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The Good, the Ugly and the Bad: What We Learned from Porting ICON to GPUs

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OpenACC Summit 2021
Sep. 14, 2021, virtual

Approaches to parallel programming from user perspective

Domain Specific Language

```
Y += A*X
```

Base language support

```
do concurrent (i = 1: n)
  y(i) = a*x(i)+y(i)
enddo
```

Directives / pragmas

```
!$acc parallel loop
do j = 1,n
  y(j) = y(j) + a * x(j)
enddo
!$acc end parallel loop
```

Language extensions / Intrinsics

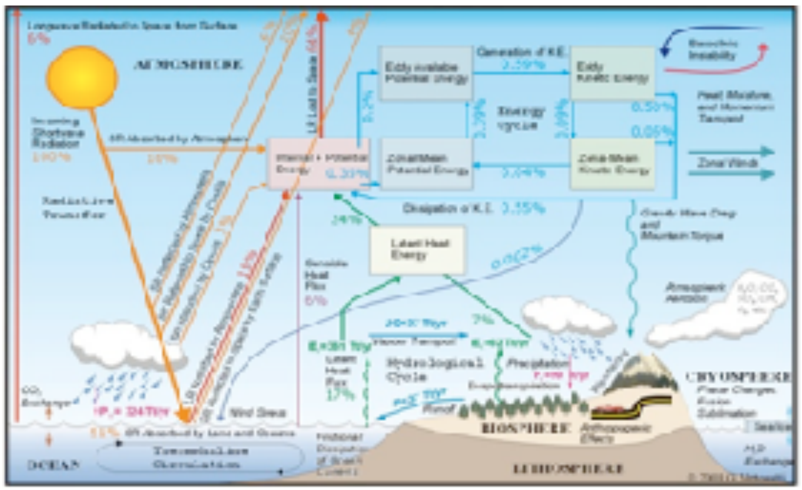
```
attributes(global) subroutine daxpy(n,a,x,y)
  double precision, dimension(*) :: x,y
  double precision, value :: a
  integer, value :: n, i
  i = (blockidx%x-1) * blockdim%x + threadidx%x
  if( i <= n ) y(i) = a * x(i) + y(i)
end subroutine
```

