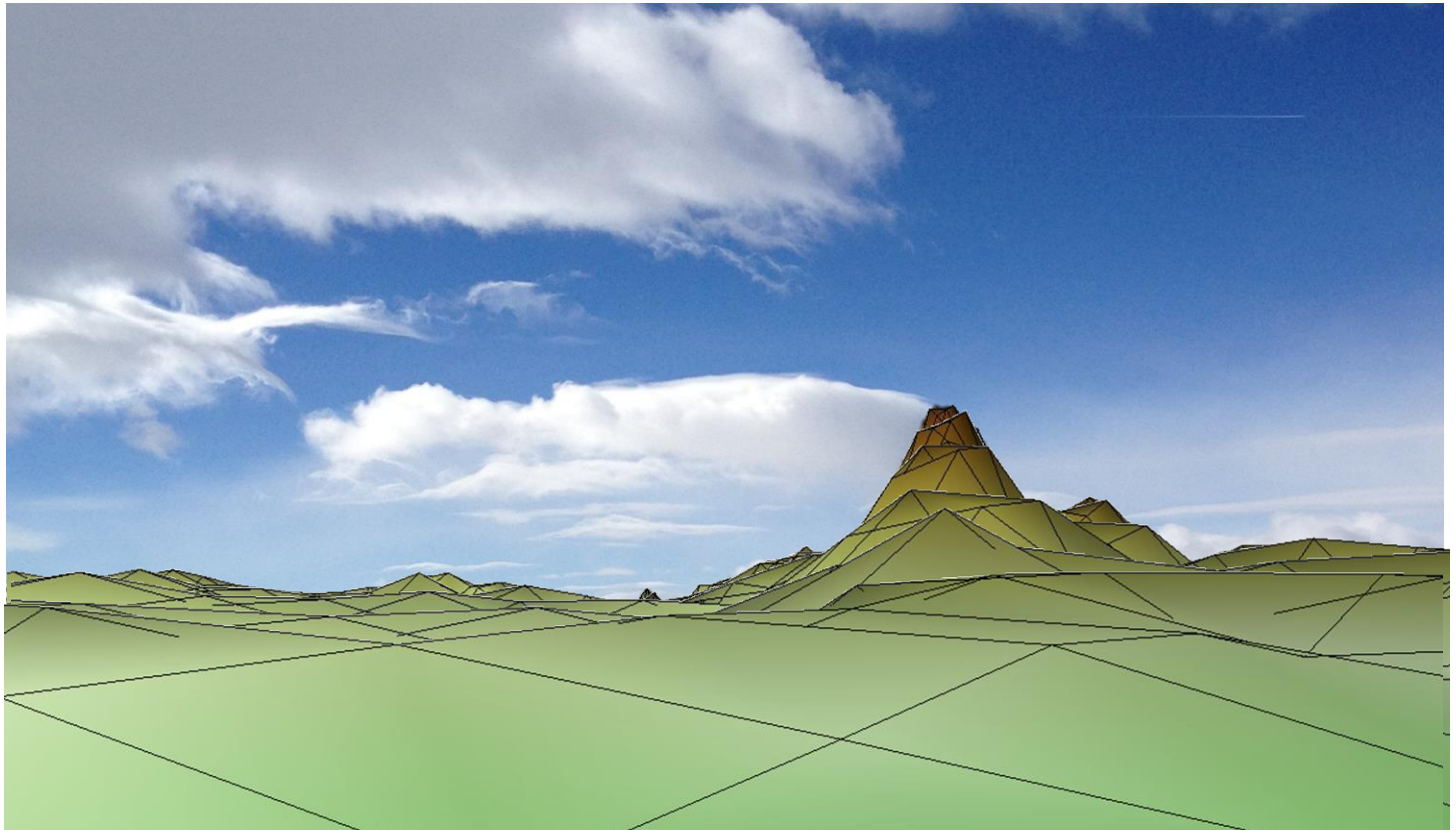
Regional weather model

2 x horizontal resolution ≈ 8 x computational cost

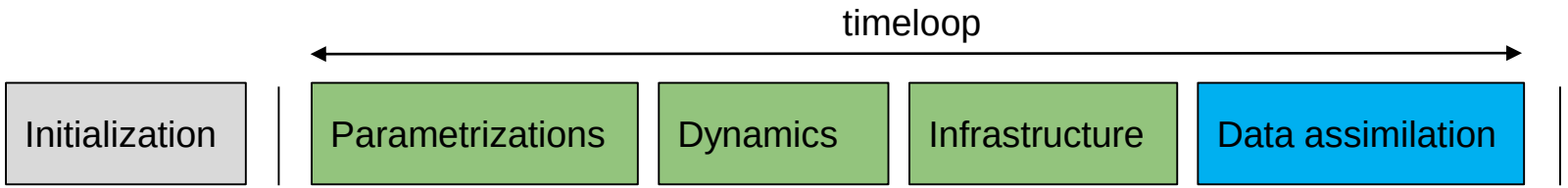
- Increase number of ensemble: better evaluation of predictability

Resolution of the computational grid

$\Delta x = 2200$ m



Numerical weather prediction using OpenACC



- Most components for NWP Regional and global application ported, optimization work ongoing
- Support for both double and mixed precision
- Regular testing on builbot infrastructure

Turbulence

Optimizations applied

- Apply ASYNC clause as much as possible
- Collapse purely nested k- and i-loops
- Fuse i-loops inside k-loop
- Replace !$ACC DATA PRESENT with DEFAULT(PRESENT) at kernel-level
- Applying GANG(STATIC:1)

