Challenges of NICAM toward the exascale era

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and

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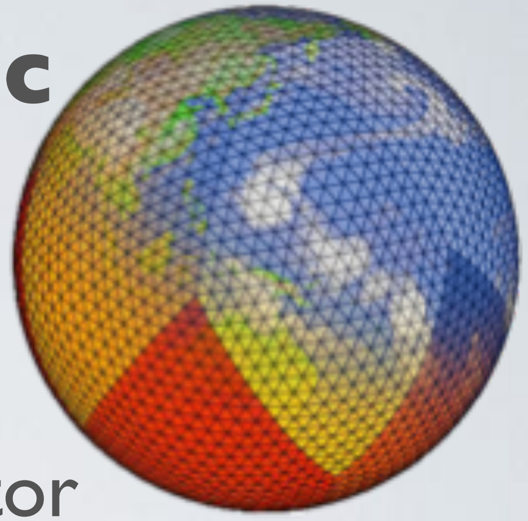
NICAM

Non-hydrostatic **I**cosahedral **A**tmospheric **M**odel (NICAM)



- Development was started since 2000
  Tomita and Satoh (2005), Satoh et al. (2008, 2014)
- First global dx=3.5km run in 2004 using the Earth Simulator
  Tomita et al. (2005), Miura et al. (2007, Science)
- First global dx=0.87km run in 2012 using the K computer
  Miyamoto et al. (2013, 2015), Kajikawa et al. (2016)

Prof. Satoh (AORI, Tokyo univ.)

Dr. Tomita (RIKEN)

- Main target : high-resolution simulation without convection parameterization, without lateral boundary
- Compressive, non-hydrostatic equations are solved using finite volume method on the icosahedral grid
  - Most part is written by Fortran90
  - ~50 users, ~10 active developers

NICAM and Supercomputers

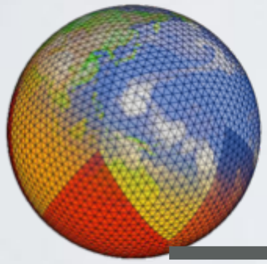
JAMSTEC
- Earth Simulator 36TFLOPS (2002)
- Earth Simulator 2 122TFLOPS
- Earth Simulator 3 ~1PFLOPS

RIKEN
- The K computer 10PFLOPS
- Post-K

The U. of Tokyo & Tsukuba U.
- T2K-Tsukuba 100TFLOPS
- Oakleaf-FX 1PFLOPS
- Oakforest PACS 14PFLOPS

JAXA
- SORA-MA 3PFLOPS

Tokyo Tech.
- TSUBAME2.5 3PFLOPS
- TSUBAME3 8PFLOPS



2000 2004 2011 2018

3.5km MJO sim.

870m run
14km 30yr AMIP run

International collaborations

- CMIP6/HighResMIP
- RCEMIP
- DYAMOND project
- SPPEXA/AIMES & GridTools-NICAM

Current development target **from the viewpoint of HPC**

Cloud-permitting (14km~3.5km) simulation + X

+ Eddy resolving ocean
+ Ensemble data assimilation system
+ Aerosol & chemistry

Keywords

- Approximate computing
- Data centric design
- Performance portability

Today's talk

Our efforts on the petascale computing era

- Practical cases of the extreme scale global simulation

Our efforts toward the exascale computing era

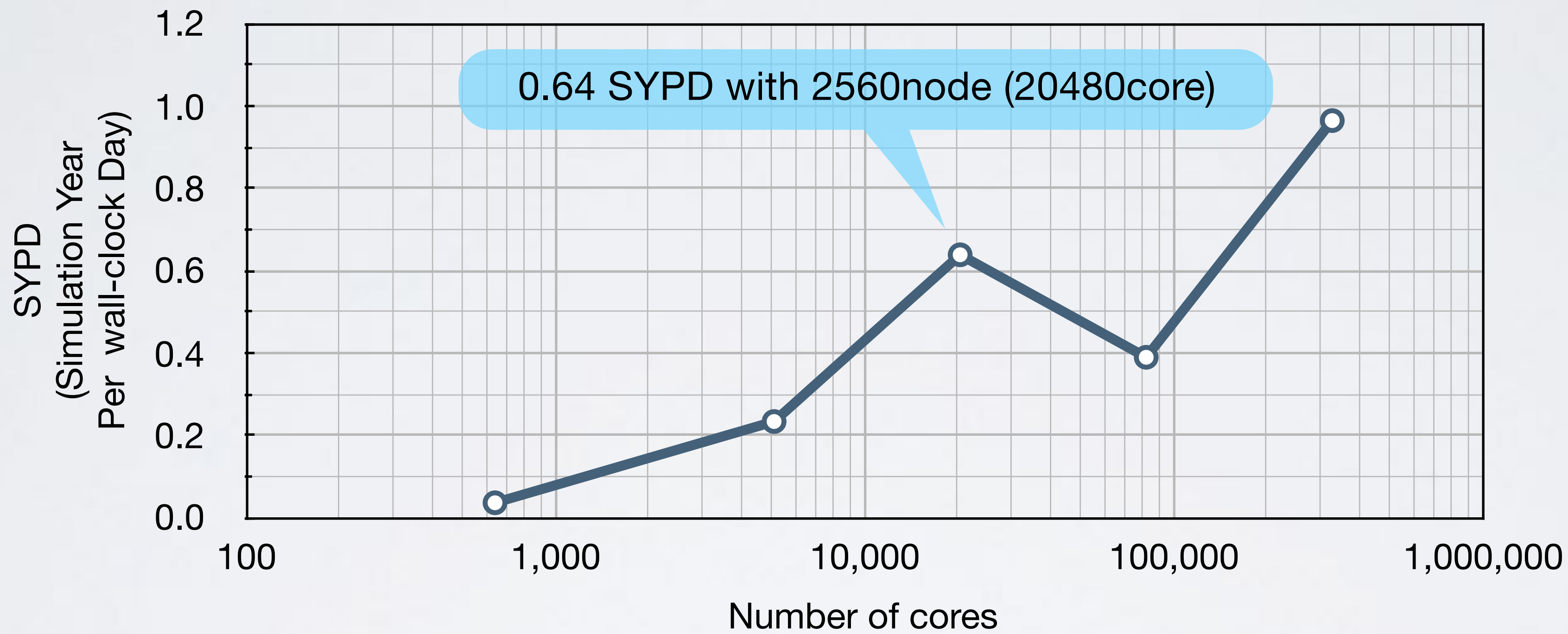
- Post-K project
- SPPEXA/AIMES & GridTools-NICAM

Efforts on the petascale computing era

NICAM on the K computer

Performance optimization (Yashiro et al., 2017, PASC'16)

- Time-consuming parts are removed: zero-filling, copying, lots of intermediate arrays, "if" in the loop
- Good weak scalability up to 81,920 nodes x 8 threads with 0.9PFLOPS
- Good strong scalability: with 14km horizontal, 38layers:



