

# WGNE – HPC/Exascale update

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European Centre for Medium Range Weather Forecasts (ECMWF)

Many thanks for the individual contributions!



# Contents

1. Overview of trends in HPC / weather & climate preparation for Exascale
2. GPU adaptation, single precision, cloud use & I/O / workflow acceleration
3. Maintainability / Performance portability
4. Annex: provided slides from members & other groups

# Trends from 20th ECMWF workshop on high performance computing in meteorology

<https://events.ecmwf.int/event/329/>



# A Changing High-P...

## Bloomberg

Subscribe

Technology | AI

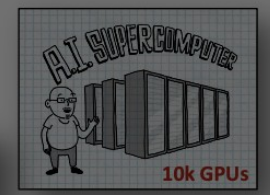
### ChatGPT to Fuel \$1.3 Trillion AI Market by 2032, New Report Says

- Bloomberg Intelligence expects generative AI market to soar
- Amazon, Microsoft, Google and Nvidia seen as biggest winners



By [Jake Rudnitsky](#)  
 June 1, 2023 at 3:00 PM GMT+2  
 Updated on June 1, 2023 at 5:50 PM GMT+2

Microsoft invests \$1 billion in OpenAI to pursue holy grail of artificial intelligence  
Building artificial general intelligence is OpenAI's ambitious goal



Chat GTP-4 Could Pass the Bar Exam  
 How Our Technology Evolves FAST  
 Source: <https://medium.com/>

AI chatbot's MBA ex business schools  
 ChatGPT earned a solid grade and out...



A robot may \_\_ injure a

0.74	not	1.00
0.28	sometimes	0.00
0.07	always	0.00

## Deep Learning Drives Future Computing Architectures!

layer-wise weight update

**Small datatypes**  
 (int + fp – 4, 8, 16 bits)  
 Example: fp8 is 33x faster than fp64

**Matrix and vector ops**  
 (tensor cores and vector units)  
 Example: NVIDIA TCs: 8.3x over CUDA cores

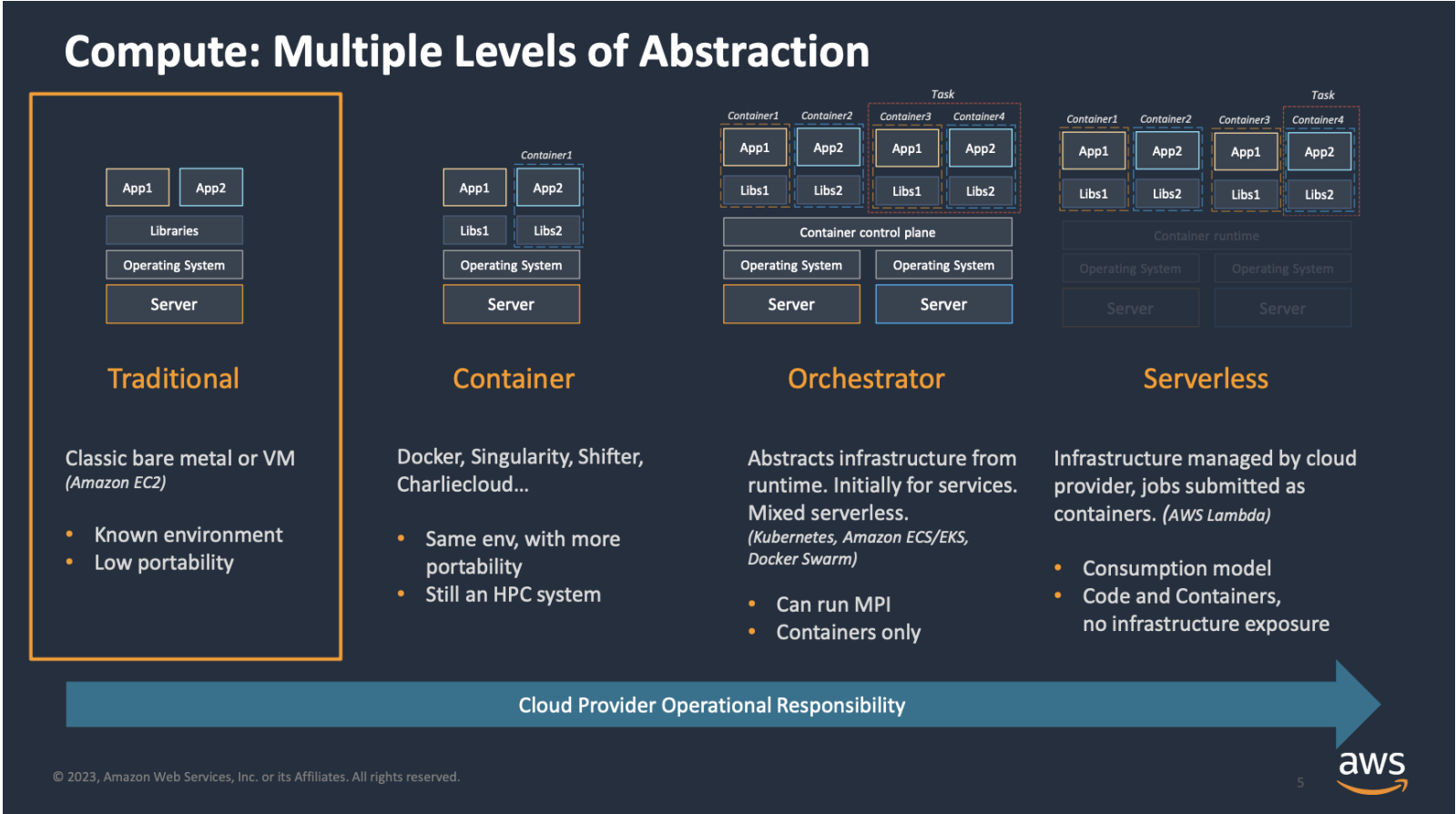
**(Structured) Sparsity**  
 (in tensor cores and vector units)  
 Example: NVIDIA TCs: 2:4 sparsity

Ben-Nun, TH: Demystifying parallel and distributed deep learning: An in-depth concurrency analysis, ACM Computing Surveys (CSUR), 2019