Source: Jonas Jucker

Problem of many small GPU Kernels

```
…
!$ACC PARALLEL LOOP GANG VECTOR ASYNC(1) DEFAULT(NONE) IF( lzacc )
DO i=ivstart, ivend
   umfl_s(i)=rhon(i,ke1)*tkvm(i,ke1)*zvari(i,ke1,u_m)
END DO

!$ACC PARALLEL LOOP GANG VECTOR ASYNC(1) DEFAULT(NONE) IF( lzacc )
DO i=ivstart, ivend
   vmfl_s(i)=rhon(i,ke1)*tkvm(i,ke1)*zvari(i,ke1,v_m)
END DO

!$ACC PARALLEL LOOP GANG VECTOR ASYNC(1) DEFAULT(NONE) IF( lzacc )
DO i=ivstart, ivend
   edr(i,ke1)=tke(i,ke1,ntur)**3/(d_m*l_tur_z0(i))
END DO
```

These lead to 3 individual kernels with the overhead of launching 3 kernels, for a very small compute time.

Source: Victoria Cherkas

Problem of many small GPU Kernels

The problem we need to solve within turbulence.

Source: Victoria Cherkas

Solution: Bundling loops into single GPU kernel

```
!$ACC PARALLEL ASYNC(1) DEFAULT(NONE) IF( lzacc )
…
!$ACC LOOP GANG(STATIC:1) VECTOR
DO i=ivstart, ivend
   umfl_s(i)=rhon(i,ke1)*tkvm(i,ke1)*zvari(i,ke1,u_m)
END DO

!$ACC LOOP GANG(STATIC:1) VECTOR
DO i=ivstart, ivend
   vmfl_s(i)=rhon(i,ke1)*tkvm(i,ke1)*zvari(i,ke1,v_m)
END DO

!$ACC LOOP GANG(STATIC:1) VECTOR
DO i=ivstart, ivend
   edr(i,ke1)=tke(i,ke1,ntur)**3/(d_m*l_tur_z0(i))
END DO

!$ACC END PARALLEL !!
```

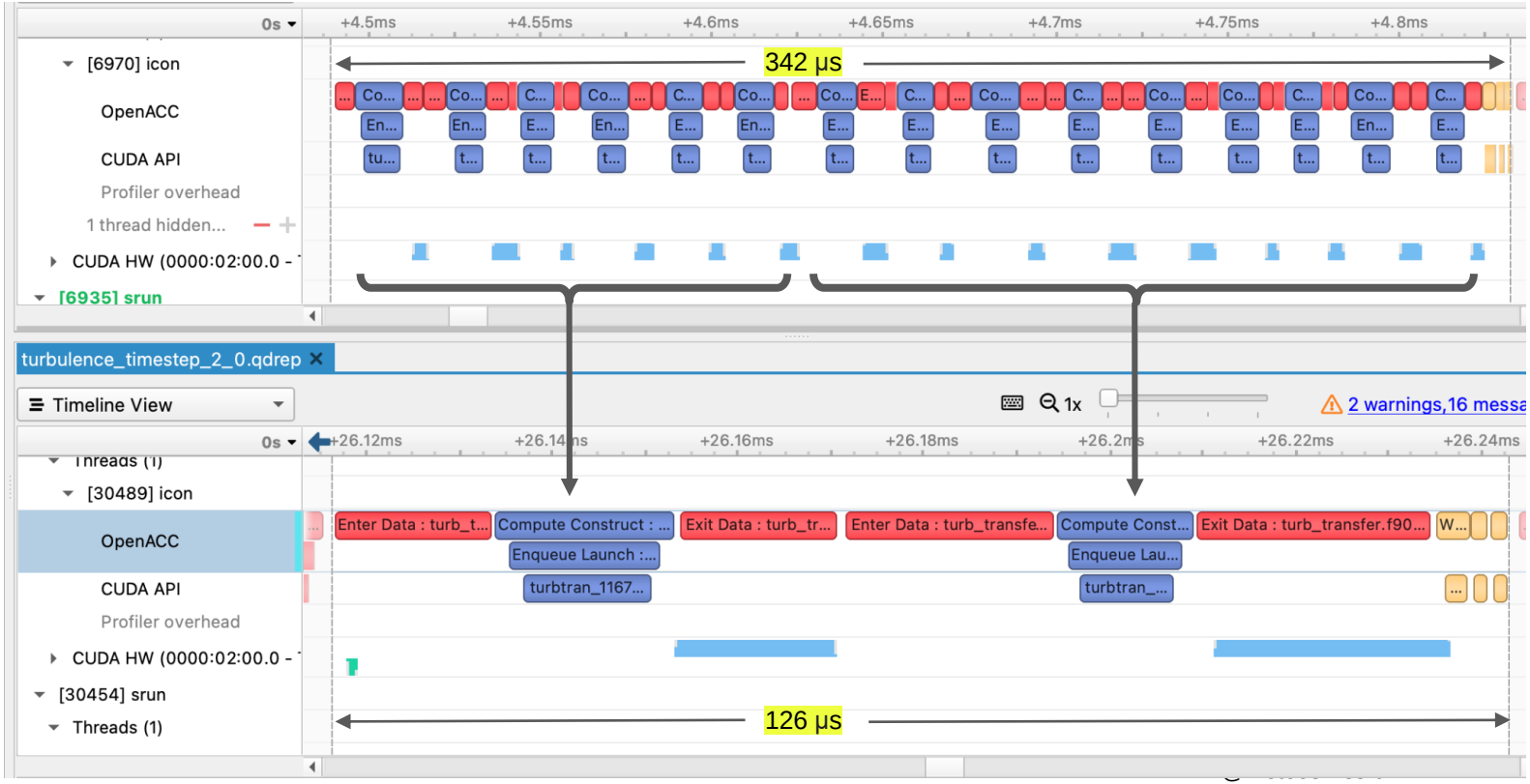
Using gang(static:1) and a single parallel region, we effectively have **one fused kernel** without the breaks in between.