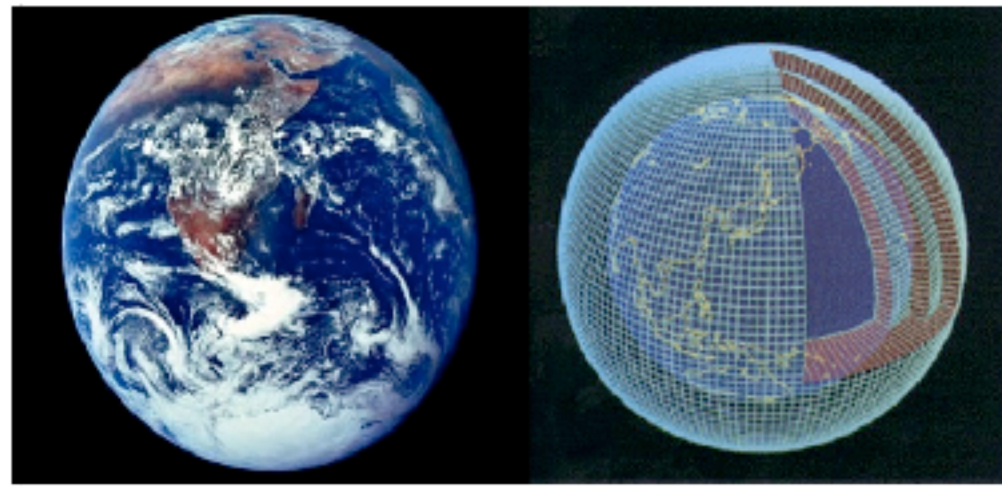

From discussions with Jeff Larkin

ICON in the nutshell

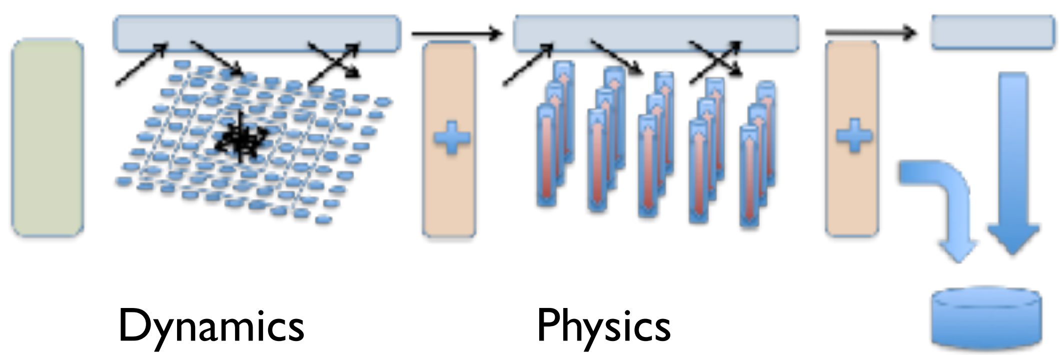
- ICON is ecosystem of atmospheric and ocean modeling software enabling climate and numerical weather prediction
- Developed by ~200 people, 4 German member institutions + numerous others, about 2M lines of code written from 2001 to today
- Successor of COSMO (regional atmospheric Climate/NWP model):
  - ICON for forecasting: DWD in 2015, MeteoSwiss in 2022
  - Also ICON for numerous climate simulations, transition in progress

One-slide introduction to (atmospheric) modeling





Dynamics: solve the 3-D equations of motion on rotating sphere
Physics: parameterize sub-grid phenomena on vertical profiles,
➔ turbulence, hydrological processes, radiation, gravity wave drag...