# Cloud provides ...

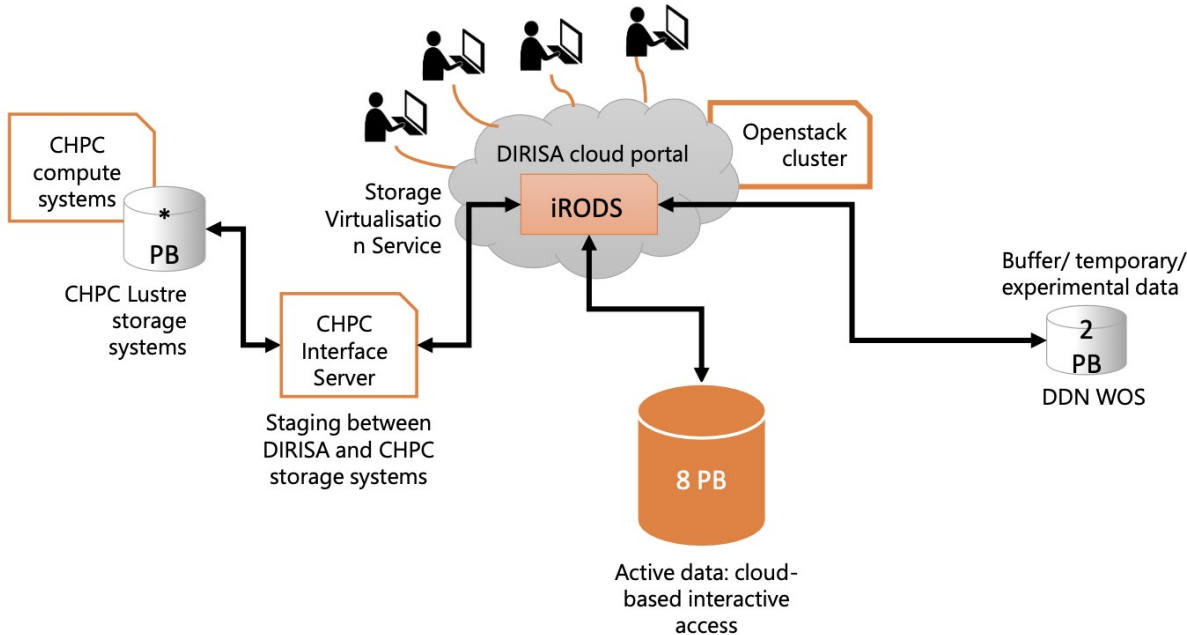
## AWS abstraction levels



# South Africa example on cloud-based system

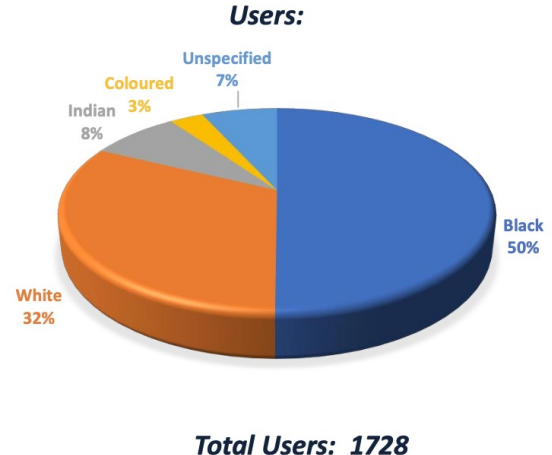
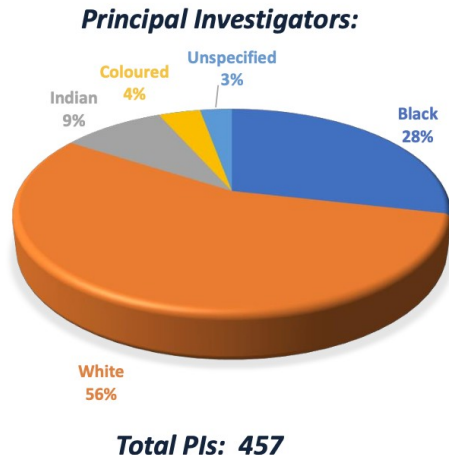
Leveraging diversity to push the boundaries of computing  
*Mthetho Vuyo Sovara*

## DIRISA Data Storage Architecture



## Demographics: Principal Investigators and Users

Past 6 Years **2016/17 – 2021/22**



Substantial increase & reaching wider range of users

# Accelerate Workflows

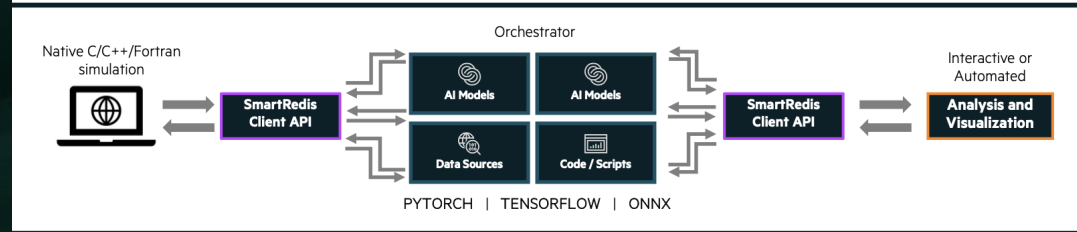
## ABOUT SMARTSIM

The SmartSim open-source library bridges the divide between traditional numerical simulation and data science

**SmartSim** enables simulations to be used as engines within a system, producing data, consumed by other services to create **new applications**

- Use Machine Learning (ML) models in existing Fortran/C/C++ simulations
- Communicate data between C, C++, Fortran, and Python applications
- Train ML models and make predictions using TensorFlow, PyTorch, and ONNX
- Analyze data streamed from HPC applications while they are running

All of these can be done without touching the filesystem, i.e., **data-in-motion**



CRAYLABS@HPE.COM | 21

## Post-Exascale Vision

### Leadership Class HPC

Productivity and agility for HPC and AI applications

Today

### Exascale Supercomputer

### Multi-dimensional, complex workflows

modeling, simulation, data analytics, and artificial intelligence

### Federated Diverse Systems

Integrate, automate, and optimize workflows that span multiple locations, organizations, and vendors

World's fastest Supercomputer

World's fastest Workflows

HPE Confidential | 27

Carpenter et al



# Different institutes – similar problems

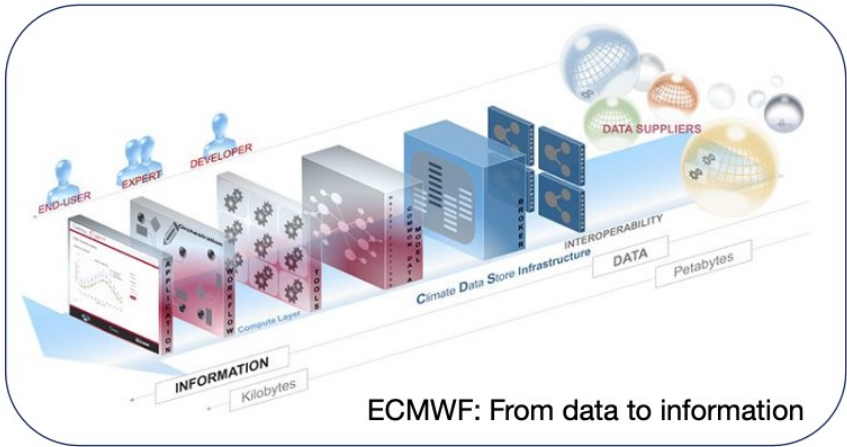
Modernization of modeling software

Co-design between scientists and computer scientists

Data Science, new workflows, AI/ML, data management

Investment in software engineering, scientific design

Adapted from UK Met Office & EPSRC: Harnessing Exascale Computing



### DOE E3SM

E3SM Workbench – Encapsulates Infrastructure

**Process Flow**

**Analysis and Visualization**

**Diagnostics**

**Provenance**

ProvEn  
Provenance Capture

**Data Management**

E3SM Input data, Maps, Obs  
SVN

### DOE Exascale project

**ECP 51 SDKs span all technology areas**

Technology Area	SDK Name	Lead	Co-Lead	Co-Lead	Co-Lead	Co-Lead	Co-Lead	Co-Lead	Co-Lead
AI/ML	AI/ML	...	...	...	...	...	...	...	...
Cloud	Cloud	...	...	...	...	...	...	...	...
Containers	Containers	...	...	...	...	...	...	...	...
DB	DB	...	...	...	...	...	...	...	...
DevOps	DevOps	...	...	...	...	...	...	...	...
File Systems	File Systems	...	...	...	...	...	...	...	...
Frameworks	Frameworks	...	...	...	...	...	...	...	...
IO	IO	...	...	...	...	...	...	...	...
Networking	Networking	...	...	...	...	...	...	...	...
OS	OS	...	...	...	...	...	...	...	...
Parallel Computing	Parallel Computing	...	...	...	...	...	...	...	...
Performance	Performance	...	...	...	...	...	...	...	...
Programming	Programming	...	...	...	...	...	...	...	...
Security	Security	...	...	...	...	...	...	...	...
Storage	Storage	...	...	...	...	...	...	...	...
System	System	...	...	...	...	...	...	...	...
Tools	Tools	...	...	...	...	...	...	...	...
Web	Web	...	...	...	...	...	...	...	...
Workflows	Workflows	...	...	...	...	...	...	...	...

Many opportunities for cross-agency and international partnership on tools and methods