- Improves cache reuse
- Reduces launch overhead

Notice loop bounds are same for the 3 loops.

Source: Victoria Cherkas

Before and after profile comparison



Source: Victoria Cherkas

Porting and optimization challenges

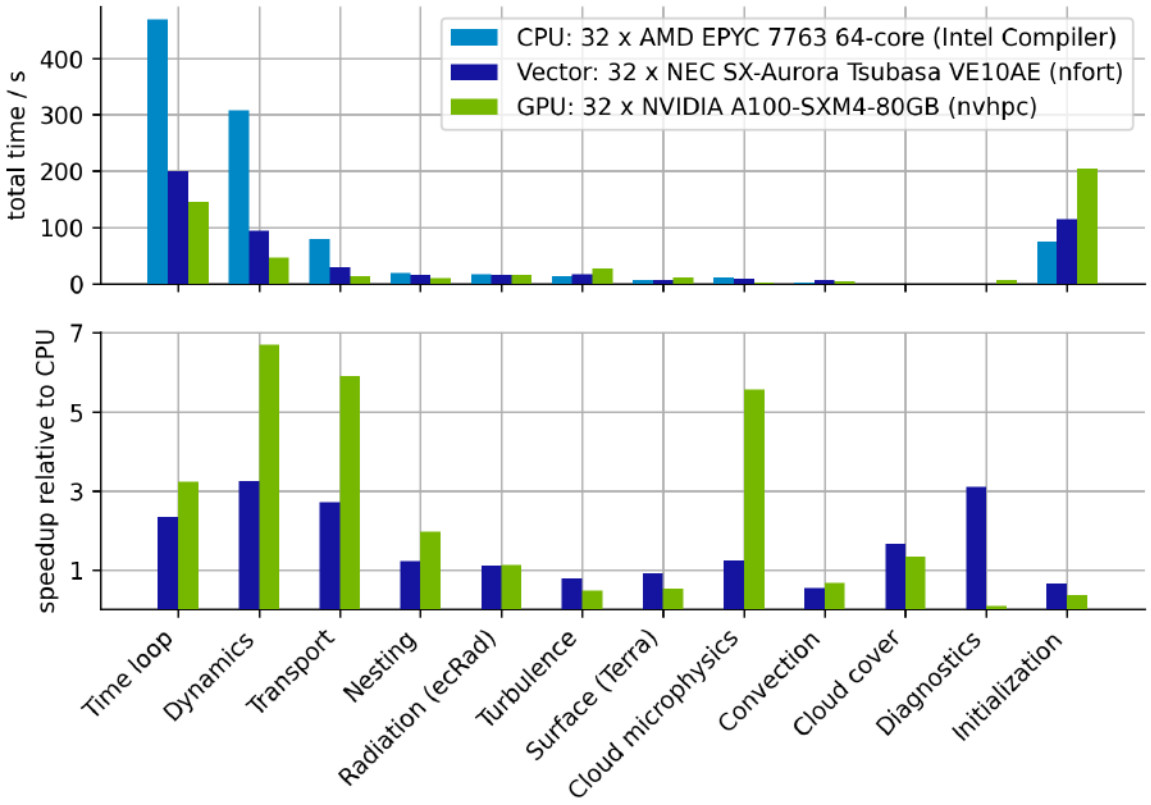
OpenACC optimizations

- GPU and CPU working asynchronously
  - Reduces launch overhead
- Bundling similar loop constructs into single GPU kernels
  - Improves cache reuse
  - Reduces launch overhead
- Compiler assisted / manual inlining of function calls
  - Required for complex (deep call-trees) GPU kernels
  - Enables optimizations above

Conceptual challenges

- Code management
  - Disruptive code changes are challenging
  - ecrad: juggling diverse Institutes

Current performance



CPU vs GPU vs NEC
Experiment:

- ~DWD deterministic forecast Global R2B**8**
- 5 242 880 cells (10 km) + Nested grid over Europe 845 340 cells (5 km)
- Output disabled

Performance and energy

- GPU 3x faster than CPU
- 32 GPUs: 663 s/day 268 Wh/day
- 32 VEs: 914 s/day 292 Wh/day

Source: Marek Jacob, DWD, using ICON branch with ecRad on GPU

Why using Domain Specific Language (DSL) in weather and climate ?

