

## Rewriting ICON for scalable development on emerging architectures

Claudia Frauen<sup>1</sup>, Jörg Behrens<sup>1</sup>, Sergey Kosukhin<sup>2</sup>, Hendryk Bockelmann<sup>1</sup>, Daniel Klocke<sup>2</sup> and the (pre)WarmWorld and ICON-C teams

ESM User Forum, March 16-17, 2022

<sup>1</sup> DKRZ, <sup>2</sup> MPI-M

## Overview of projects and initiatives

- WarmWorld: German national project initiative proposed to the BMBF hopefully starting in September 2022. Project partners: DKRZ, DWD, KIT, MPI-M, AWI, ECMWF, FZJ, JSC, Uni Köln, Uni Hamburg, Uni Leipzig
- ICON-C: Coordinated effort involving all ICON partners (C2SM, DKRZ, DWD, KIT, MPI-M) to rewrite ICON for scalable development on emerging architectures
- preWarmWorld: Preparatory project for WarmWorld; separately funded by BMBF; started in 2021; project partners: DKRZ, JSC, MPI-M



# ICON (ICOsahedral Nonhydrostatic model)

- ICON is a weather and climate model with atmosphere, ocean and land components
- Almost 2 decades development; initially by DWD and MPI-M, later also KIT and DKRZ and now also in collaboration with C2SM
- Mostly written in Fortran using MPI/OpenMP for parallelisation
- ~ 2 Million lines of code



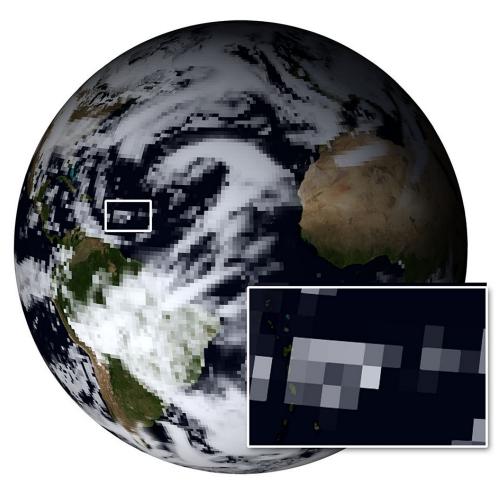


- HD(CP)<sup>2</sup> project enabled efficient km and hectometre (hm) scale applications over large regional domains
- These efforts enabled the use of ICON to perform the first global storm-resolving (SR) simulations in Europe
- ICON is one of only four models worldwide to have been run as an SR-ESM, i.e., coupled with km-scale resolution in the atmosphere and ocean

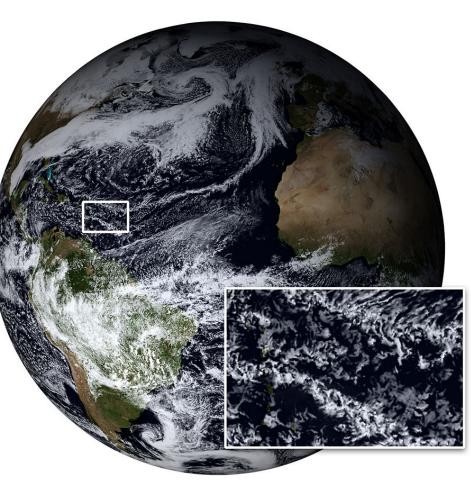


### Simulation of clouds

#### MPI-ESM HR, 80km



#### ICON R2B10, 2.5km



Florian Ziemen, DKRZ



- Huge efforts especially by CSCS, Meteo Swiss, Nvidia have lead to a GPU-enabled version of ICON-A (e.g. through the PASC ENIAC and IMPACT projects)
- Use of OpenACC directives + CLAW tool for the land model
- Successfully runs on Piz Daint and JUWELS Booster (QUBICC and Monsoon 2.0 projects)



## Current ICON performance

$\Delta_{h}$	L <sub>atm</sub>	L <sub>ocn</sub>	Nodes	Machine	SDPD
5.0 km	90	n/a	300	Mistral (2xIntel BDW 36-cores)	28
2.5 km	90	n/a	510	Mistral (2xIntel BDW 36-cores)	7
2.5 km	n/a	112	262	Mistral (2xIntel BDW 36-cores)	51
5.0 km	90	128	420	Mistral (2xIntel BDW 36-cores)	25
5.0 km	90	n/a	77	JUWELS Booster (4xNVIDIA A100)	120
2.5 km	90	n/a	600	Levante (2xAMD 7763 128-cores)	20
5.0 km	n/a	128	250	Levante (2xAMD 7763 128-cores)	375
5.0 km	90	128	420	Levante (2xAMD 7763 128-cores)	96

Performance characteristics of ICON for different horizontal ( $\Delta_h$ ) and vertical ( $L_{atm}$  and  $L_{ocn}$ ) resolutions.



Assess the detailed trajectory of global warming and the quantitative implications of this warming for human and natural systems

- Coupled ICON running with an acceptable simulation quality on km scale > 0.5 SYPD by 2026
- ICON-C: A free and open source software implementation of the fully (land, ocean, atmosphere) coupled ICON to enable scalable development
- Integrated workflow to expose information of ICON alongside IFS-based solutions and observational data



## WarmWorld Modules

- Better: Responsible for defining and testing the model configurations
- Faster: Responsible for transforming the ICON code base into an open, scalable, modularized and flexible code
- Easier: Responsible for developing novel methods to make information visible, accessible, and interoperable
- Smarter: Aims to involve the applied maths and informatics communities, to improve the workflow and the model performance

WarmWorld collaborations

#### **CECMWF** Bonn

ATLAS

WARM

WORLD

**Mod1:** Support for continuing development cycles from NextGEMS to shadow ICON developments (*simulation ghosts*), aid evaluation, provide robust information systems, and strengthen workflow.