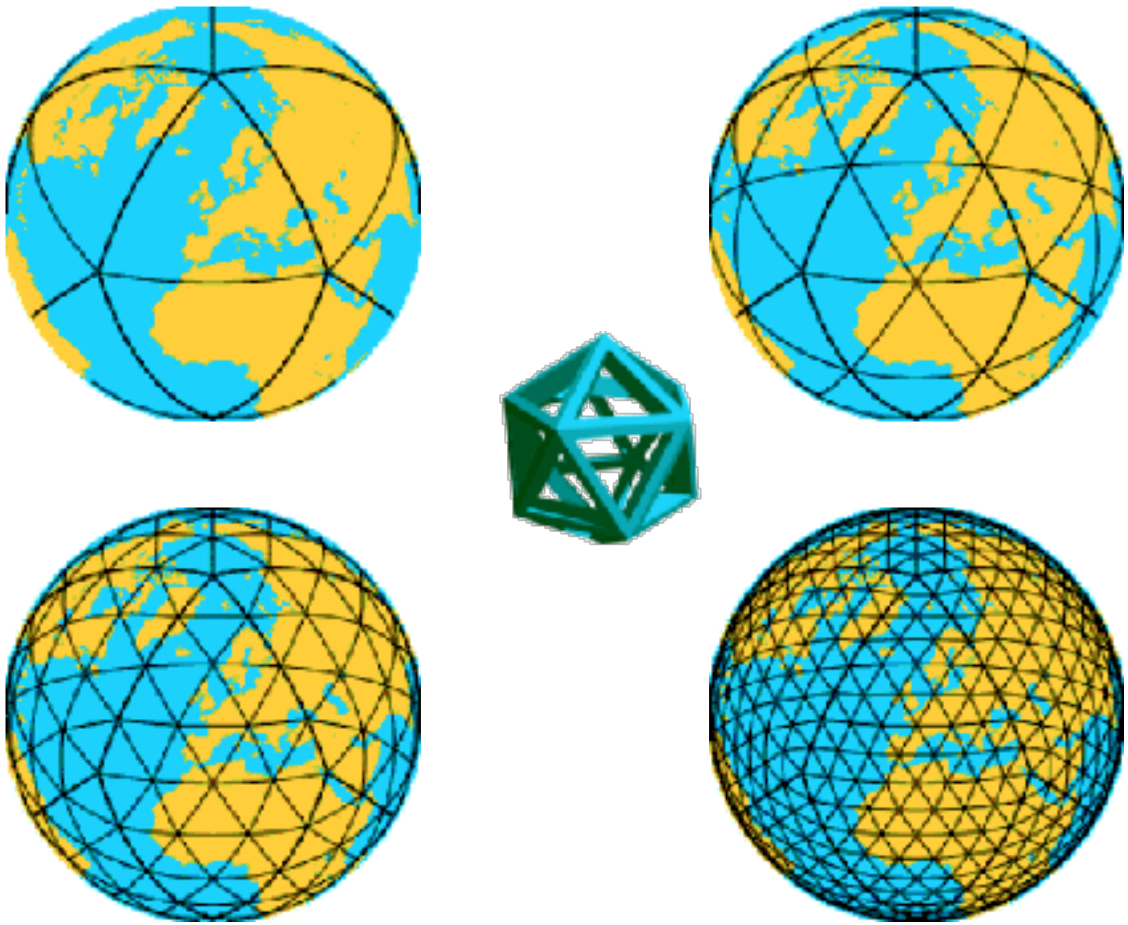


Timeline: ICON GPU port
Large CSCS investment

2010-2019: Port of COSMO with DSL (dynamics) and OpenACC (physics)
2011: ICON dycore (solves atmos. eqns) prototypes (CUDAFortran / OpenCL)
➡ *ICON developers insist on directive-based approach*
2013-2016: PRACE 2IP Work Package 8: ICON dynamical core, one of ~15 applications chosen for HPC refactoring, based on *OpenACC directives*
2015-2017: Effort to port physics of ICON-HDCP^2 to GPUs *unsuccessful* : scientific development too fast, no component testing infrastructure
2015-2019: (Pincus, Norman et al.) OpenACC port RRTMGP radiation: advice
2017-2020: PASC ENIAC project to *port climate-physics, partially with new tools*
2017-2018: ENIAC port of PSrad physics *unsuccessful,* reverted to RRTMGP
2018-2019: *dynamical core refactored* to match physics data layout
2019: "final push" GPU-programming 'hackathon', intensive effort to incorporate RRTMGP, additional optimizations, extensive testing, system integration
2020-2021: ***QBO simulations in production at CSCS (support effort)***

Enabling ICON for Kilometer-Scale Global Climate on GPU Systems; Sawyer, William, PASC19 MS08 - "Bridging the Software Productivity Gap for Weather and Climate Models, Part II of II"