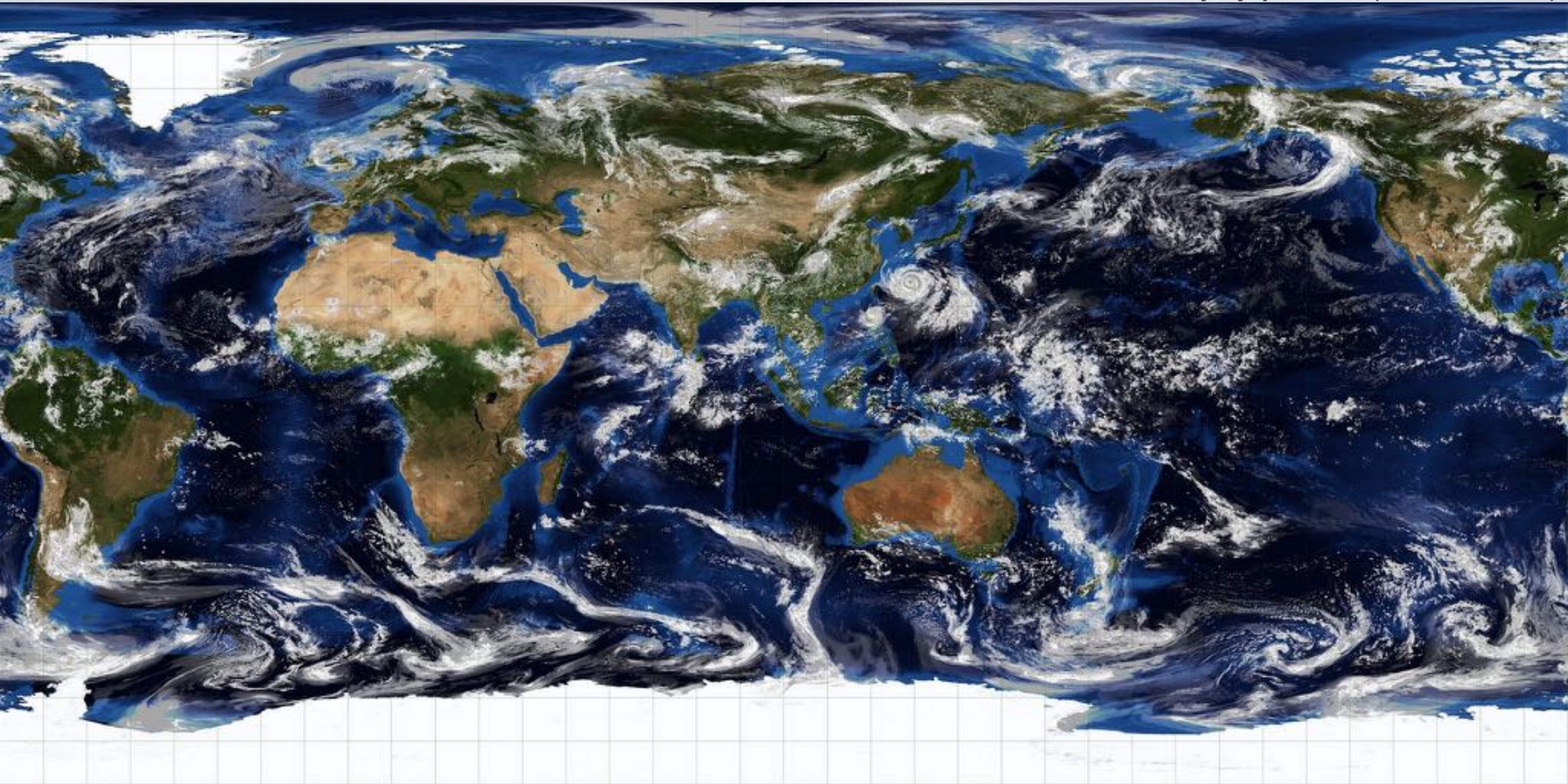
The cost ranking cannot find the time-consuming part

- Tiny "time eaters" are hiding everywhere in the code
- It is necessary to collect the information about the elapsed time, the memory throughput, and the number of floating operations for each loop nests

The first global sub-km weather simulation on the K computer

Miyamoto et al., 2013, GRL

Visualized by Ryuji Yoshida(RIKEN,Kobe U.)



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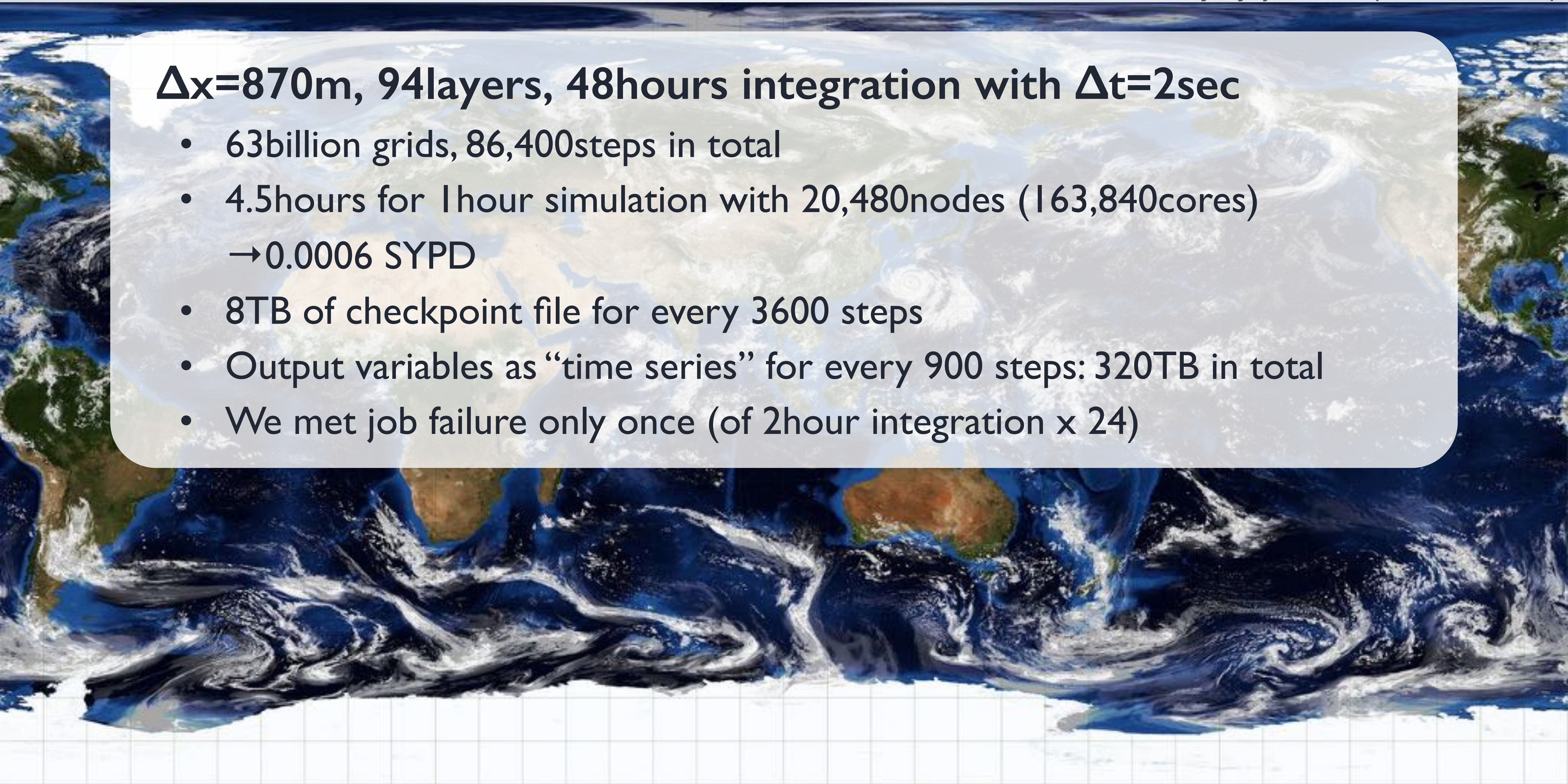

Δx=870m, 94layers, 48hours integration with Δt=2sec

- 63billion grids, 86,400steps in total
- 4.5hours for 1hour simulation with 20,480nodes (163,840cores)
  →0.0006 SYPD
- 8TB of checkpoint file for every 3600 steps
- Output variables as "time series" for every 900 steps: 320TB in total
- We met job failure only once (of 2hour integration x 24)

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Our simulation didn't have any problems in I/O: Why?