- DSL : computer language restricted to a particular domain
- We need performance to reach time to solution
- Separation of concern between domain and computer scientist
- Single source code for multiple target architectures
- Possible to write a new backend when a new technology emerged
- Allow aggressive optimization without degrading readability of user code
- Allow optimization across components – data centric optimization

High level DSL for ICON

- Need to support unstructured grid, such as ICON grid
- New abstraction (e.g. neighbors operations)
- Focus on usability, productivity. Should be usable for domain scientist
- High level python dsl (gt4py)
- Development work in the EXCALIM project
  - High resolution use cases
  - Re-write code components using python DSL framework

Motivation

$$\nabla_{\underline{n}}\psi(e) = \frac{\psi(c_1(e)) - \psi(c_0(e))}{\hat{l}}$$

```
#ifdef _OMP
!$OMP ....
#else
!$ACC ....
#endif
DO jb = i_startblk, i_endblk
 CALL get_indices_e(ptr_patch, ...)
 #ifdef __LOOP_EXCHANGE
 DO je = i_startidx, i_endidx
   DO jk = slev, elev
 #else
   DO jk = slev, elev
     DO je = i_startidx, i_endidx
 #endif
     grad_norm_psi_e(je,jk,jb) =  &
       ( psi_c(iidx(je,jb,2),jk,iblk(je,jb,2)) -
         psi_c(iidx(je,jb,1),jk,iblk(je,jb,1)) )
       / ptr_patch%edges%lhat(je,jb)
   ENDDO
 END DO
END DO
#ifdef _OMP
!$OMP ...
#else
!$ACC ...
#endif
```

Motivation

$$\nabla_{\underline{n}}\psi(e) = \frac{\psi(c_1(e)) - \psi(c_0(e))}{\hat{l}}$$

```
grad_norm_psi_e = neighbor_sum(
        psi_c,
        axis=E2CDim,
        weights=[-1, 1]
)/lhat
```

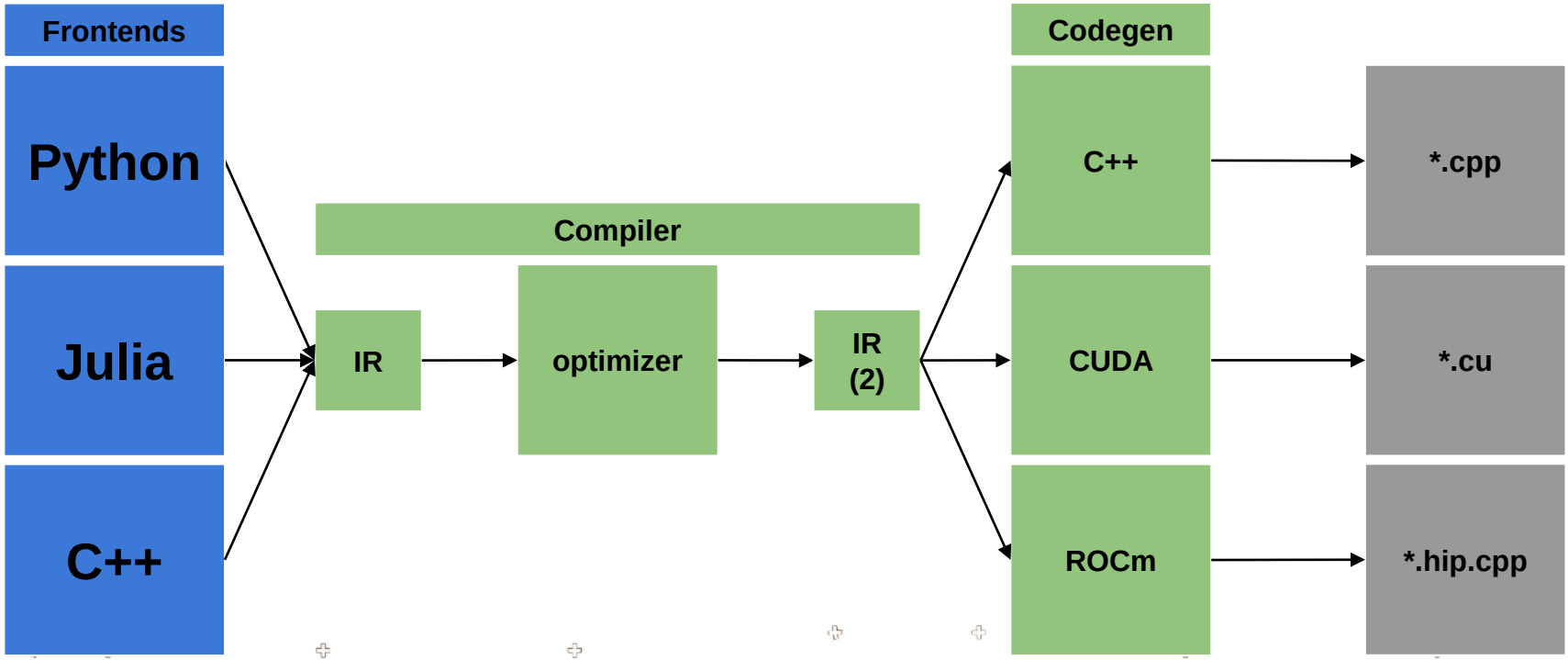
```
#ifdef _OMP
!$OMP ....
#else
!$ACC ....
#endif
DO jb = i_startblk, i_endblk
 CALL get_indices_e(ptr_patch, ...)
 #ifdef __LOOP_EXCHANGE
 DO je = i_startidx, i_endidx
   DO jk = slev, elev
 #else
   DO jk = slev, elev
     DO je = i_startidx, i_endidx
 #endif
      grad_norm_psi_e(je,jk,jb) =  &
        ( psi_c(iidx(je,jb,2),jk,iblk(je,jb,2)) -
          psi_c(iidx(je,jb,1),jk,iblk(je,jb,1)) )
        / ptr_patch%edges%lhat(je,jb)
   ENDDO
 END DO
END DO
#ifdef _OMP
!$OMP ...
#else
!$ACC ...
#endif
```