ICON Horizontal Grid



R2B0

R2B1

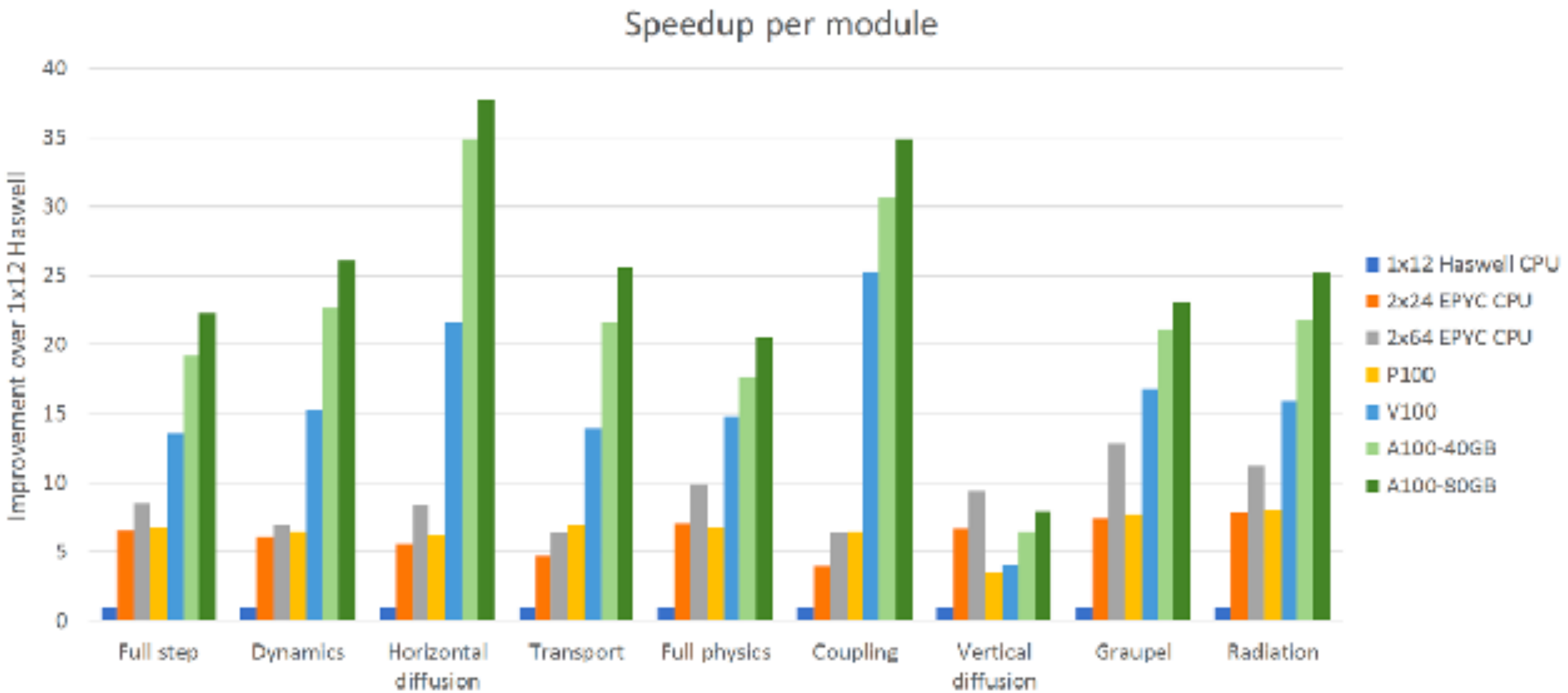
R2B2

ICON the Good: OpenACC

- *It works with good performance after careful optimization*
- Good initial support from Cray for CCE compiler
- Subsequent vendor support from PGI/Nvidia
  - 2013 - 2017: PGI cannot compile ICON for CPUs; *Dave Norton tracks down and reports ~20 compiler bugs.* PGI 18.x works
  - 2019: OpenACC *Atomics* in index list generation too slow. *Dmitry Alexeev replaces atomics with calls to CUB library*
  - 2019-21: *Dmitry introduces ASYNC and other OpenACC optimizations* (e.g., A100), in particular in RRTMGP radiation
- CSCS has strong bonds to OpenACC community
  - Participate in weekly technical calls (user perspectives)
  - Thomas Schulthess elected board member (2019)
- GPU port for climate simulations (QUBICC) ultimately successful
  - Roughly 5x speedup on P100 w.r.t., single-socket Haswell
  - Port from CSCS Daint (P100) to JSC Juwels Booster (A100) straightforward