- File staging : isolated from the crowded global file system
  - A different storage disk is assigned to each MPI rank
- I/O node : we don't have to wait writing due to the large buffer
- Distributed file I/O : each MPI rank writes the files

The diurnal cycle of precipitation over land in the tropics

Yashiro et al., 2016, SOLA

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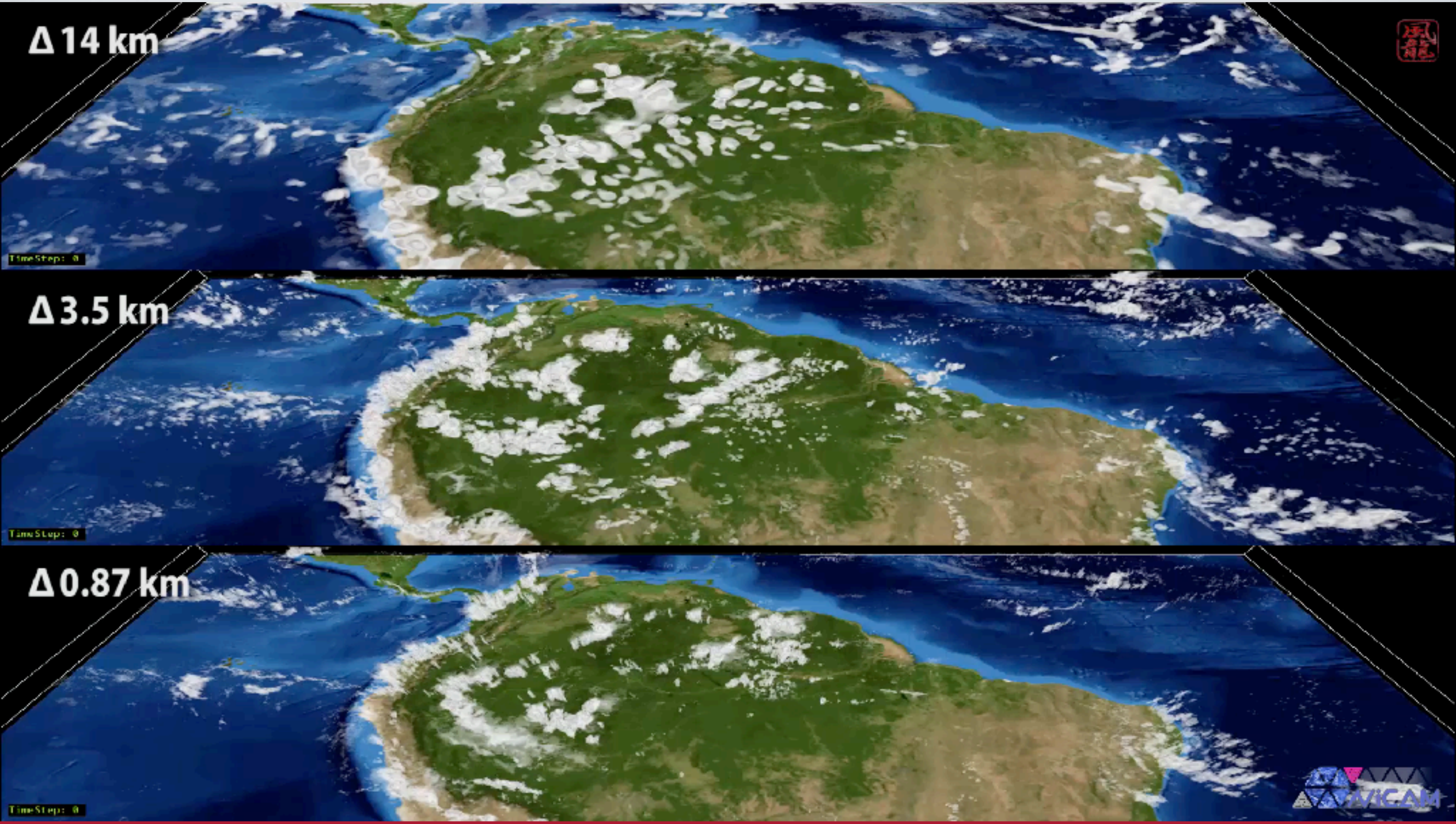

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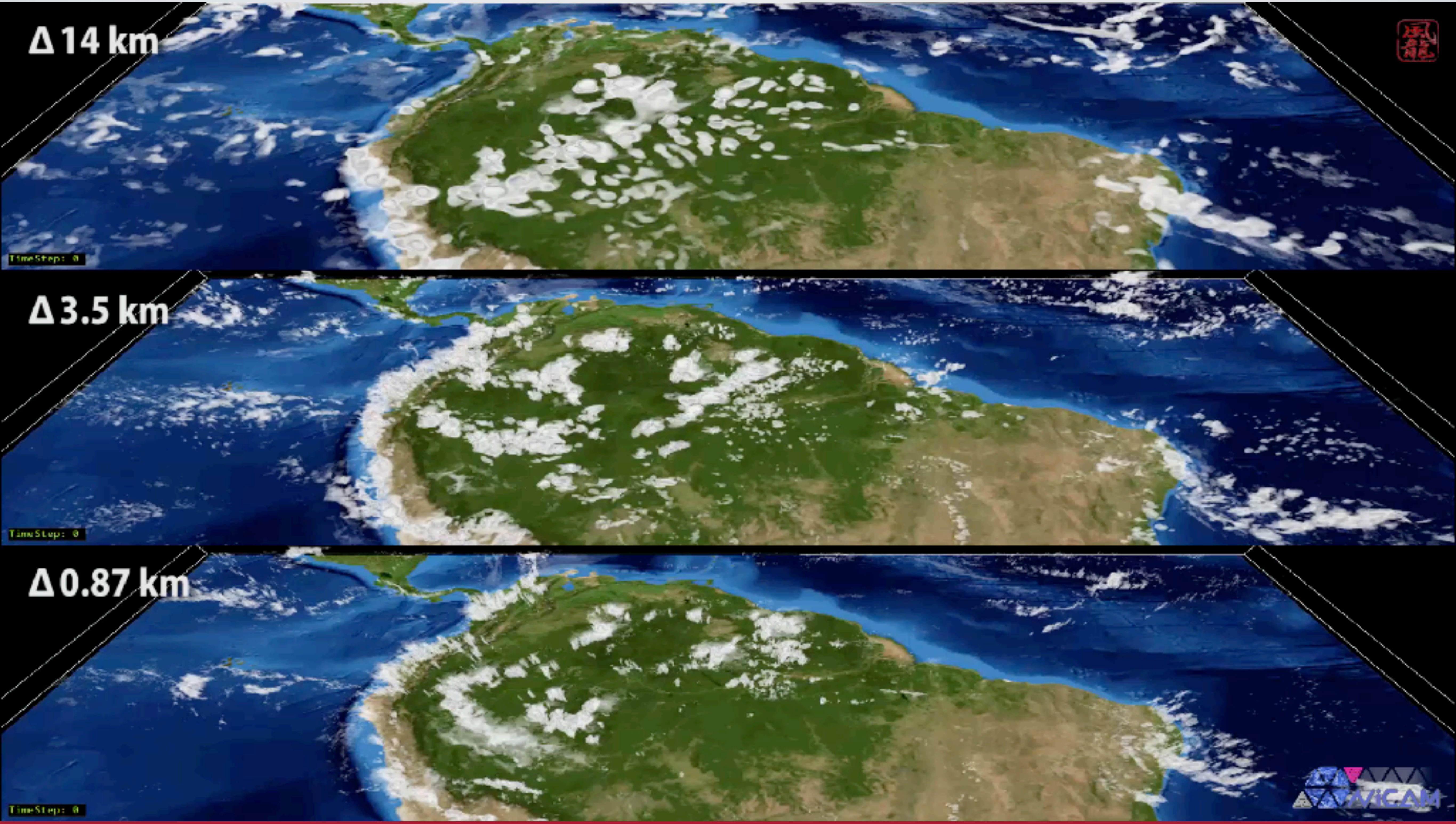