High level DSL for ICON

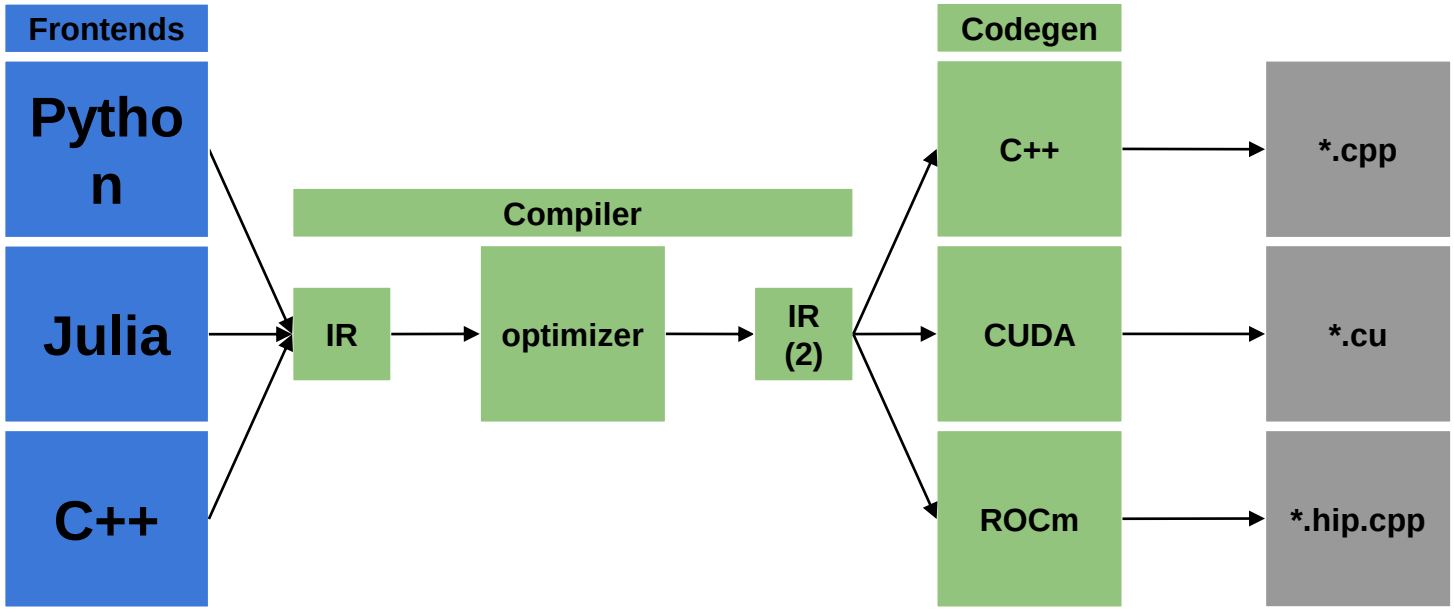
- Need to support unstructured grid, such as ICON grid
- New abstraction (e.g. neighbors operations)
- Focus on usability, productivity. Should be usable for domain scientist
- High level python dsl (gt4py)
- Development work in several projects, ESCAPE, EXCLAIM(ETHZ)

- Performance :
  - CUDA code generation for GPU : allow more optimization than OpenACC
  - long term perspective - data centric optimization across components, e.g. fusion …