Intel Haswell, AMD EPYC, Nvidia P100/V100/A100 Performance

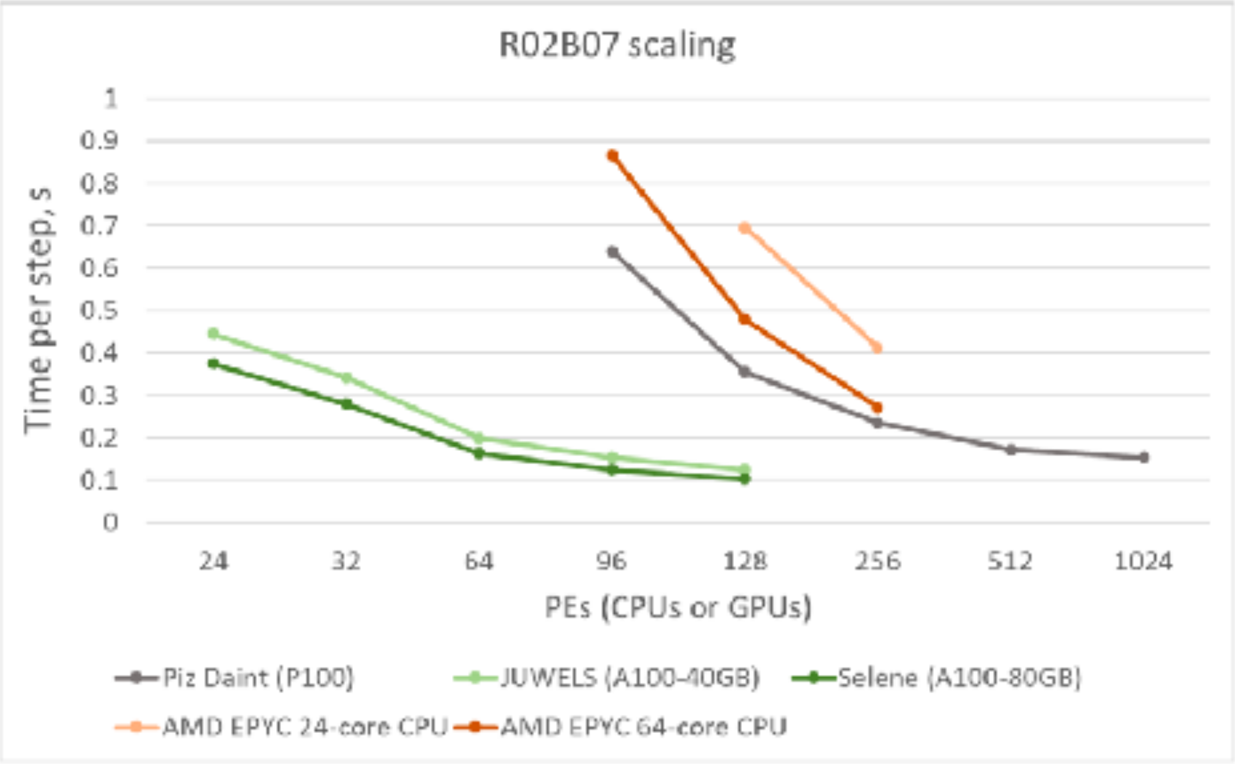
Single-node performance (R2B04 = 160km)



Benchmarking: Dmitry Alexeev

Intel Haswell, AMD EPYC, Nvidia P100/V100/A100 Performance

Strong-scaling (R2B07 == 20km)



ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

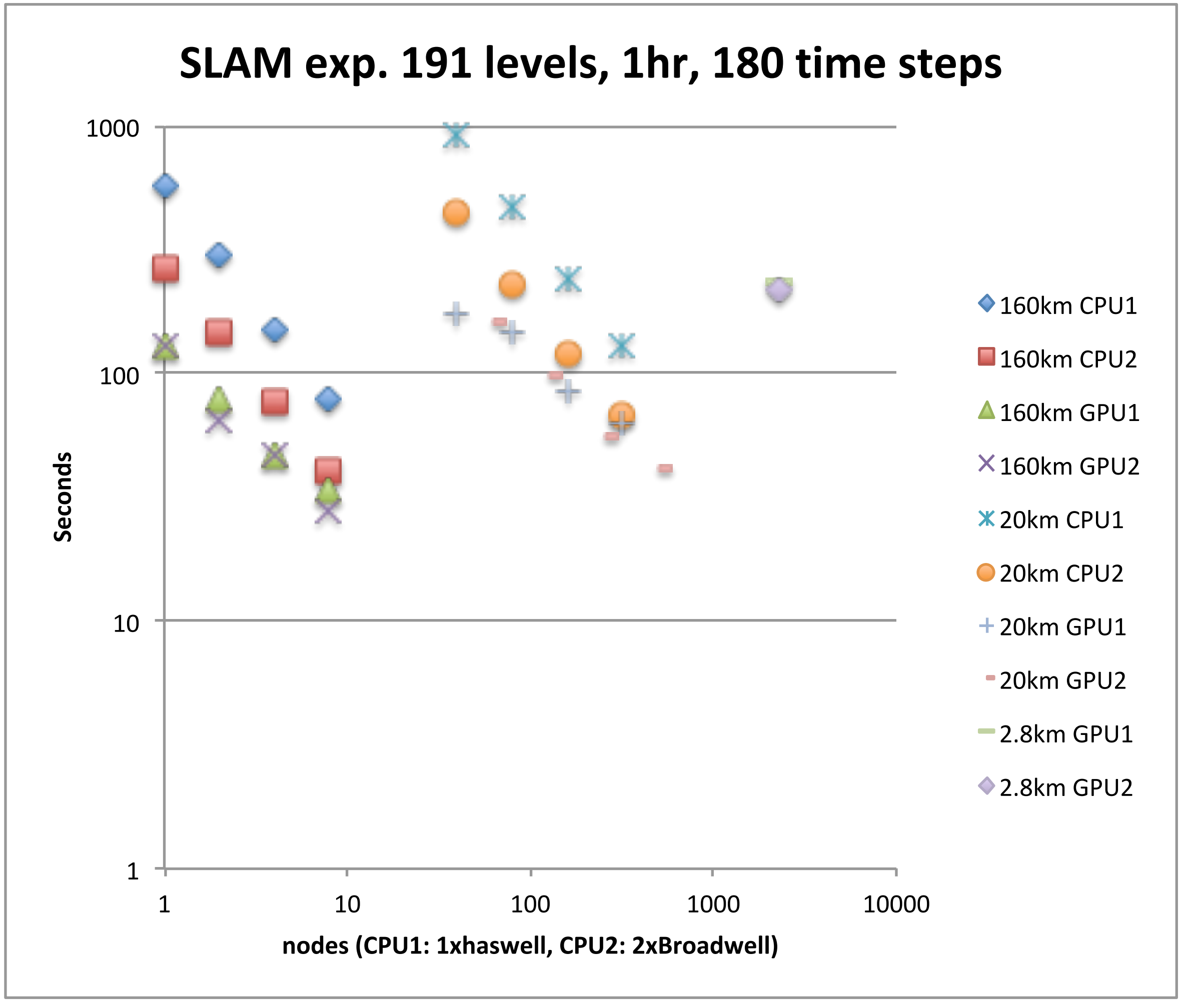
Benchmarking: Dmitry Alexeev

CSCS Swiss National Supercomputing Centre

End-to-end benchmarks (QUBICC proposal)

CPU1: nodes 1xHaswell

CPU2: nodes 2xBroadwell



GPU1: P100 communication G->C->C->G

GPU2: P100 communication G->G

ICON the Ugly

- ICON is a monolithic code; no unit/component tests (or lost after initial development). Similar to COSMO in this respect
  - ➡ Testing infrastructure needed for GPU development (months)
- Original PRACE 2IP dynamical core parallelization not designed with with entire model in mind
  - ➡ Dycore required refactoring during port of full model (weeks)
- PASC funding for GPU port time-limited
  - ➡ ENIAC delayed, team barely completed port of climate "Physics"
  - ➡ Component integration into full model by CSCS

Ugly: Dynamics refactoring needed for large block sizes

Original OpenMP code

```
SUBROUTINE solve_nonhydrostatic_eqns
  …
  !$OMP PARALLEL
  !$OMP DO PRIVATE( lots of vars )
  DO jb = 1, nblocks
    DO jk = 1, nlev
      DO jc = 1, nproma
        prog_var(jc,jk,jb) = f(jc,jk,jb)
      END DO
    END DO
  END DO
  !$OMP END DO NOWAIT
   :
  !$OMP DO PRIVATE( lots of vars )
  DO jb = 1, nblocks
   :
  END DO
  !$OMP END DO NOWAIT
   :
  !OMP END PARALLEL
END SUBROUTINE solve_nonhydrostatic_eqns
```

Original OpenACC

```
SUBROUTINE solve_nonhydrostatic_eqns
  …
  !$ACC PARALLEL LOOP GANG
  DO jb = 1, nblocks
    !$ACC LOOP VECTOR COLLAPSE(2)
    DO jk = 1, nlev
      DO jc = 1, nproma
        prog_var(jc,jk,jb) = f(jc,jk,jb)
      END DO
    END DO
  END DO
  !$ACC END PARALLEL
   :
  !$ACC PARALLEL LOOP GANG
  DO jb = 1, nblocks
   :
  END DO
  !$ACC END PARALLEL
   :
END SUBROUTINE solve_nonhydrostatic_eqns
```