'Big' data analysis in the weather/climate study

Every 30min Snapshot for 0.87km run: ~3TB
x 48 steps (for last 1day output) = 160TB

↓

Grid remapping
from icosahedral
to latitude-longitude

2 months on the post-process cluster

↓

Analysis on
latitude-longitude grid

2 months on the post-process cluster

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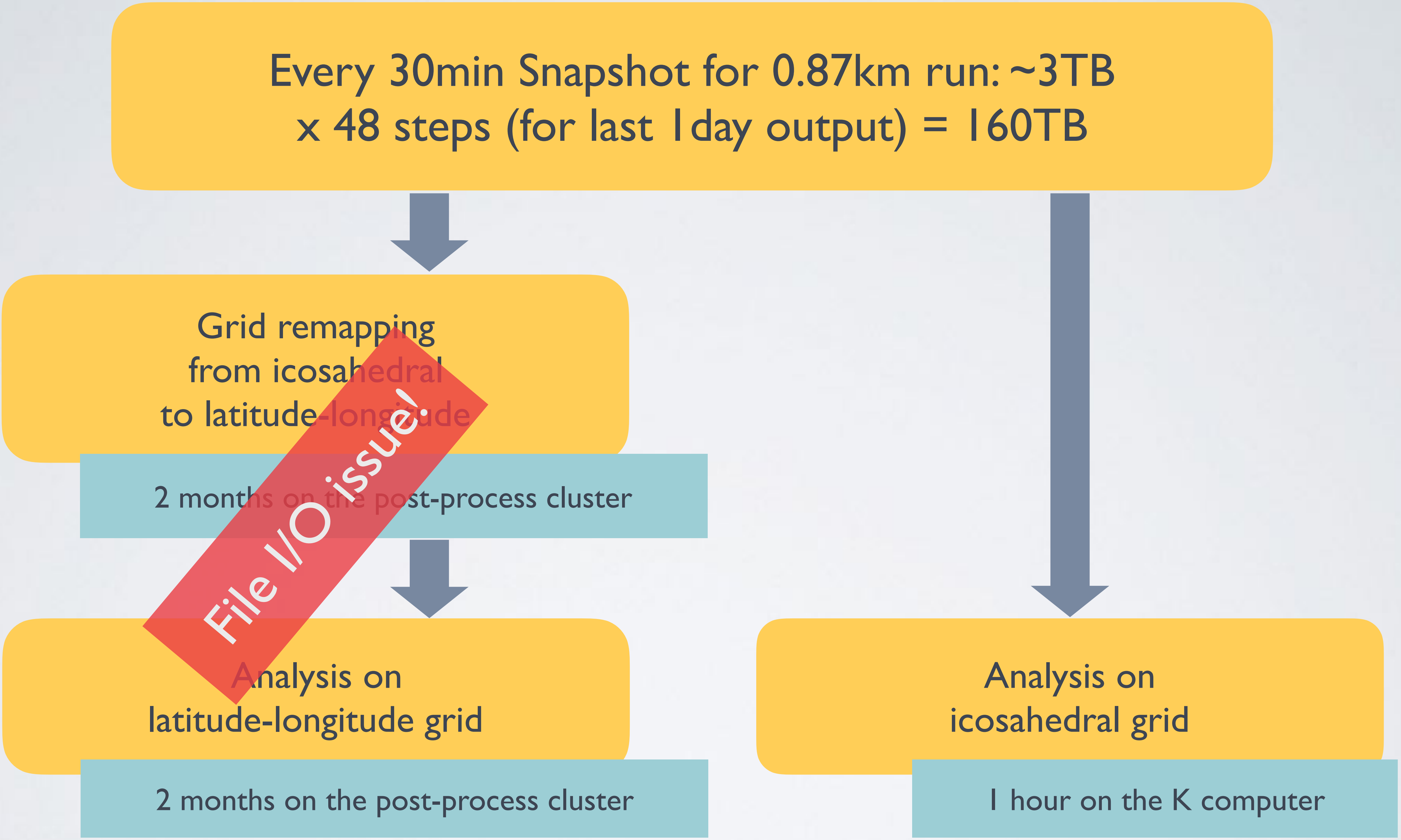