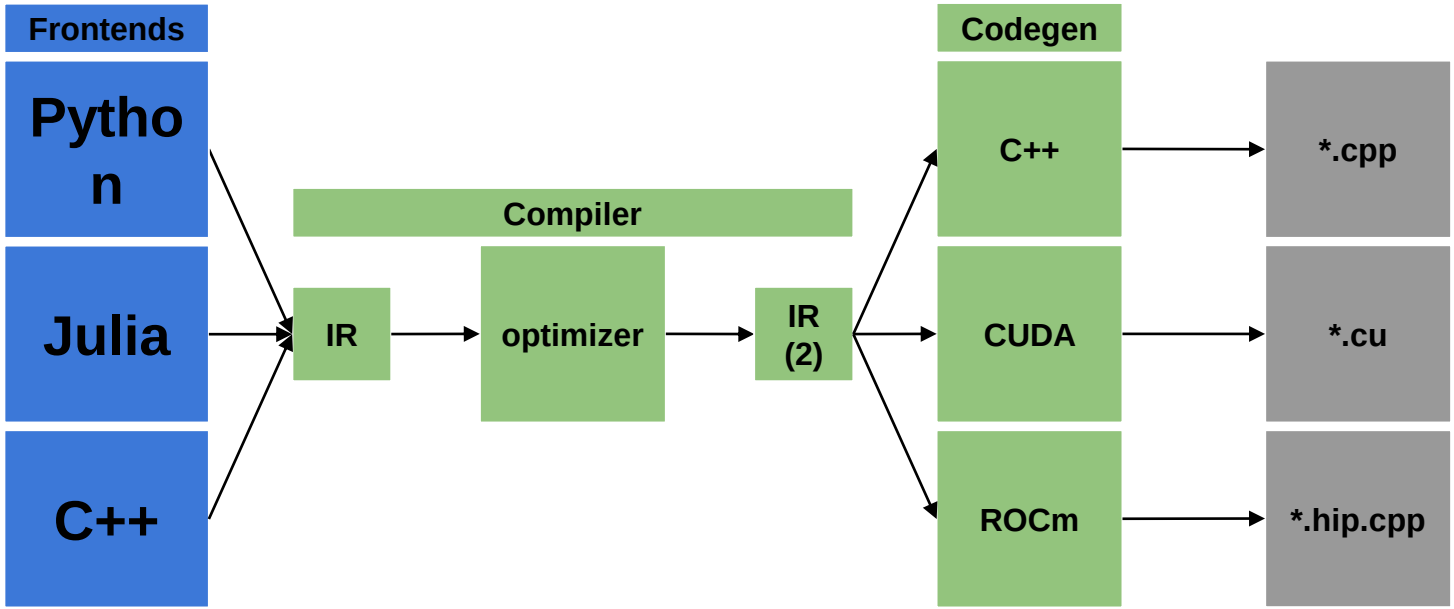
General DSL toolchain



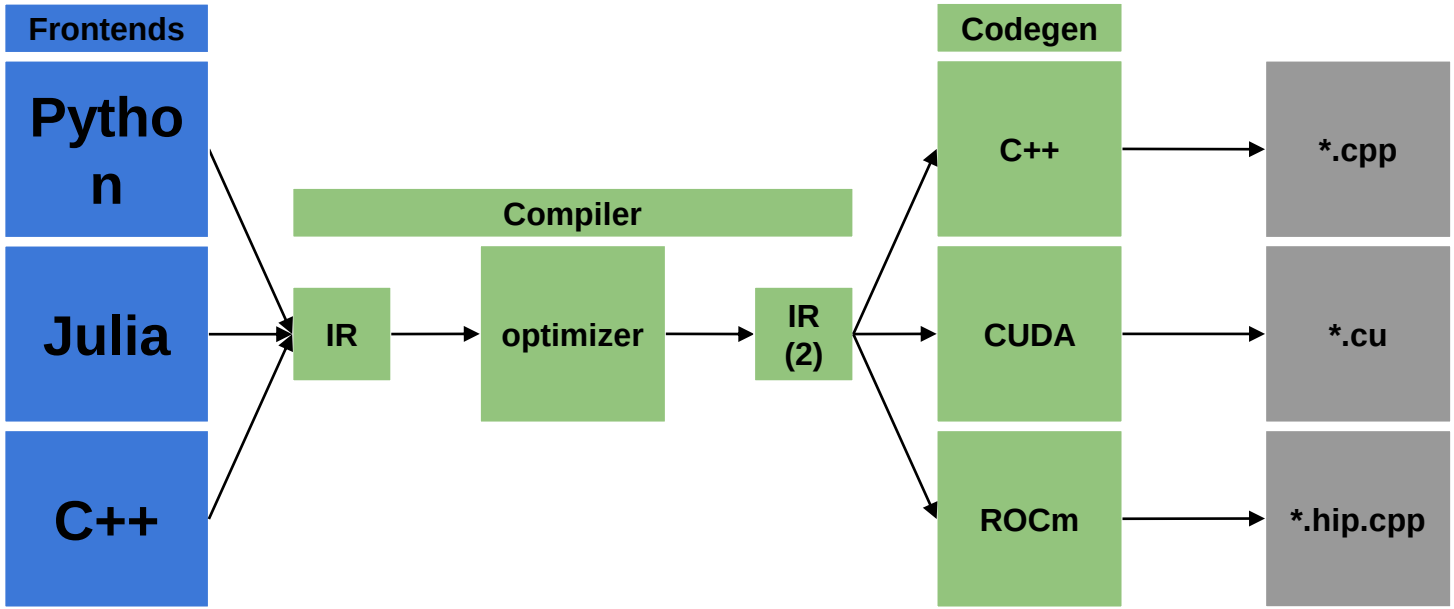
Task 1: Higher order stencil



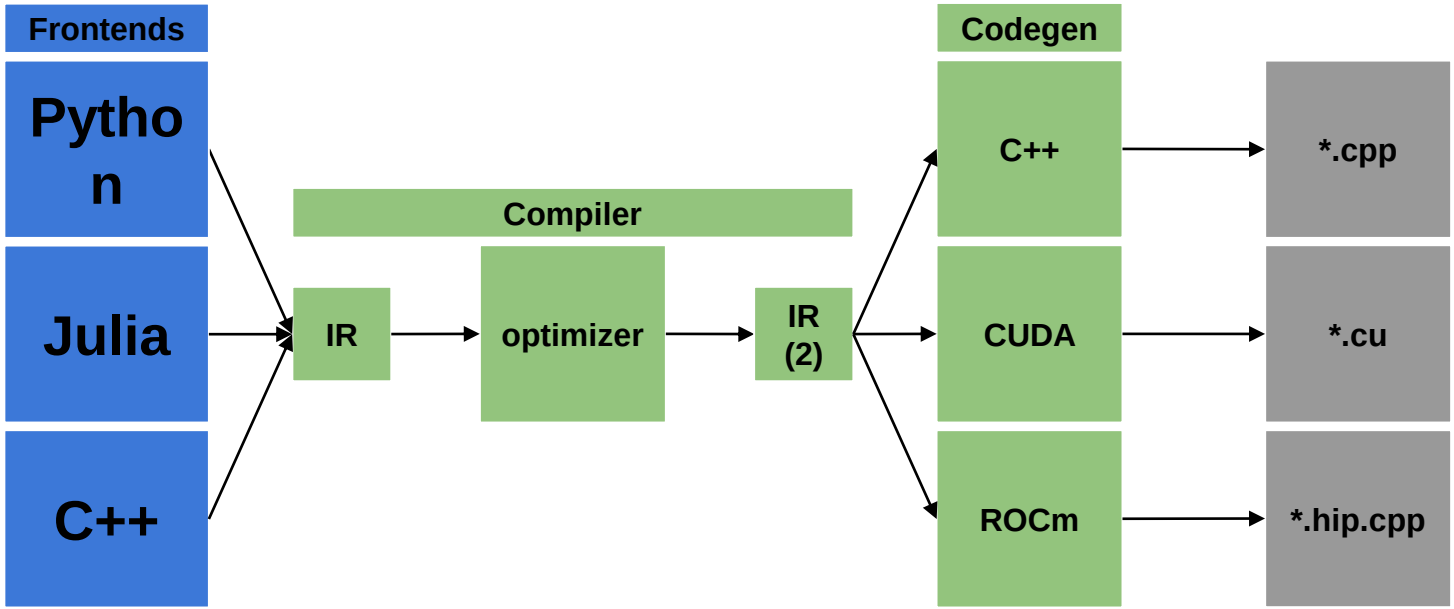
Task 2: Another architecture



Task 3: Substitute mesh library



Task 4: Fusing stencils



GT4Py Code Sample

- Definition of operators isolated
  - Can be composed from existing ones
- Programs use the operators
  - And compose them
- Infrastructure is user defined