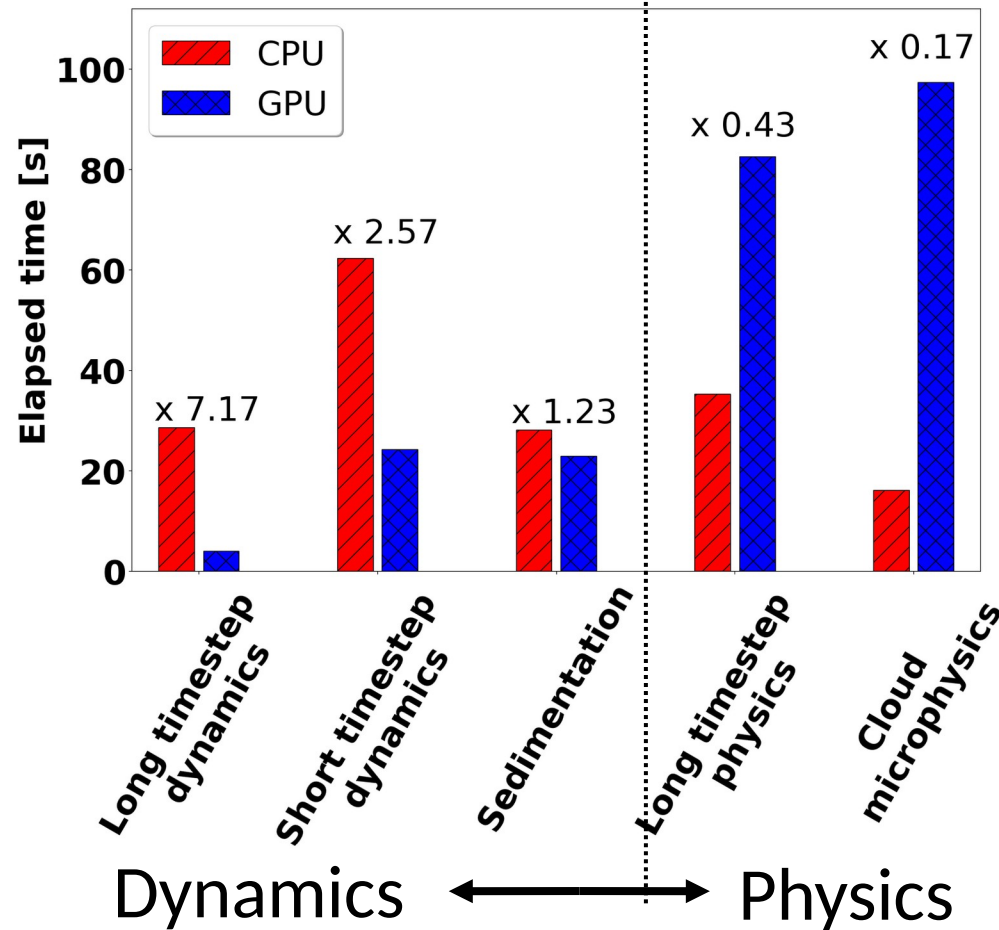
Hauser et al

# Results of GPU porting

CPU: Intel Xeon Gold 6226 2.7GHz 12C/24T x2 with DDR4 memory (140GB/s)

GPU: NVIDIA Tesla V100-PCIe-32GB x1 with HBM2 memory (900GB/s)

(nx,ny,nz) = (150,150,76) ~ grid size / node in the operational configuration



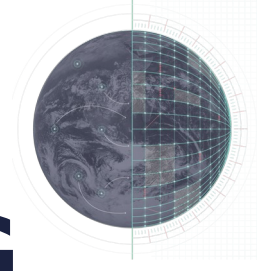
## Dynamical process

- ✓ **High** acceleration rate
- ✓ **A few** workloads
- ✓ Issues : Optimizing MPI communications

## Physical process

- ✓ **Low** acceleration rate
- ✓ **A lot of** workloads
  - Modifying a lot of work arrays to arguments
- ✓ Issues : Hard to vectorize innermost loop, Saving GPU memory





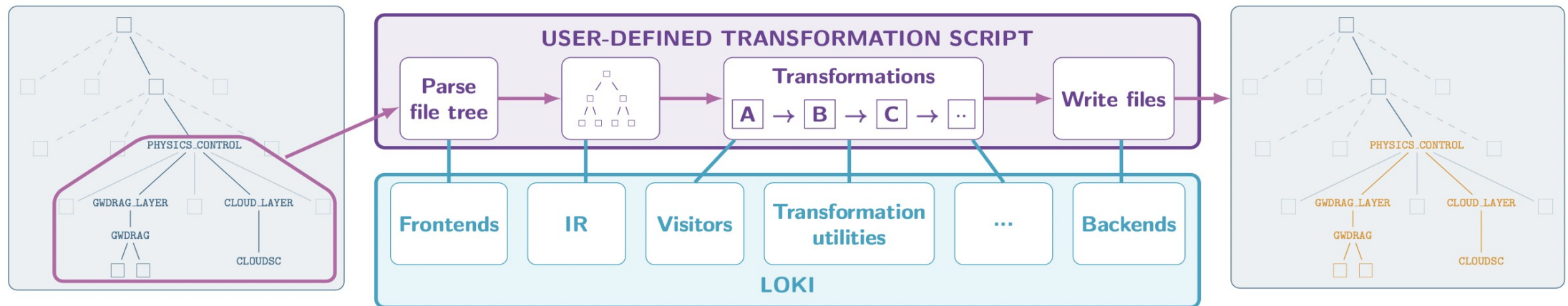
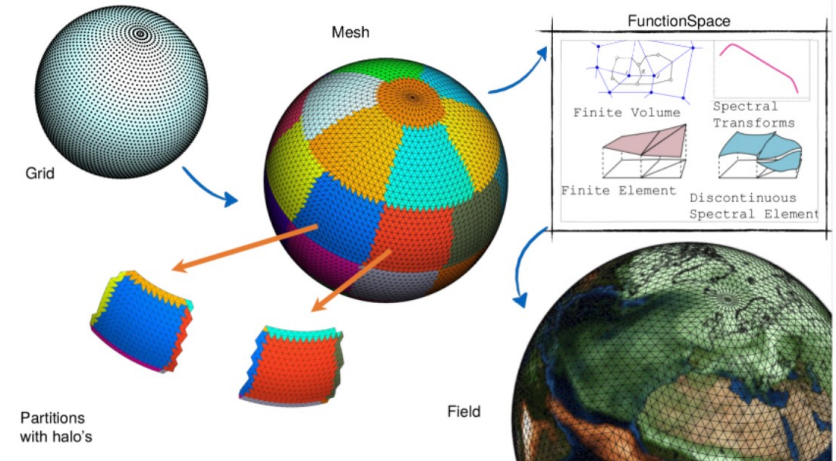
# HIGH PERFORMANCE COMPUTING

## Atlas - A library for NWP and climate modelling

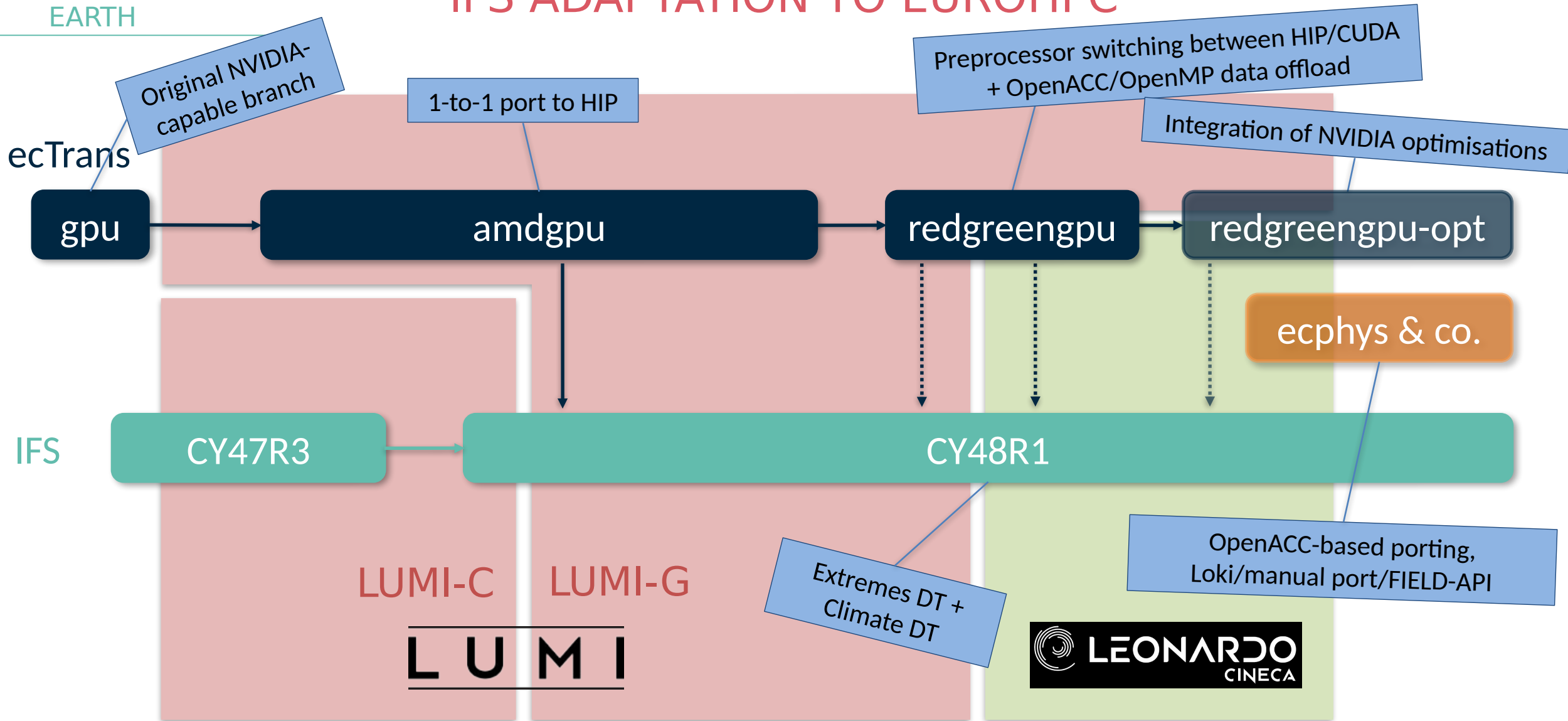
- Modern C++ library with Fortran interfaces
- Data structures for numerical algorithms:
  - Increasing accelerator-awareness