NICAM on KNL cluster

Oakforest-PACS: the largest KNL cluster in Japan

- 8208 nodes, Intel Xeon Phi 7250

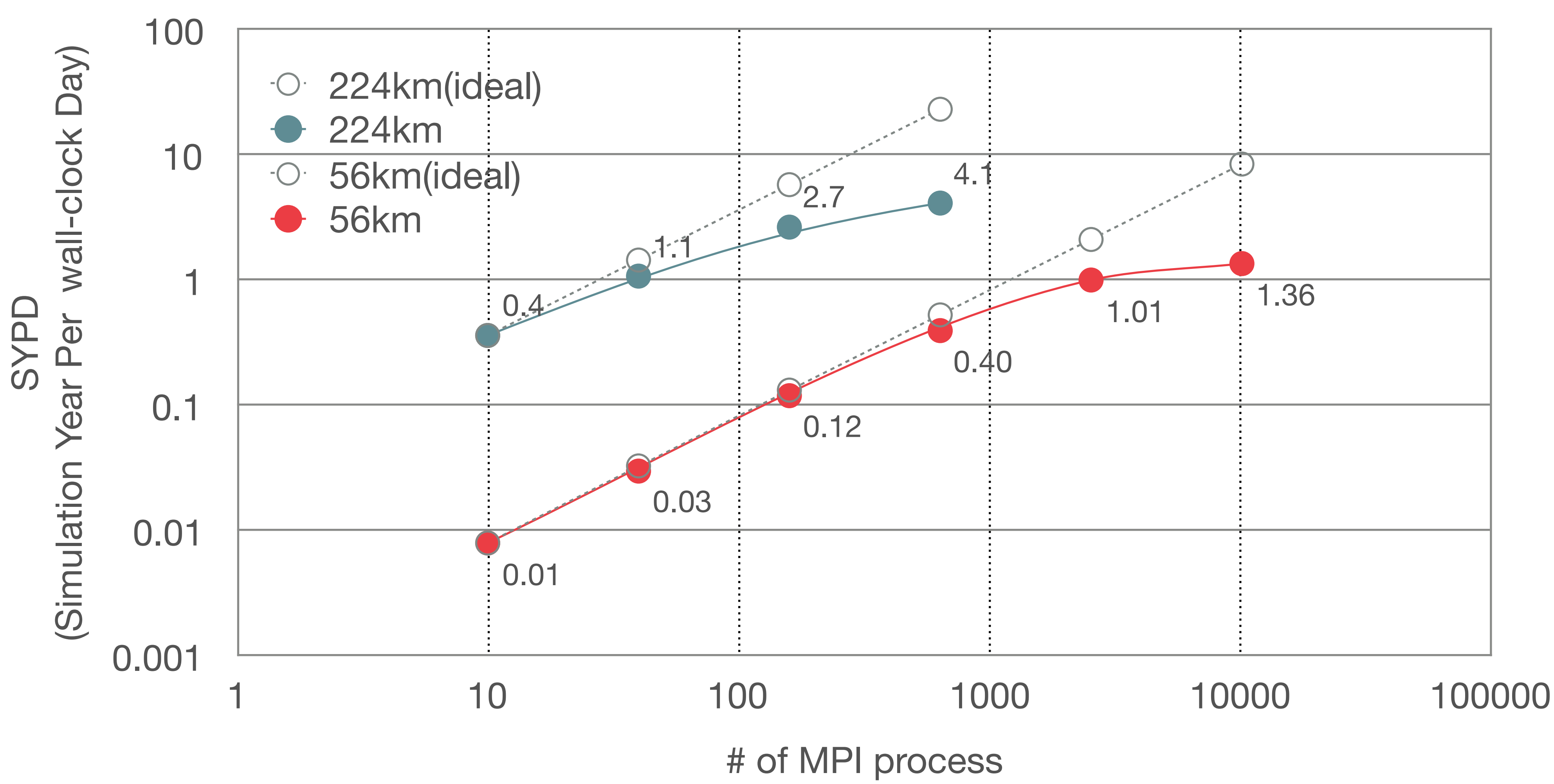
Optimization on Oakforest-PACS

- This was the first time that we inserted OpenMP directives in the NICAM code
- Fine-grained thread parallelization → **worse** thread scalability
  :The cost of fork/join is large on the KNL
- The flat-MPI execution shows fairly good performance
  - The Omni-Path is good at handling many small p2p communications?
  - I/O did not become critical issue

NICAM on KNL cluster

Weak scaling w/ low resolution run on Oakforest-PACS

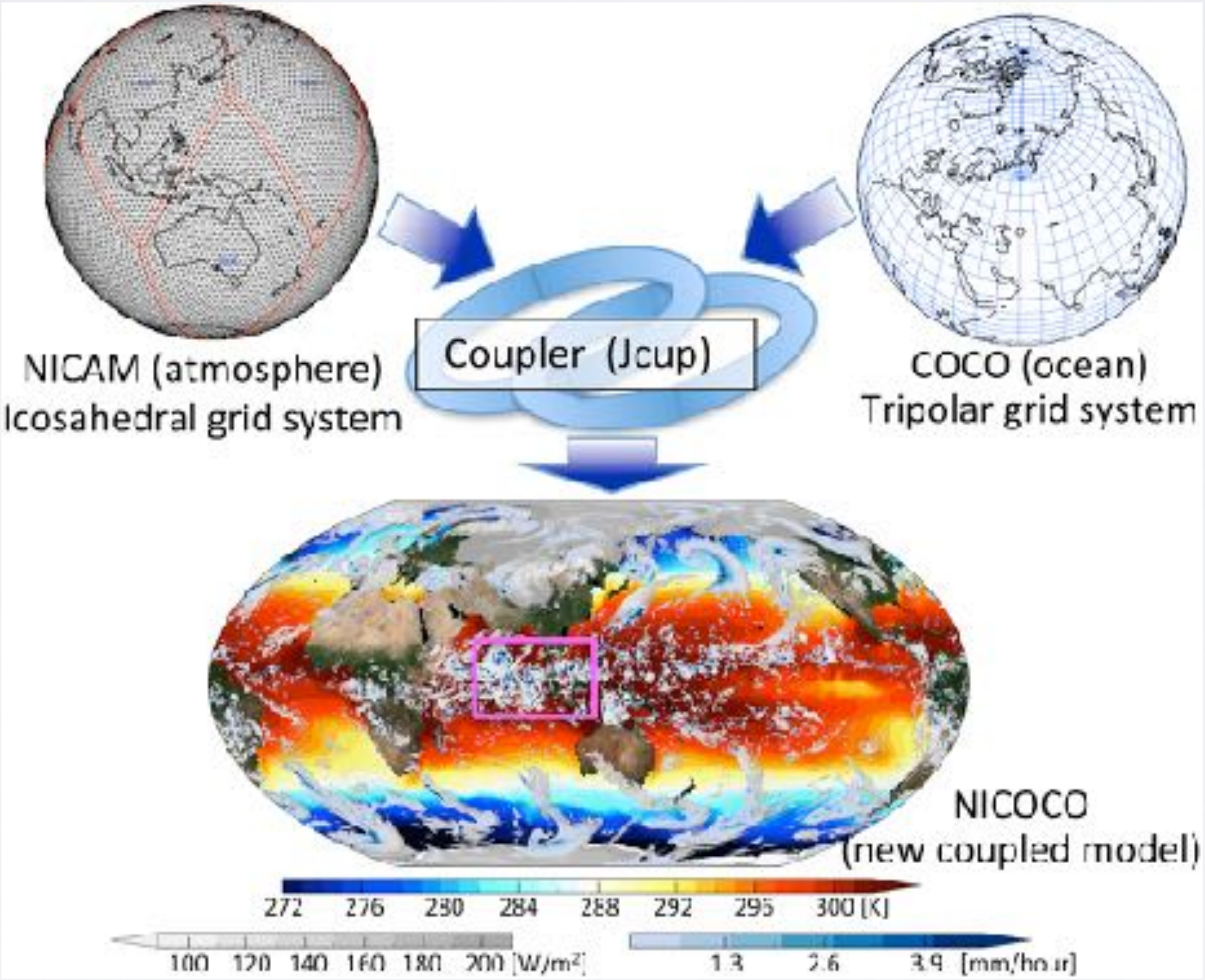
- Result shows good scalability when the grid point size per process is enough
- More process → less grid per proc. → lack of parallelism



NICAM on KNL cluster

Atmosphere-Ocean coupling studies on Oakforest-PACS

- A whole-year simulation with 14km atmosphere (NICAM) + 0.1deg ocean (COCO)
- Atmosphere: 0.3 billion grid points, 0.8 million steps, 10240 MPI processes
- Ocean: 0.6 billion grid points, 0.2 million steps, 1600 MPI processes



Picture from Miyakawa et al., 2017, GRL

Efforts toward the exascale computing era

From "K" to "post K"

Post K is…

- Next Japanese flagship supercomputer
- Manycore architecture
  - ARM v8 + Scalable Vector Extension
  - No accelerators
- 6-D mesh/torus network

- Designed for general purpose
  - The proxy applications are selected from nine priority research fields
  - ➡ System-Application co-design