C<sub>2</sub>SM

Center for Climate Systems Modeling

next GEMS

WORLD

**Mod3:** Developing next Generation workflows to create scalable workflows that give German researchers transparent access to ICON- and IFS-based information systems.

**ACROSS** 

Pre-Marnwold Mod2: Enabling a scalable development to benefit from parallel efforts in the C2SM (ETH) project EXCLAIM, and eventually other (DestinE) projects.

**Mod4:** Open call to strengthen links to applied math and informatics communities, and other EU projects to improve performance of model and analysis systems.







- Transform the ICON code base into an open, scalable, modularized and flexible code named ICON-C ("ICONconsolidated").
- Refactor ICON with the goal of scalable development to enable portable performance improvements ultimately making ICON faster
- Initiate target performance ports to meet throughput (>0.5SYPD on a 2.5km or finer grid) goals
- Progressively redefine the ICON code structure to expose areas of performance improvement for targeted exploration of new programming concepts



- WarmWorld is just one piece of the puzzle towards ICON-C; larger coordinated effort involving all ICON partners
  - Balancing between different needs: Operational numerical weather forecast and cutting-edge climate modelling
- EXCLAIM (ETH Zürich): Extreme scale computing and data platform for cloud-resolving weather and climate modelling
  - Approach: Re-write ICON code into a descriptive user code based on Python, which is then translated into standard imperative language (e.g. C++) for specific architectures using a toolchain based on GT4Py (GridTools for Python)



- ICON is largely monolithic:
  - Huge code base is compiled in
  - Namelists are used to (de-)activate large tracts of code
  - Minimal unit testing
- Git submodules are used, but only few can be decoupled from compilation
- Components are not cleanly separated
- Uses complex derived types
- Contains unused code

## ICON-C first development steps

- Refining the Development Process
- Implementation of a disable functionality, initially via #ifdef, and clean-up
- Modularisation of components: Proposal and prototypes
- Prototype Data Management
- Infrastructure Measures
- Testing Hierarchy and Tools



- Funded by the BMBF as a separate project to prepare for WarmWorld and to facilitate timely coordination with external projects such as EXCLAIM
- Provide a technical blueprint in terms of modularization and programming paradigms
- Overlap between the latter phase of preWarmWorld and the start of WarmWorld allows these plans to be coordinated before delivering the development environment (repository, test structure, licenses) for use in WarmWorld

# Planned assessment of programming paradigms in preWarmWorld

- Evaluation, comparison and prototypical implementation of selected modules using modern programming paradigms targeting heterogeneous hardware
- Implement granule using GridTools framework
- ▶ Implement granule using a *generic DSL*, like AnyDSL
- Implement granule using a domain independent generic library, like Kokkos and/or DPC++ / SYCL
- Implement granule using the concept of an embedded DSL
- Analyse the applicability and, if suitable, implement the interfacing of the above concepts to the front-end developed in the ESCAPE2 project

## C++ Data / Memory Management - Why?

- Need to move away from Fortran-centric view of memory management to open up ICON for new possibilities
- Better compiler support for C/C++ than for Fortran
- Enable easier language interoperability with e.g., Gt4Py, Kokkos, ...
- But: Legacy Fortran code still needs to be able to access data in the same way

## C++ Data / Memory Management - Why?

- ICON variables and their meta-data are organized in a linked list (varlist) implemented in Fortran
- Current functionality includes adding and removing elements and searching the list
- A C++ varlist implementation based on a quasi ordered map can make use of existing standard C++ functionality
- Future extension of functionality will also be simpler than a Fortran implementation



- Exploring the CFI (C-Fortran-Interface) in ISO\_Fortran\_binding.h
- Agnostic creation of arrays in C and their later clean use in Fortran
- Using the Fortran Standard (2018) or TS29113 (2012)
- Not yet supported by all compiler vendors



- Atmospheric tracer advection ideal example to test new concepts and develop software blueprint:
  - Representative for whole ICON, has 3D-stencil operations
  - Extensively utilizes ICON infrastructure
  - But conceptionally could be own submodule
  - OpenACC implementation exists for some methods



Problems with current implementation:

- More than 100 Fortran module dependencies
- Data flow through global model data is not obvious
- Complex interface, e.g.: step\_advection(p\_patch, p\_int\_state, + 19 simple args)
- Complexity comes from huge derived types: t\_patch, t\_int\_state, but derived type content mostly not used or not used directly



#### Goals:

- pool together "advection-owned" code and data
- make data flow obvious
- minimize interface complexity
- have a stand-alone version using the same advection code as in the full model



- Significant rewriting and refactoring of ICON is needed for scalable development on emerging architectures => ICON-C
- preWarmWorld: Assessment of programming paradigms and modular software blueprint
- Steps are underway in preWarmWorld together with partners in ICON-C and EXCLAIM to
  - rewrite the memory management in C++ with a C-Fortran interface
  - prepare a stand-alone version of the atmospheric tracer advection as a playground, on which to try out different programming paradigms



## Thank you for your attention!