## Loki - Programmable source-to-source translation package written in Python

- Library of tools and APIs to build custom transformation recipes
- Built on basic principles of compiler technology (IR trees, visitors, transformers)



# IFS ADAPTATION TO EUROHPC





# HPC efforts at Météo-France



## *Towards a general use of single-precision (32 bits) in operational NWP systems.*

1. Operational use in all AROME<sup>1</sup> operational systems (forecast component only)
2. Next steps: operational use, whenever possible,
  - i. in all ARPEGE forecasts
  - ii. in all trajectories within the assimilation cycle
  - iii. parts of assimilation

## *Adaptation to hybrid processors with accelerators:*

3. Significant code refactoring (e.g., new memory structure)
4. Development of automatic source-to-source code transformation tools (Loki, Fxtran)
5. ARPEGE forecast with physics (except radiation) running on GPU-Nvidia  
>> next steps: semi-implicit, semi-lagrangian and radiation schemes
6. Work done in collaboration with ECMWF and ACCORD<sup>2</sup> partners
7. Hectometric LAM configuration developed within DestinE On Demand project (phase 1)
8. TRACCS<sup>3</sup>: 8-year (2023-2030) French national project for advancing climate modelling for climate services.
  - 1 WP devoted to new computing paradigms (portability, efficiency, composability, trainable)

<sup>1</sup> Météo-France LAM NWP operational system

<sup>2</sup> A Consortium for convective-scale modelling Research and Development

<sup>3</sup> Transformative Advances of Climate Modelling for Climate Services

# Met Office Physics Schemes

1. Radiation - Socrates (done - ORNL)
2. Micro Physics – Casim (done - ORNL)
3. UKCA – Excalibur
4. Land Surface – Jules (Excalibur?)
5. Aerosols - RADAER
6. Boundary Layer – slow and fast
7. Convection – CoMorph
8. Stochastic physics
9. Cloud Physics
10. Spectral Gravity Wave Drag (GWD)
11. Orographic GWD

```
!$acc parallel loop collapse(2)
do j = js, je
  do i = is, ie
    ...
    !$acc loop seq
    do n = 1, nsubsteps
      do k = 1, nz
        ....
      end do
    end do
  end do
  ...
end do
end do
```

Change  
loop order  
to increase  
parallelism

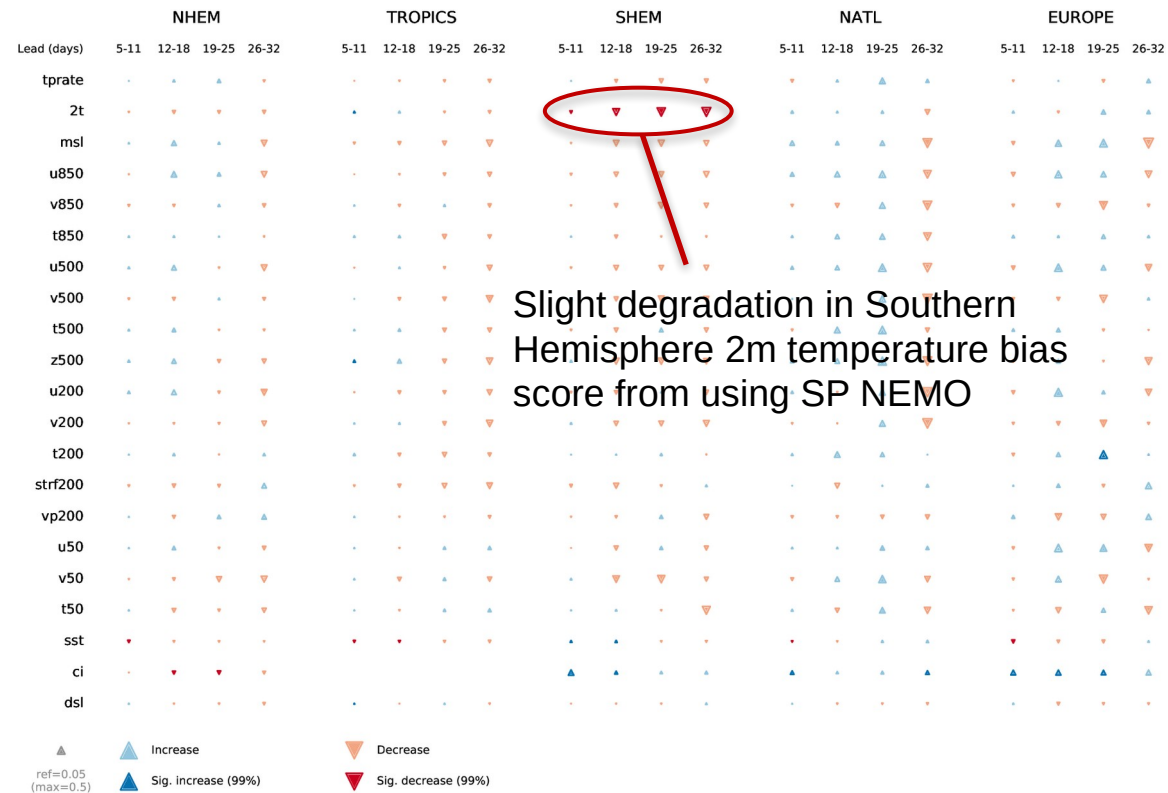
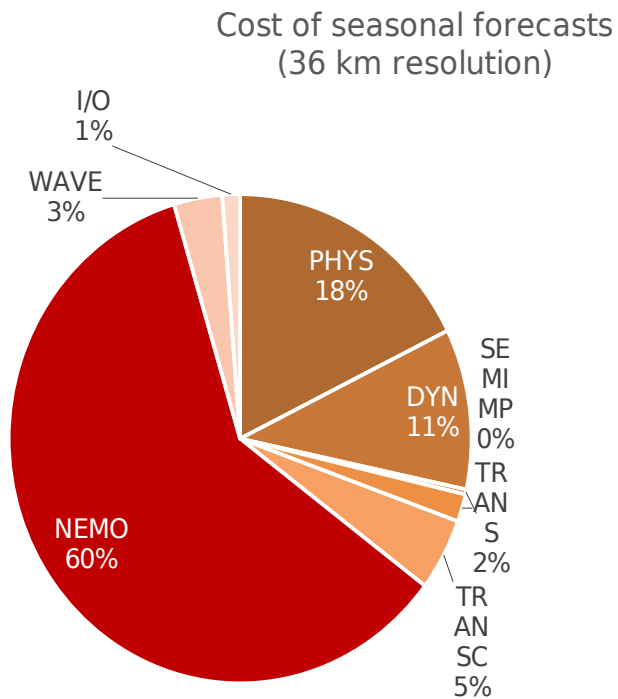
W. Zhang

Keep single  
source code  
but don't  
back port to  
UM

```
do n = 1, nsubsteps
!$acc parallel loop
collapse(2)
  do j = js, je
    do i = is, ie
      !$acc loop vector
      do k = 1, nz
        ....
      end do
    end do
  end do
end do
end do
```

# Single precision in the ocean

- For seasonal runs the ocean is over half the cost – could we use single precision there too?
- Coupled tests show minimal differences up to seasonal lead times
- However, some small but detectable effects on ocean mean state from single precision



# Single precision in SOM advection

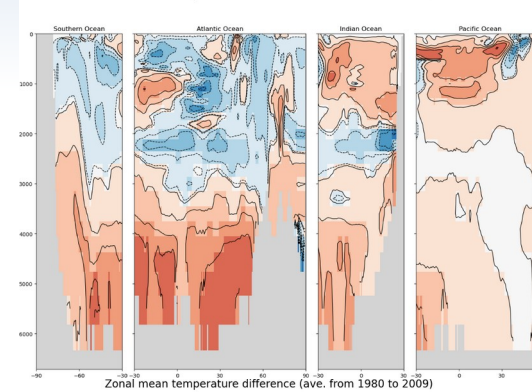
- SOM (Second Order Moment) advection (Prather, 1986) for tracers
  - High accuracy, but one of the bottlenecks in MRI.COM (~30% of total costs)
  - A scalar variable with a grid cell ( :grid size) is expressed as second-order orthogonal polynomials, then the moments are advected.

$$\phi(x) = m_0 + m_1 K_x + m_2 K_{xx}$$

$$K_x = x - \frac{X}{2}, \quad K_{xx} = x^2 - xX + \frac{X^2}{6}$$

- Less risks of “loss of digits” than finite difference methods
- Several variables need to be kept as double precision to obtain both speed up and accuracy.