Co-design in post-K project

Estimation of computational performance

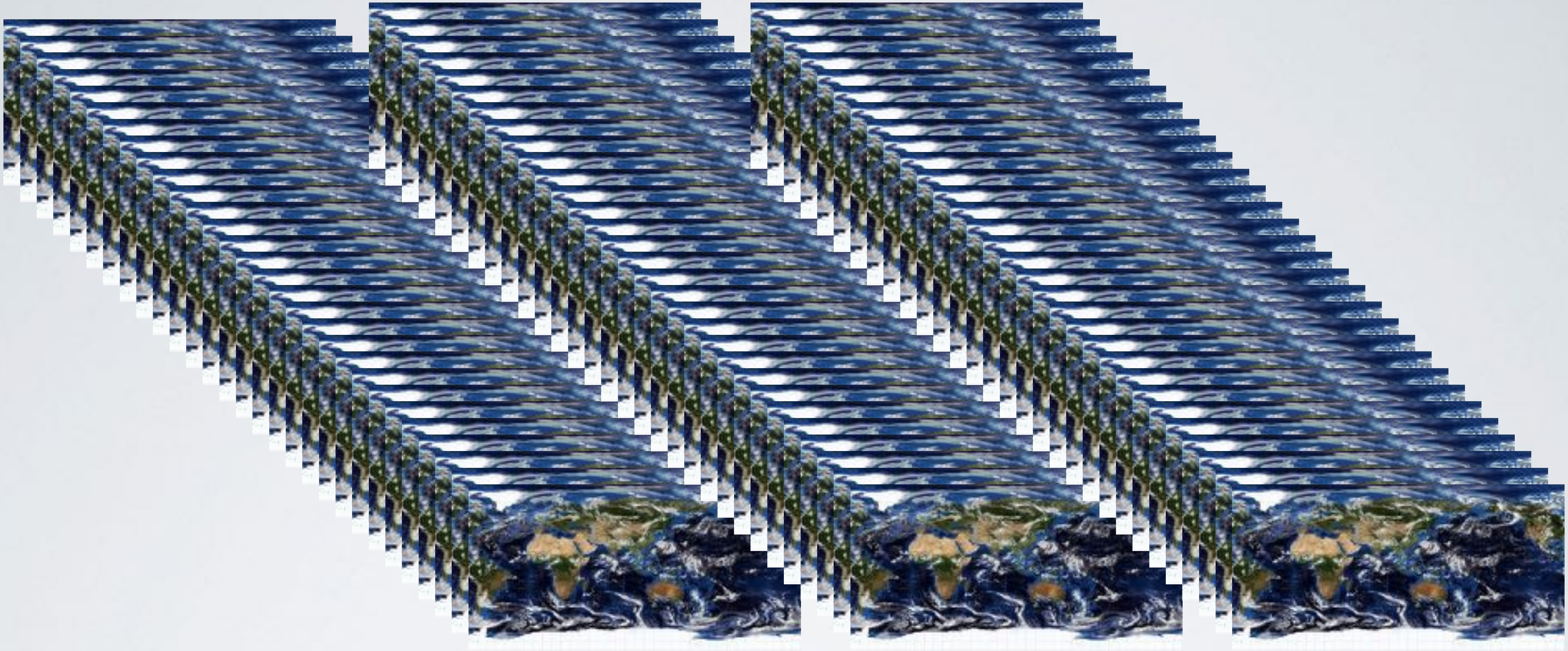
- ~10 kernels are extracted from dycore & physics
- Estimation using a performance profiler of FX100 and parameter of post-K
- Evaluation using post-K software simulator

- Basic design phase (~2015): Contribute to the decision of machine parameter
- Detailed design phase (2015~): Contribute to the compiler development

Change of application side

- All of things beyond the subroutine-level optimization
  : refactoring, data layout, algorithm, framework, etc.
- Optimization with the risk of deterioration of simulation results: precision

Grand challenge on the post-K computer



- 3.5km-mesh, 100 layers x 1000 members
  - It takes **2 weeks** for 1 DA cycle using full node of the K computer
  - **3 PByte** of the data will be exchanged between NICAM and LETKF for 1 DA cycle
- 1 million observation including satellite data

New design of the DA system

Data centric design

Problem:
Huge amount of data exchange/transpose occurs between the weather model and the ensemble DA system

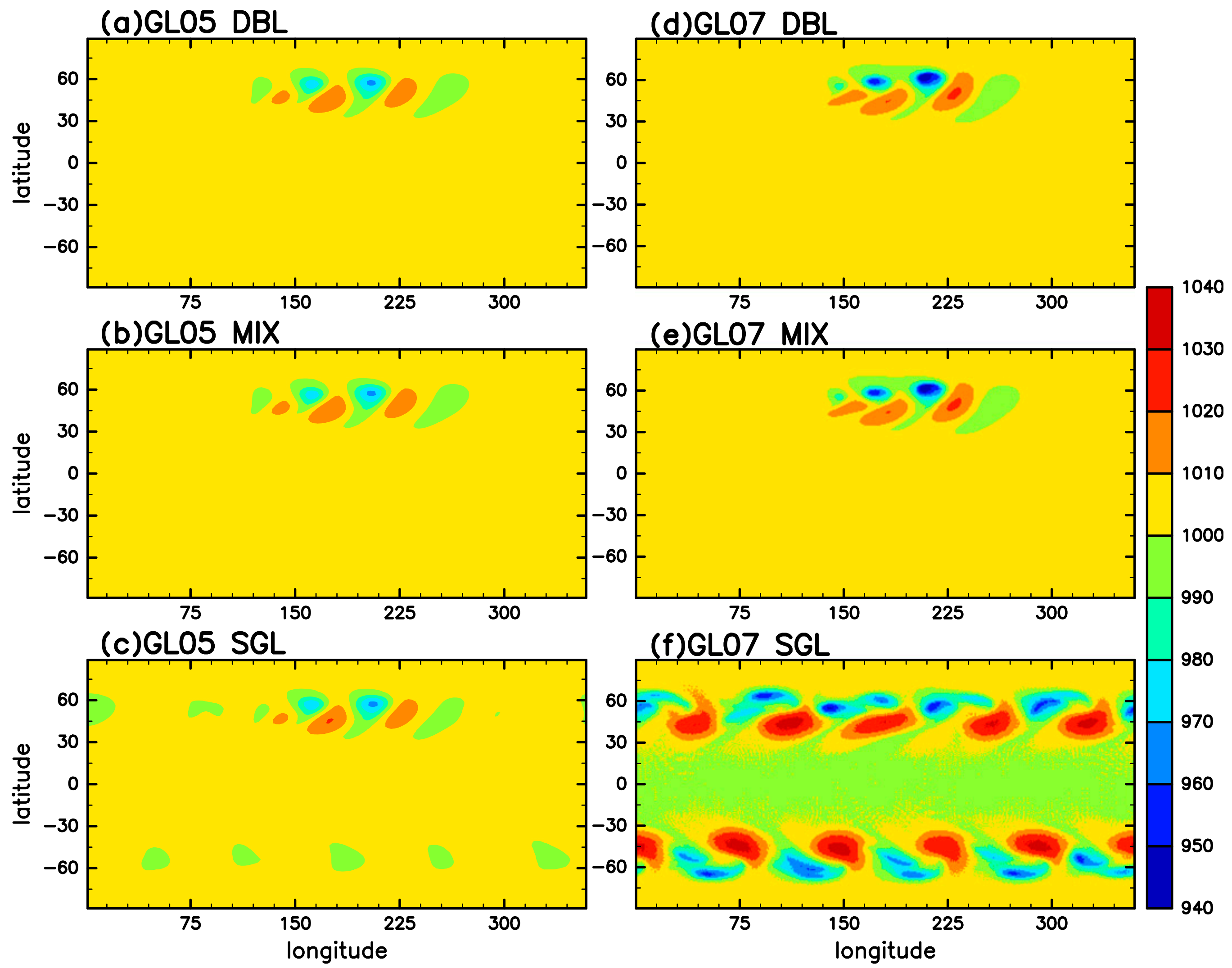
"Throughput-aware" design of the DA system
(Yashiro et al., 2016, GMD)