New OpenACC

```
SUBROUTINE solve_nonhydrostatic_eqns
  …
  DO jb = 1, nblocks
  !$ACC PARALLEL
  !$ACC LOOP GANG VECTOR COLLAPSE(2)
  DO jk = 1, nlev
    DO jc = 1, nproma
      prog_var(jc,jk,jb) = f(jc,jk,jb)
    END DO
  END DO
  !$ACC END PARALLEL
  END DO
   :
  DO jb = 1, nblocks
  END DO
   :
END SUBROUTINE solve_nonhydrostatic_eqns
```

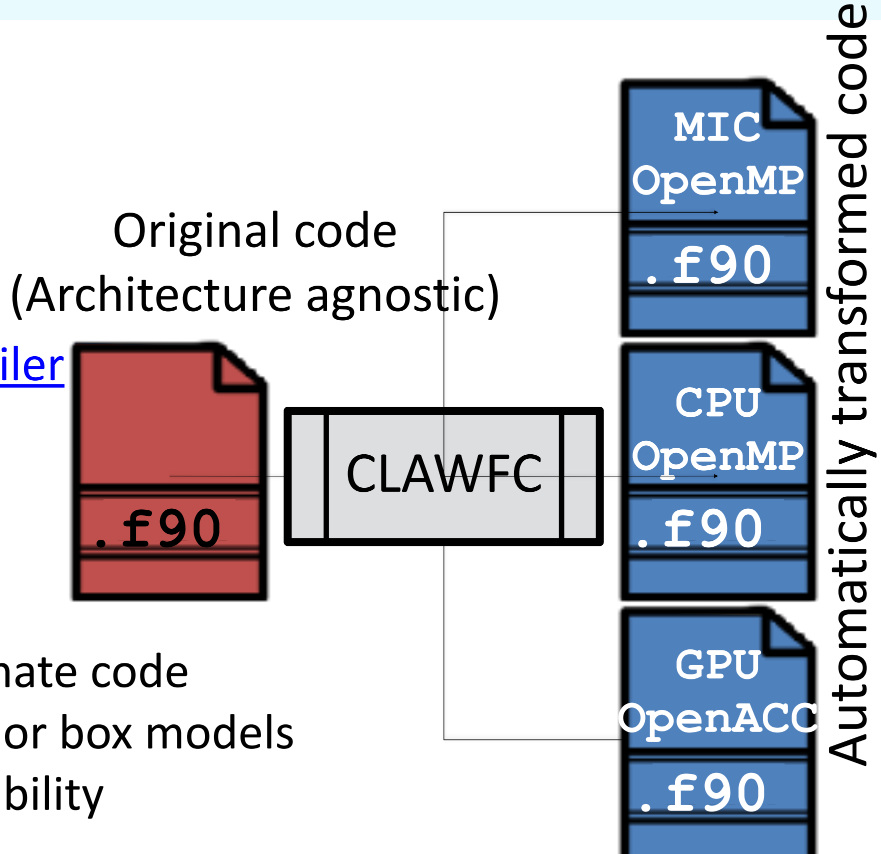
Scientists are not Software Engineers

- ICON developers generally do not write unit tests
- New code features are directly incorporated into model, often with a namelist flag to toggle them
- But: refactoring the feature requires compilation of all of ICON (remember PGI compilation problems)
- For GPU porting: it is *much* easier to port code (e.g. physics) in standalone driver, with serialized data from real model run
- https://github.com/GridTools/serialbox (Arteaga, et al.) serialization, includes `ppser.py` to preprocess serialization directives
- https://github.com/fortesg/fortrantestgenerator (Hovy) generating unit tests for subroutines of existing Fortran applications

Ugly: Long-term support needed for tools

CLAW Compiler (Clement et al.)