  - Mesh, locations and connectivities

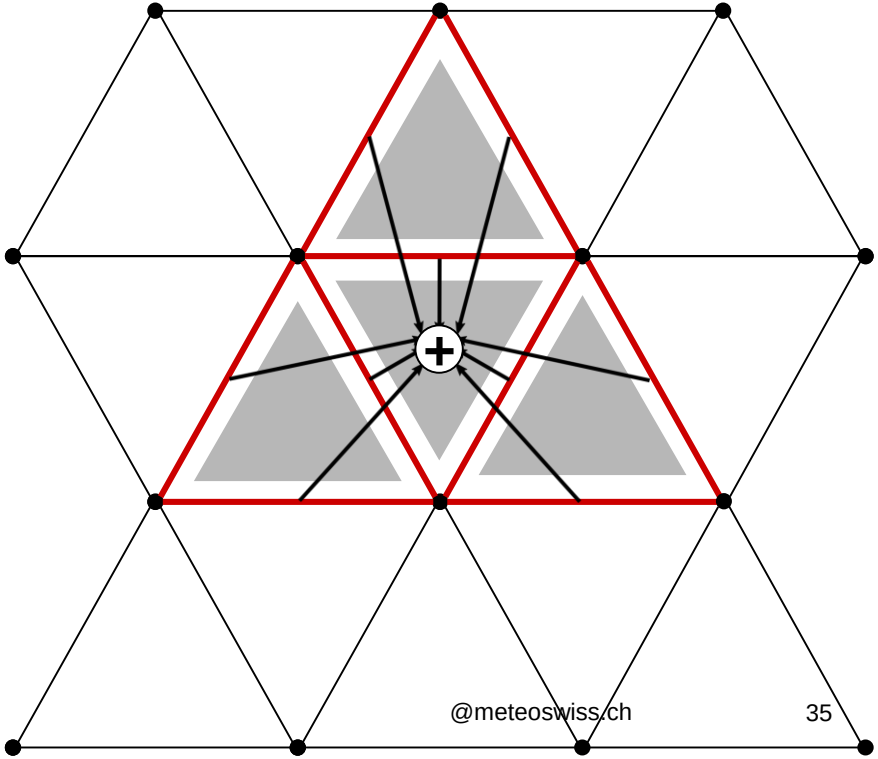
```python
from icon4py.common.dimension import (
    V2C,
    CellDim,
    KDim,
    V2CDim,
    VertexDim,
)
```

```python
@field_operator
def op_interpolation_cells2verts(
    p_cell_in: Field[[CellDim, KDim], float],
    c_intp: Field[[VertexDim, V2CDim], float],
) -> Field[[VertexDim, KDim], float]:
    p_vert_out = neighbor_sum(c_intp * p_cell_in(V2C), axis=V2CDim)
    return p_vert_out
```