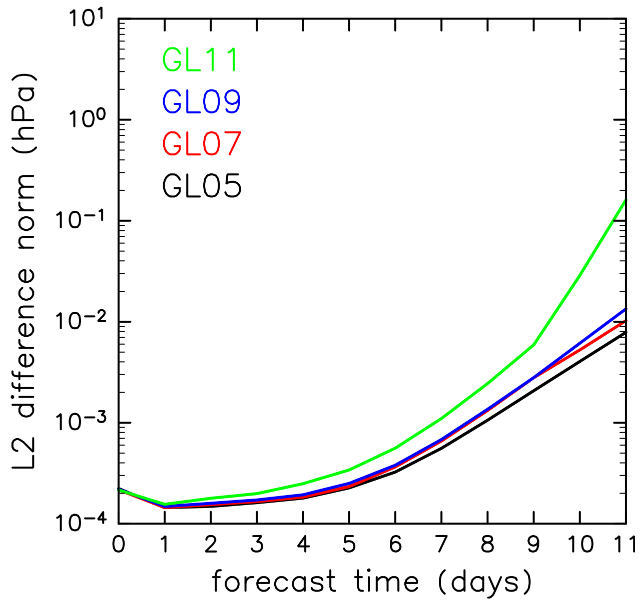
- reduce data movement
- use local storage
- avoid global communication

Evaluation of mixed precision

We had better utilize the single/half precision more

- More evaluation of physical performance is necessary
  : Ideal/real case, deterministic/statistic case, unit/total tests, etc.

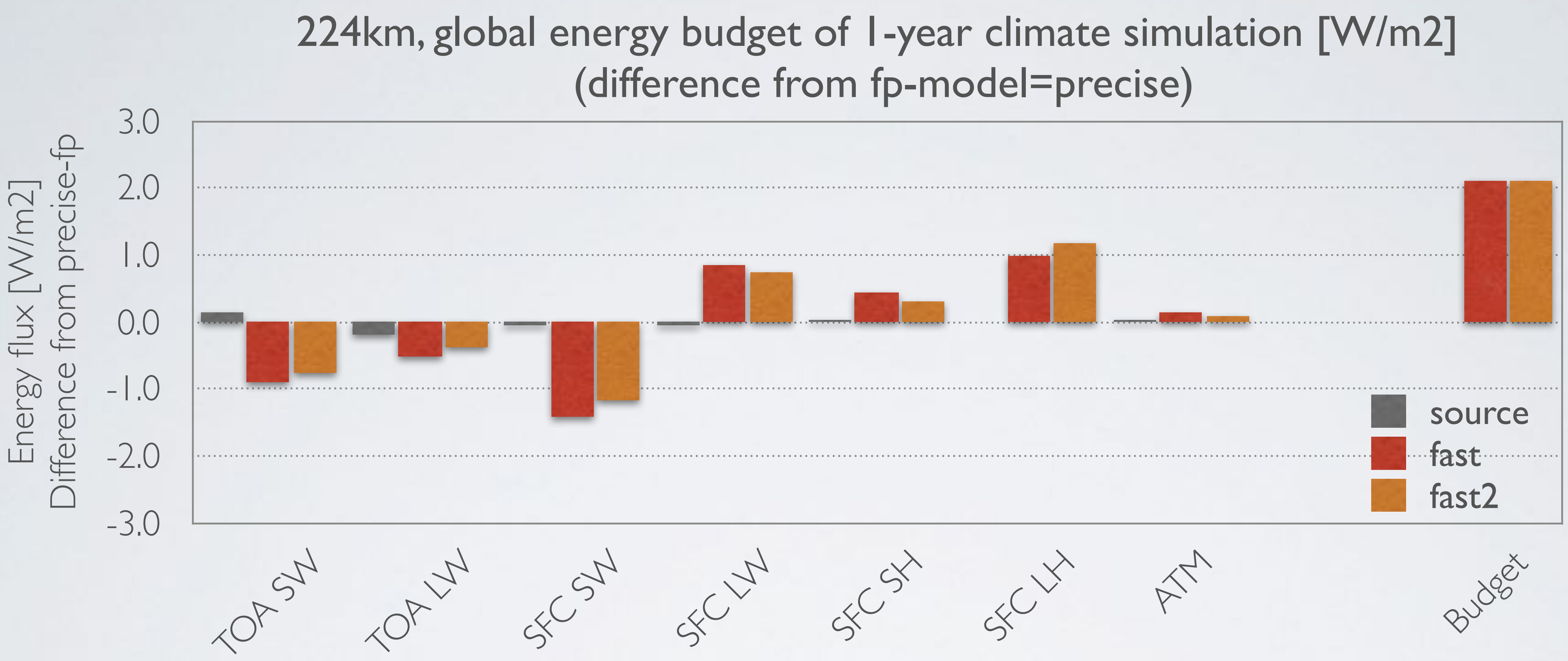




Baloclinic wave test with single precision
(Nakano et al., 2018, MWR)

Approximate Computing

Scientific performance evaluation is important

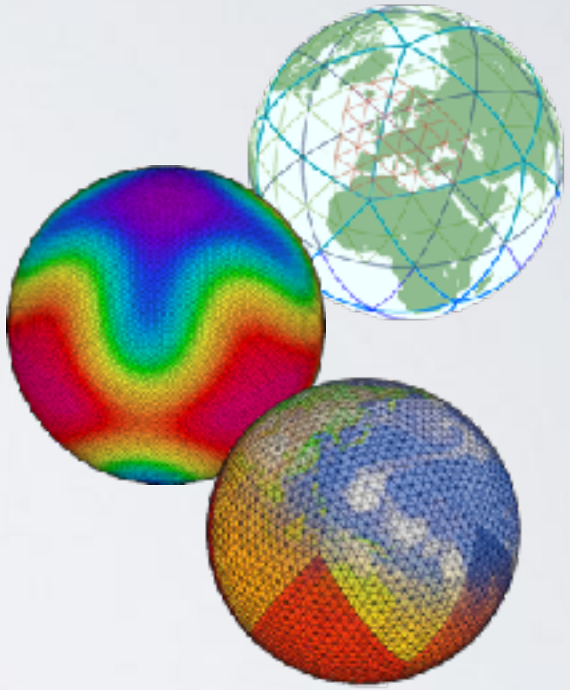


- For intel Fortran compiler, fp-model=fast2 is x1.6 faster than precise mode
- However, the budget imbalance occurs in the cases of fp-model=fast/fast2
  - We know there are few lines to keep precision in radiation scheme

SPPEXA/AIMES project (1)

AIMES **(Advanced Computation and I/O Methods for Earth-System Simulations)**

- Tri-lateral collaborative project funding
- Collaboration of icosahedral atmosphere model
  - U. Humburg, DWD, DKRZ (German) : ICON
  - IPSL (France) : DYNAMICO
  - RIKEN, Tokyo Tech., U. Tokyo (Japan) : NICAM