- Source-to-source translator
- Based on the OMNI Compiler Project
- Fortran 2008
- Open source under the BSD license
- https://github.com/claw-project/claw-compiler
- Generation of OpenACC/OpenMP directives on the fly



CLAW Single-Column Abstraction (SCA)

- High-level abstraction for weather and climate code
- Targets physical parameterization: column or box models
- Achieve portability and performance portability

Valentin Clement, Sylvaine Ferrachat, Oliver Fuhrer, Xavier Lapillonne, Carlos E. Osuna, Robert Pincus, Jon Rood, and William Sawyer. 2018. The CLAW DSL: Abstractions for Performance Portable Weather and Climate Models. In Proceedings of the Platform for Advanced Scientific Computing Conference (PASC '18). Association for Computing Machinery, New York, NY, USA, Article 2, 1–10. DOI:https://doi.org/10.1145/3218176.3218226

ICON the Bad: Changing messages on OpenACC

- OpenACC commitment based on Cray's early enthusiasm (e.g., John Levesque's presentations ~2012), requirements of community
- Luiz DeRose intimates shift from OpenACC to OpenMP (2015)
- 2019: Cray announces OpenACC unsupported in CCE 9.x
  - ➡ MeteoSwiss/CSCS already in multi-year transition to PGI (painful, but successful)
- 2020: For LUMI, HPE/Cray promises 'sufficient' CCE support to compile ICON benchmark code (but no more than that)
- July 2021: HPE commits to support OpenACC 3.x / OpenMP 5.x in "directive-agnostic" fashion

Bad: we used unofficial extensions

```
#if defined( _OPENACC )
  CALL init_gpu_variables( )
  CALL save_convenience_pointers( )
!$ACC DATA COPYIN( p_int_state, p_patch, p_nh_state, prep_adv ), IF
( i_am_accel_node )
  CALL refresh_convenience_pointers( )
#endif
  TIME_LOOP: DO jstep = (jstep0+jstep_shift+1), (jstep0+nsteps)
   :
  ENDDO TIME_LOOP
#if defined( _OPENACC )
  CALL save_convenience_pointers( )
!$ACC END DATA
  CALL refresh_convenience_pointers( )
  CALL finalize_gpu_variables( )
#endif
```

Cray CCE full automated deep copy

Bad: Transition to manual deep copy

- Fortran full automated deep copy: unsupported feature in Cray CCE, proposal (2013, Beyer, et al.) for inclusion into standard
- Protracted discussion in OpenACC committee
- In 2018 we stopped waiting

```
!$ACC ENTER DATA &
!$ACC       COPYIN( p_int(j)%lsq_high, p_int(j)%lsq_lin,                               &
!$ACC               p_int(j)%c_bln_avg, p_int(j)%c_lin_e, p_int(j)%cells_aw_verts,     &
!$ACC               p_int(j)%e_bln_c_s, p_int(j)%e_flx_avg, p_int(j)%geofac_div,       &
!$ACC               p_int(j)%geofac_grdiv, p_int(j)%geofac_grg, p_int(j)%geofac_n2s,   &
!$ACC               p_int(j)%geofac_rot, p_int(j)%lsq_high%lsq_blk_c,                  &
!$ACC               p_int(j)%lsq_high%lsq_dim_stencil, p_int(j)%lsq_high%lsq_idx_c,    &
!$ACC               p_int(j)%lsq_high%lsq_moments, p_int(j)%lsq_high%lsq_moments_hat,  &
!$ACC               p_int(j)%lsq_high%lsq_pseudoinv, p_int(j)%lsq_high%lsq_qtmat_c,    &
!$ACC               p_int(j)%lsq_high%lsq_rmat_utri_c, p_int(j)%lsq_high%lsq_weights_c &
  :
  :
```

Subsequently: all CCE-specific code removed

Take home messages

- Good:
  - OpenACC is a successful approach in the absence of base language support
  - Successful collaboration; CSCS integrated into development
  - We built good relationships with the OpenACC community
  - Great support from Nvidia; good performance (QUBICC)
  - Partners now see value in GPUs; allocation requests to follow
  - Follow-on efforts (EXCLAIM, ESiWACE) have good promise
- Ugly:
  - ICON is monolithic, component testing and porting difficult
  - OpenACC has serious deficiencies, but also other tools like CLAW
  - Personnel bottlenecks (short-term contracts), long-term support needed
- Bad:
  - Cray dropped OpenACC support in 2018; *HPE reverses strategy in July 2021*
  - Usage of non-standard features for automated deep copy
  - Bottlenecks / refactoring meant bigger CSCS effort than foreseen
  - CSCS lost the high-visibility PRACE QUBICC project to Jülich Juwels Booster

Thanks for your attention