Zonal mean temperature difference for the last 30-yr average of the 366-yr integration [K](single - double)



Full single in SOM

Single in SOM (but only mass and volume kept double)

Single in SOM (mass and volume: double)

Double

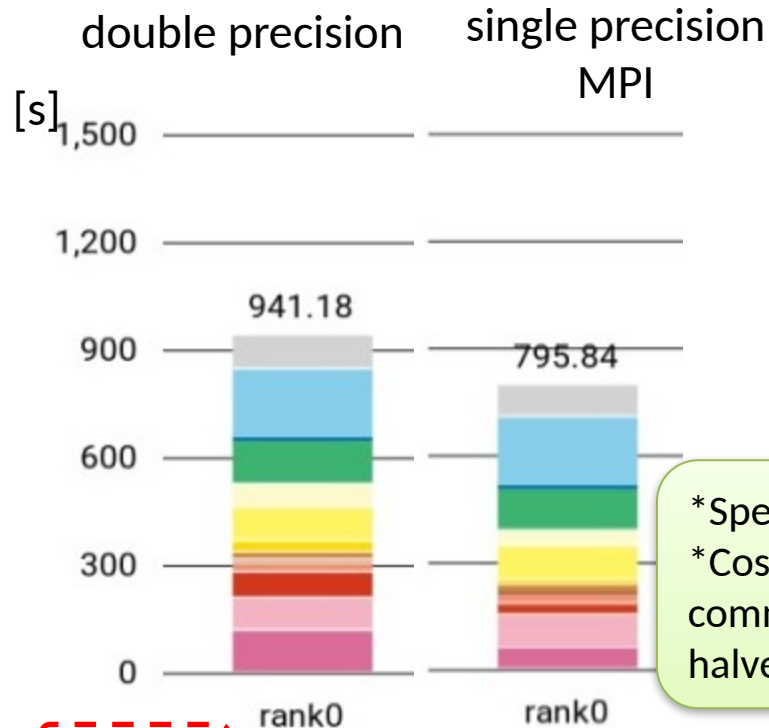
	ave[sec]
%	
TOTAL	1.30E+03
100.00	
TRACER	4.50E+02
34.67	

	ave[sec]
%	
TOTAL	1.12E+03
100.00	
TRACER	3.23E+02
28.76	

Speed up by 30% in the tracer schemes

# Impacts of single precision (only MPI) GSM

## Computational costs of Tq959L128 GSM



\*Speed up by 15%  
\*Costs for MPI comm. almost halved

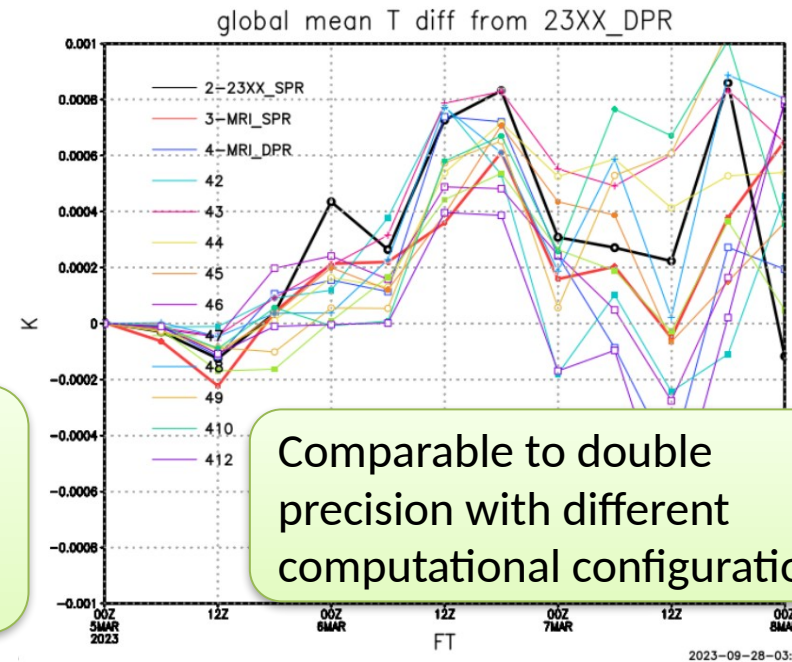
MPI comm.



## Global mean T at 500hPa diff.

Red and black : single precision MPI GSM

Others: double-precision GSM with different compilers / compile options / libraries (FFT, matrix)



Comparable to double precision with different computational configuration



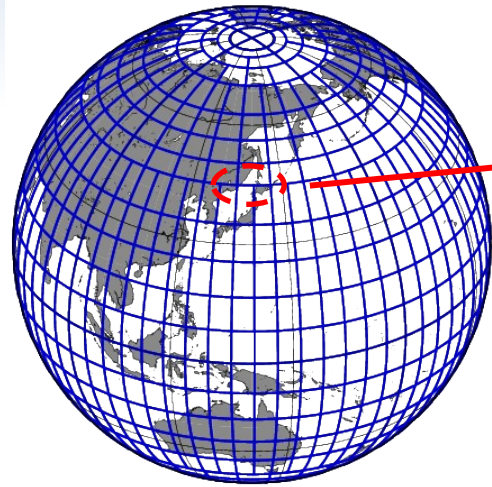
# Preparing for exascale computing at Hydrometcentre of Russia



- Since 2022, more single precision computations and memory access optimizations in many routines: current gain of ~18% for the global SLAV10 model (operational since 10/23,  $0.1^\circ$  lon,  $0.08-0.13^\circ$  lat, 104 lev) at Cray XC40. These works are ongoing
- Data handling: offline compression using **ncks** utility of output NetCDF files, with compression depending on variable

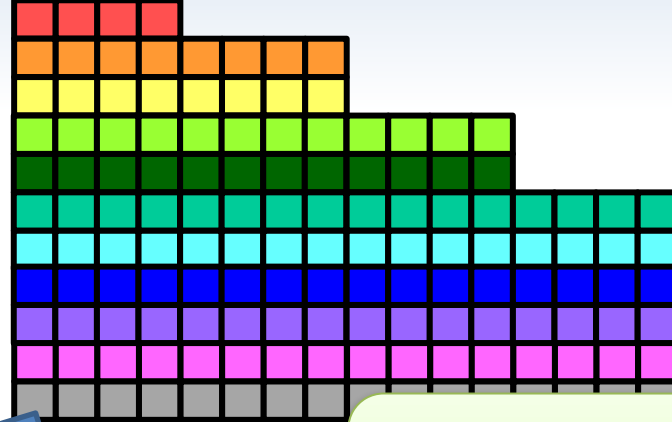


# Flexible (I, K, J) array structure for non-stencil calculation (e.g. physics, I/O etc) for both CPU and GPU



Lon. →  
 Lat. ↓

Horizontal grid boxes in a MPI process

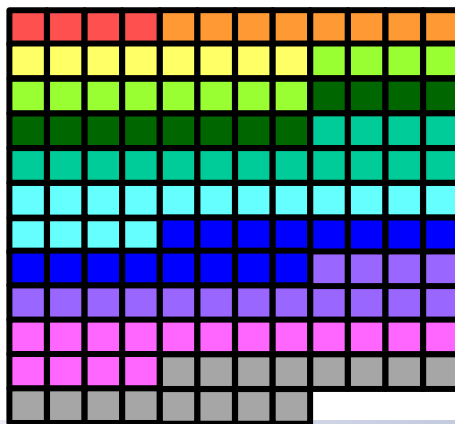


NUMI\_I=12

NUMI\_I=36

Max array size of array in the "i" direction is controlled by a parameter "NUMI\_I"