Targets

- DSL benefit for icosahedral atmospheric models
- Massive I/O
- Kernel suites and mini-apps from three state-of-art climate models

SPPEXA/AIMES project (2): Benchmarking

IcoAtmosBenchmark

- https://aimes-project.github.io/IcoAtmosBenchmark_v1/
- Ver.1: A kernel package from icosahedral models
  - For the performance evaluation of stencil calculation
  - For the development of domain specific languages (DSLs)

SPPEXA/AIMES project (3): I/O

Approximate Computing

Data centric design

SCIL: Scientific Compression Interface Library

- User can control precision of output data for each model variable
- Library selects compression algorithm (lossy/lossless)
- HDF5/NetCDF4 integration

Integration into NICAM

- History output: evaluation of compression efficiency is ongoing
- Checkpoint input/output: planned

Performance Portability

GridTools-NICAM(1)

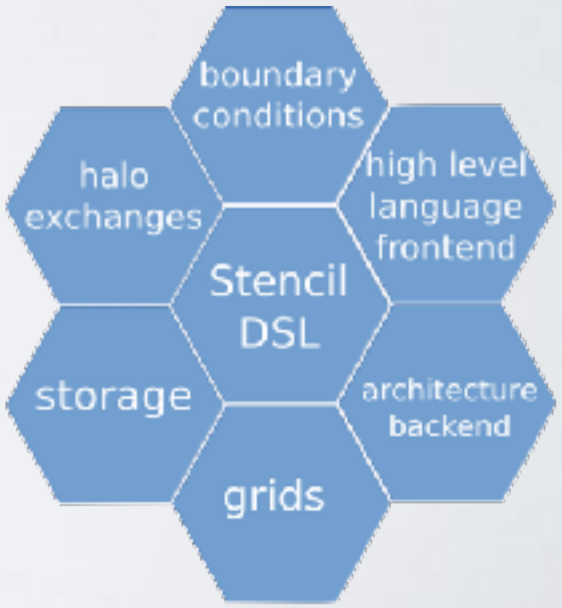
Can we become released from the curse of directives?

- Maintenance of directives is costful

```
!OCL XFILL
!$acc kernels pcopy(PROGq00) pcopyin(PROGq) async(0)
!$omp parallel do default(none),private(g,k,l,nq), &
!$omp shared(gall,kall,lall,nall,PROGq00,PROGq), &
!$omp collapse(3)
do nq = 1, nall
do l  = 1, lall
do k  = 1, kall
do g  = 1, gall
   PROGq00(g,k,l,nq) = PROGq(g,k,l,nq)
enddo
enddo
enddo
enddo
!$omp end parallel do
!$acc end kernels
```

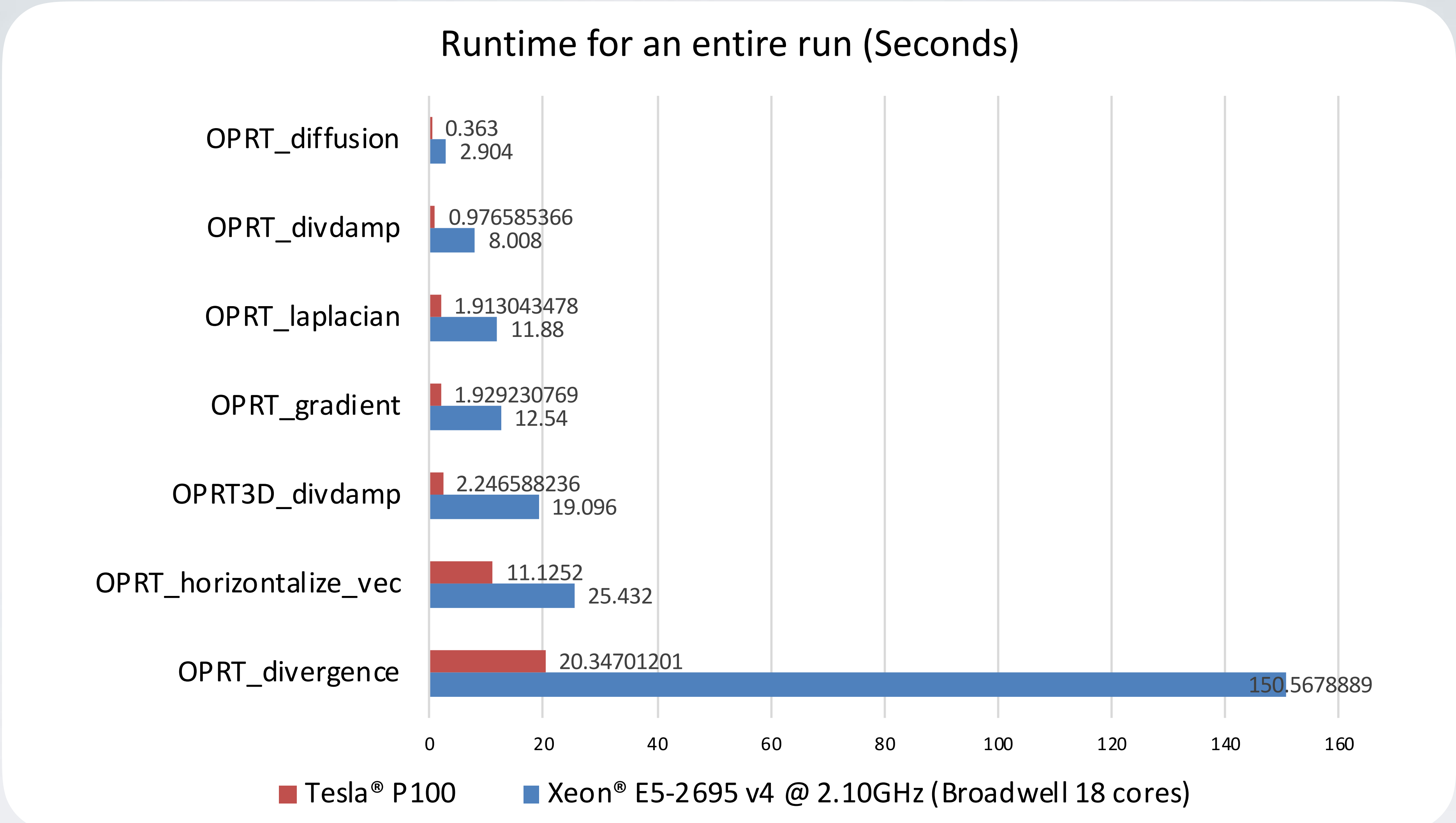
GridTools-NICAM project

- Collaboration started in the AIMES project
- NICAM is favorable for GridTools
  - Structured grid in tile: cartsian-like data layout



GridTools-NICAM(2)

Performance Portability



The way to full implementation with GridTools

- The full-dycore is almost finished: very good results on GPU
- Communication part is more difficult: node topology is complex
- Physics library? : exploring solutions using Python

Summary

- **In the petascale era, the efforts on the performance have meant the utilization of more cores and accelerators**
  - Labor intensive works were effective: code refactoring and directives

- **In the exascale era, the efforts will mean how the application developers accept trade-offs.**
  - ~~Sub-grid parameterization vs super high resolution~~
  - The floating-point precision vs simulation result
  - DSL affects everything of the ecosystem of weather/climate studies: from education to operation.
    - Can we change the mind of community people?

"Rebuild myself while running at full speed"