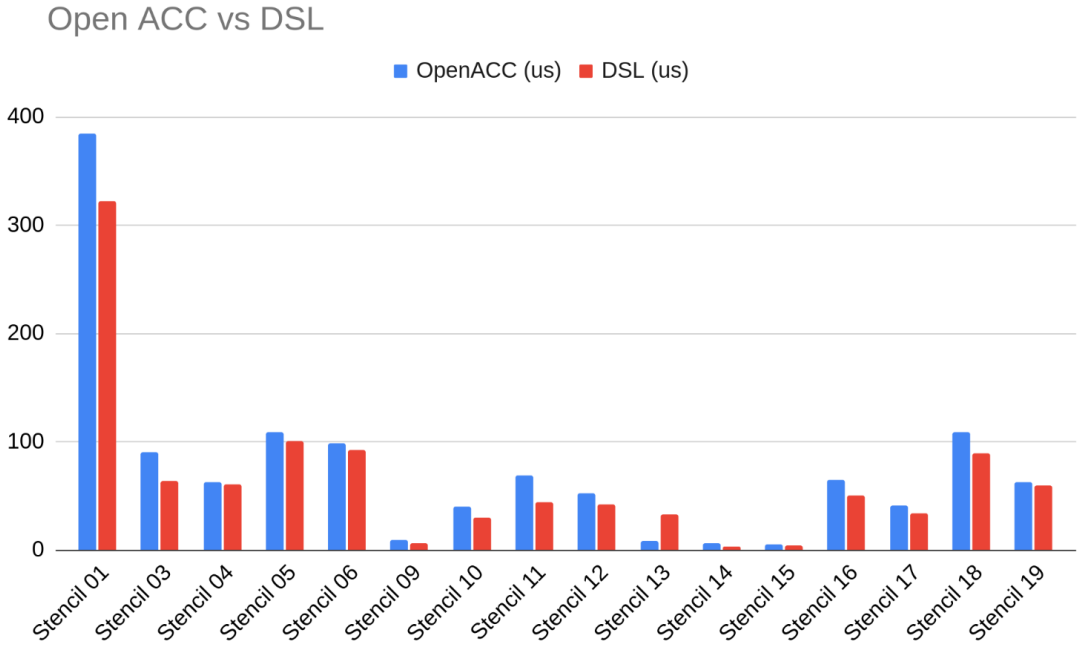
```python
@program
def interpolation_cells2verts(
    p_cell_in: Field[[CellDim, KDim], float],
    c_intp: Field[[VertexDim, V2CDim], float],
    p_vert_out: Field[[VertexDim, KDim], float],
):
    op_interpolation_cells2verts(
        p_cell_in, c_intp, out=p_vert_out
    )
```

Python DSL notation example (gt4py) : Neighbor Chains

```python
@field_operator
def intp(
    fe: Field[[EdgeDim], float],
    w: Field[[CellDim, C2E2C2EDim], float],
) -> Field[[CellDim], float]:
    f_c = neighbor_sum(w * f_e(C2E2C2E), axis=C2E2C2EDim)
    return f_c
```



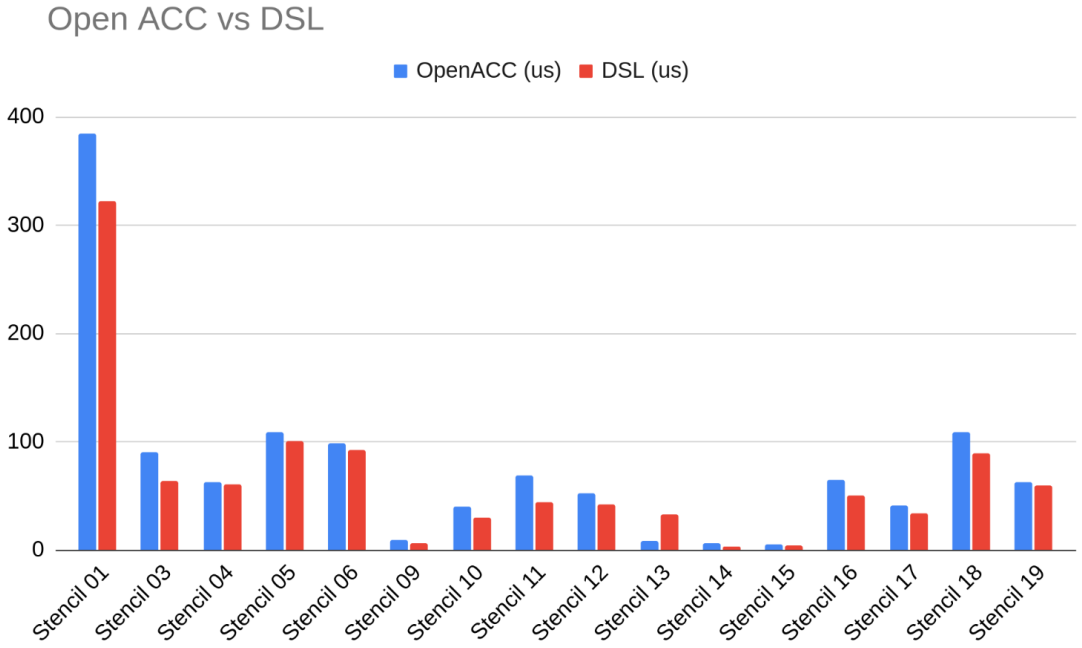
Performance of ICON dycore (DSL) prototype



DSL : Dusk/ Dawn

- Stencil by stencil translation 10-20% faster DSL compared to OpenACC.
- Prototype DSL dycore about 40% (1.4x) faster then OpenACC - not fully optimized. Dry dycore only.

Performance of ICON dycore (DSL) prototype



DSL : Dusk/ Dawn

- Stencil by stencil translation 10-20% faster DSL compared to OpenACC.
- Prototype DSL dycore about 40% (1.4x) faster then OpenACC - not fully optimized. Dry dycore only.

Conclusions

- First version of ICON model ported to GPU using OpenACC compiler directives
- Most components for global and regional NWP ported, and shall be soon available
  - basic version: Q4 2022
  - complete version: std NWP configurations tested with buildbot: Q4 2023
- Reasonable first performance, 3x faster than CPU, but still potential for optimization as still 2x time slower than COSMO
- Training of the ICON developers to work with OpenACC will be organized
- NWP application can likely benefit from DSL development in EXCLAIM, in particular for the dynamical core which shall be used once available

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