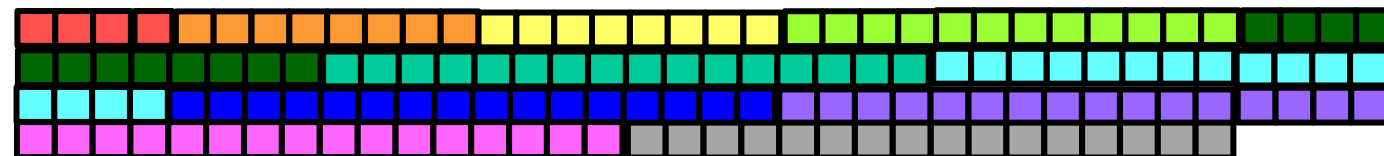
For CPU with OpenMP  
 (larger outermost loops  
 for thread parallelization)



i →  
 j ↓

For Vector machines or GPU with OpenACC:  
 (larger innermost loops for vectorization)

NUMI\_I





# CMC HPC/Exascale Projects: Science

- Planned upgrades to the existing modelling system:
  - SLIMEX : semi-Lagrangian Implicit-Explicit time integrator
    - Combine SL and IMEX BDF2 time integrator
    - Second order in time, no extra off-centering and only one elliptic solve per step
  - Single-core performance evaluation and optimization for the physics
- Development of new algorithms:
  - Moving from a Yin-Yang grid to a rotated cubed-sphere grid
  - A space-time tensor formalism is used to express the equations of motion covariantly
  - The spatial discretization with the direct flux reconstruction method
  - New multistep exponential and implicit/Rosenbrock time integrators
  - Low-synchronization matrix-free Krylov solver
- Building a network of academic collaborators for the development of a hybrid physical/AI NWP system
  - Establish a close working relationship with the universities and private sector – joint projects in the next 5 years.
  - Goal: explore the spectrum of possibilities in applying numerical methods and ML to develop an optimal hybrid NWP model that will use the best of the two worlds.
  - Develop approaches in high-performance computing – the best numerical algorithms on today's supercomputer could be suboptimal in the future – and work with GPUs.

# CMC HPC/Exascale Projects: Infrastructure

- Development of a new non-blocking IO server to solve increased IO bottleneck
- New more efficient MPMD multi-model coupling system
- Update to internal data format to enable parallel IO and multiple compression scheme allowing higher data compression
- Enable efficient check pointing on all model suites (standalone/coupled)

# NOAA Unified Forecast System

- **UFS components:** Atmos (fv3 dycore), Land (Noah-MP), Ocean (MOM6), Ice (CICE6), Wave (WAVEWATCH III), Aerosol (GOCART), Air Quality (CMAQ), CMEPS mediator, CCPP physics
- **UFS Applications:**
  - **Global:** GFS (medium-range NWP), GEFS (ensemble), SFS (seasonal), UFS-aerosol, [Whole Atmosphere Model \(WAM\) for Space Weather Prediction](#)
  - **Regional:** HAFS (hurricane), RRFs (regional NWP), Online-CMAQ (air quality), [Atmospheric River \(AR\)](#).

## Improvement for I/O and computational efficiency

- Parallel NetCDF with data compression applied to history files, [and expanded to hurricane moving nests](#)
- ESMF managed threading -- apply different threads for different UFS components
- Single and double precision dycore
- 32-bit physics (project just gets started)
- [Exchange grid capability](#)

## HPC upgrade

- **Old:** WCOSS, Dell, 73K x 2 cores, 4302 x2 TF peak performance
- **New as of June 2022:** WCOSS2, CRAY EX, 2560x2 nodes, 327Kx2 cores, 12,100 x2 TF peak performance.
- **New as of Aug 2023:** WCOSS2, CRAY EX, 3060x2 nodes, 392Kx2 cores, 14,400 x2 TF peak performance.

## On the Cloud

- [Running experimental hurricane ensemble forecast \(HAFS\) and regional high-res ensemble forecast \(RRFS\) on the Cloud.](#)
- [Plan to run global ensemble GEFS.v13 reanalysis and reforecast on the Cloud as well.](#)



# Azure HPC On-Demand Platform

Common platform for LFRic, Marine and UKCA based GPU 10 instances – 6 GPU each (NVIDIA V100 initially)

**Interactive Apps**

- Desktops
- Linux Desktop
- GUIs
- ParaView
- Servers
- Code Server
- Jupyter

**Code Server (193.scheduler)** 1 node | 1 core | Running

Host: [>\\_ndv2-1](#) Delete

Created at: 2023-10-23 10:42:28 UTC

Time Remaining: 51 minutes

Session ID: 9fac6835-75f6-4afb-9ac1-a86bb24d3c37

Connect to VS Code

EXPLORER | Get Started | hello\_world.f90

```

1 program hw
2   write(*,*) "Hello, World"
3 end program
4

```

TERMINAL

```

bash
HINT: Might try "module unload nvhpc-hpcx-cuda12/23.9" first.
[cmaynard@ndv2-1 ~]$ which nvfortran
/lustre/mdalvi/nvhpc/Linux_x86_64/23.9/compilers/bin/nvfortran
[cmaynard@ndv2-1 ~]$ nvfortran -o hw hello_world.f90 [cmaynard@ndv2-1 ~]$
[cmaynard@ndv2-1 ~]$ ./hw
Hello, World
[cmaynard@ndv2-1 ~]$

```

**pbs1**

Terminate    State **Started** at 9/29/23 5:06 PM (up 23d 18h 41m) - [View in Port](#)  
 Edit    Nodes **2** ready  
 Access    Users **1** admin ✔ | [Show](#)  
 Refresh    Scalesets **2** created  
 Size **2** instances, **48** cores (\$27.99 per hour)  
 Usage **31.8** core-hours (~\$2) in the last 24 hours  
 Alerts [Create new alert](#)  
 Issues No issues found

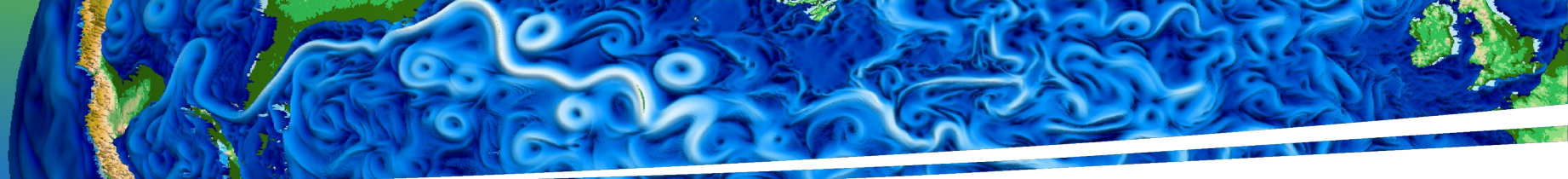
Nodes	Arrays	Activity	Scalesets	
View: Template <span style="float: right;">Search</span>				
Template	Nodes	Cores	Status	Last Status Message
ndv2	1	40		...
viz	1	8		...

View: Details Show Detail Edit Connect Actions

Show: Active ▾ Instances ▾ by MachineType ▾

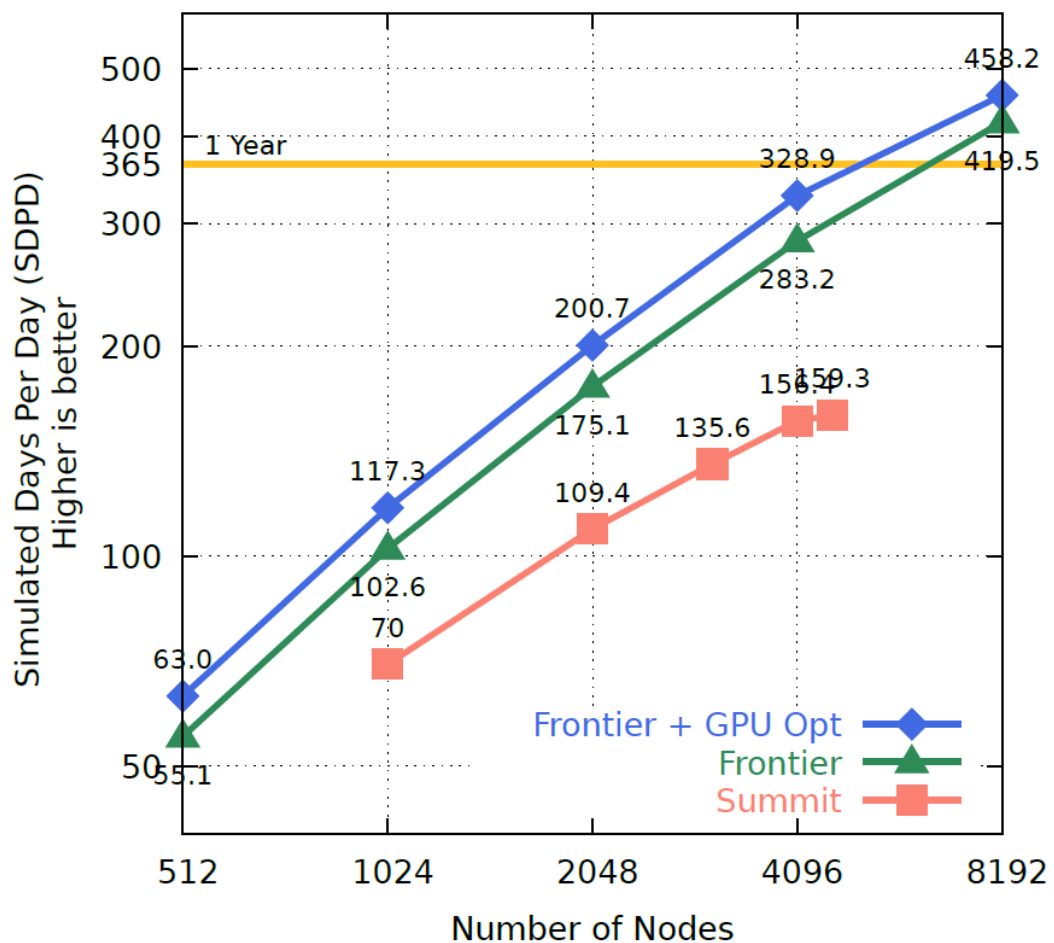
**Show Detail** Search

Time	Message
11:47 AM	Node ndv2-1 has started
11:43 AM	Added 1 Standard_ND40rs_v2 node ir
8:02 AM	Node viz-1 has started
8:00 AM	Added 1 Standard_D8s_v5 node for vi
10/20/23 6:26 PM	Terminated 1 node
10/20/23 3:47 PM	Terminated 1 node
10/20/23 3:04 PM	Node viz-2 has started
10/20/23 3:01 PM	Added 1 Standard_D8s_v5 node for vi



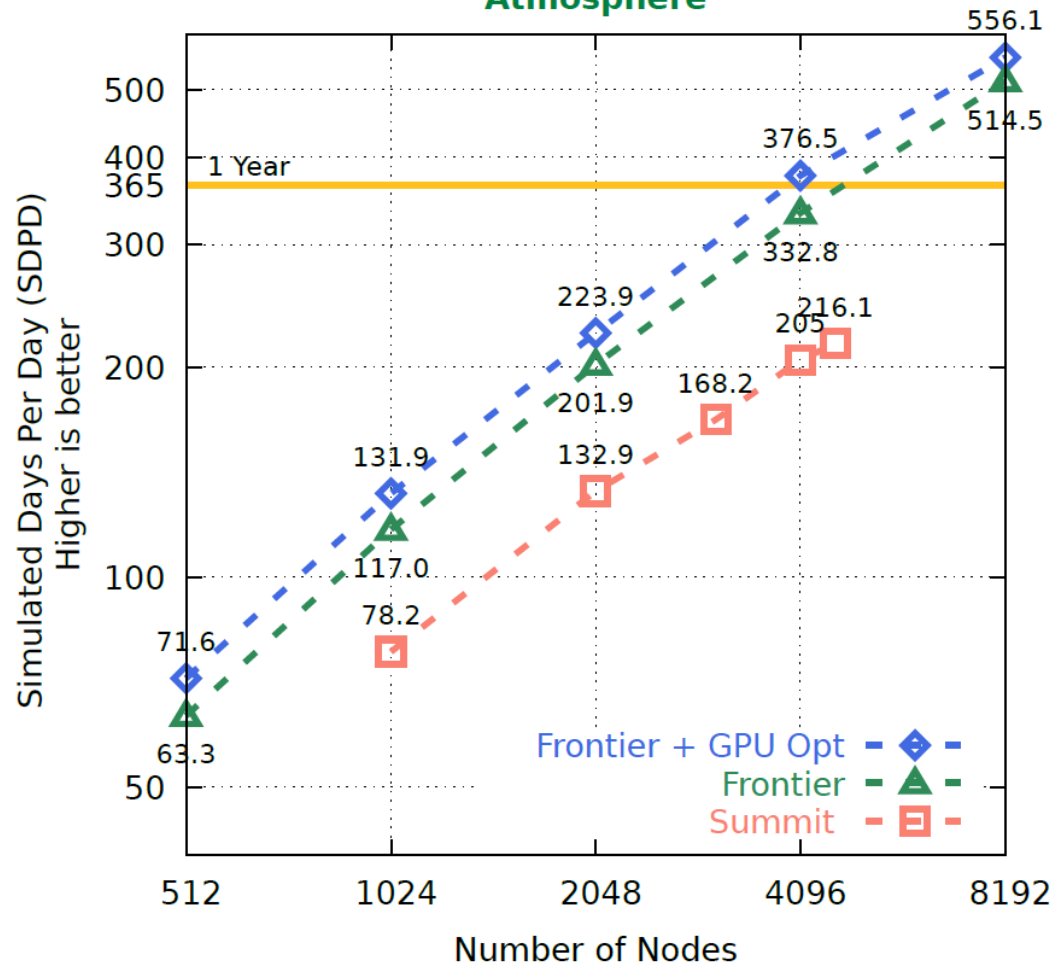
SCREAM GCRM (3.25 km) Benchmark Performance

**Full Model**



SCREAM GCRM (3.25 km) Benchmark Performance

**Atmosphere**





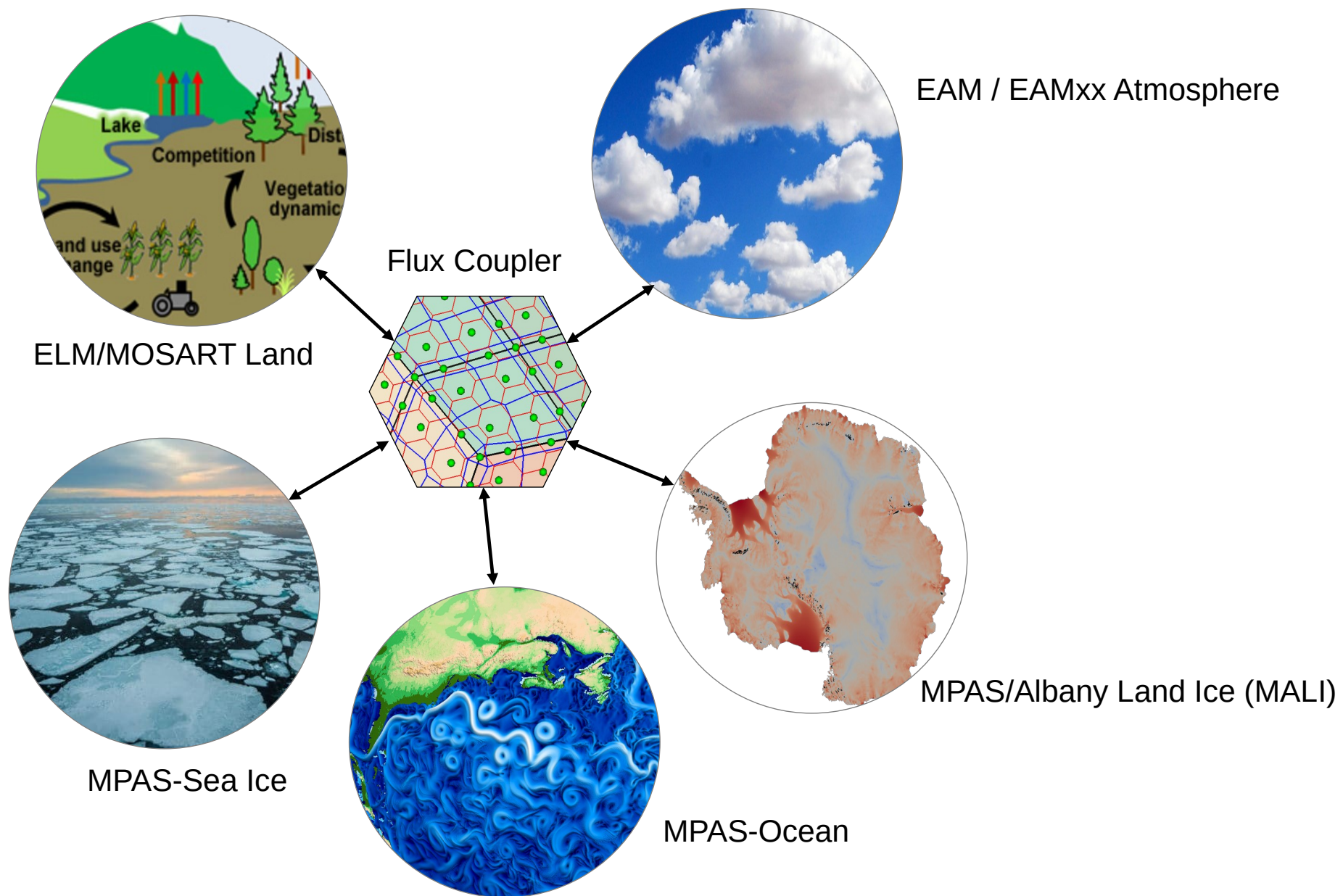
# Summary

- First Global cloud-resolving model (GCRM) to run on an Exascale supercomputer
- First GCRM to run at scale on both NVIDIA and AMD GPU systems (and hopefully soon Intel GPUs)
- First nonhydrostatic GCRM to exceed 1 simulated-year-per-day (SYPD) of model throughput
- 2023-2024: Running some of the first decadal length cloud resolving simulations

Horizontal resolution	Vertical resolution	No. of $p = 3$ spectral elements	timestep dynamics	timestep physics	dof dynamics	dof physics
110 km	128 Layers	5400	300s	1800s	6.2M	2.8M
3.25 km	128 Layers	6.3M	8.33s	100s	7.2B	3.2B



# Modern Earth System Models







# MONAN dyn core's choice



- **MONAN**

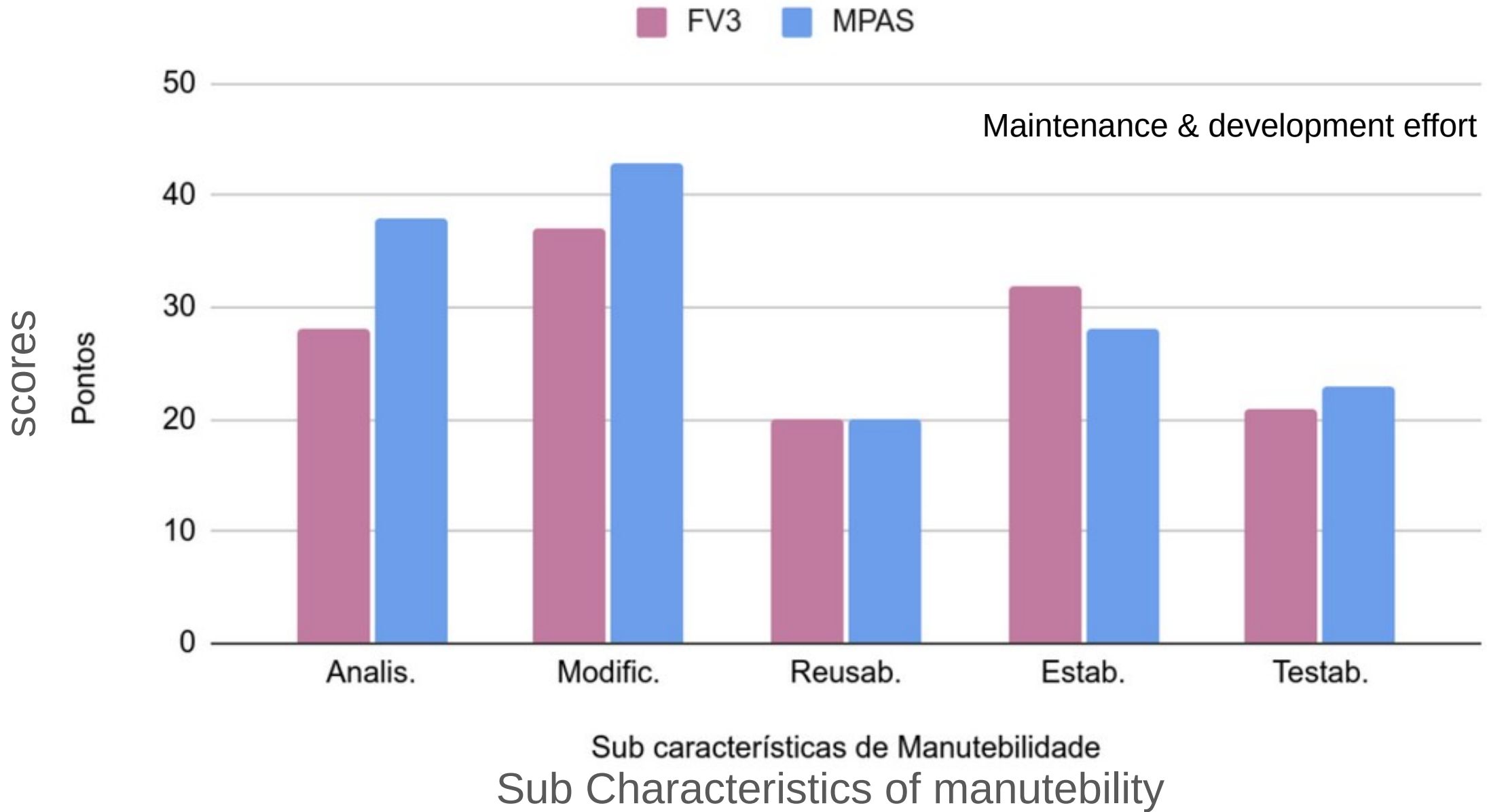
- Model for Ocean-land-Atmosphere prediction

“Monan's representation is like something infinite. For the Tupi-Guarani-speaking nations, there is no notion of Christian Paradise, heaven, or hell as in Christian beliefs, but the "Land without evils" or Ybymarã-e'yma, the place where they live with their ancestors and gods, without war, famine, or any human ailments.”

MONAN symbolizes the search for a better, sustainable, fraternal world with social justice.

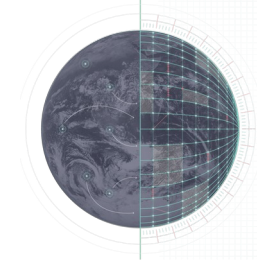


# Quality of software evaluation: Model manutability scores



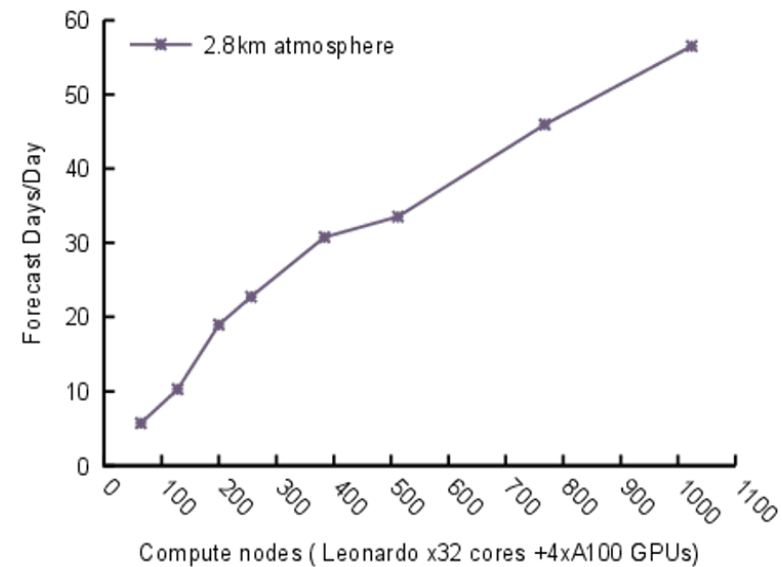
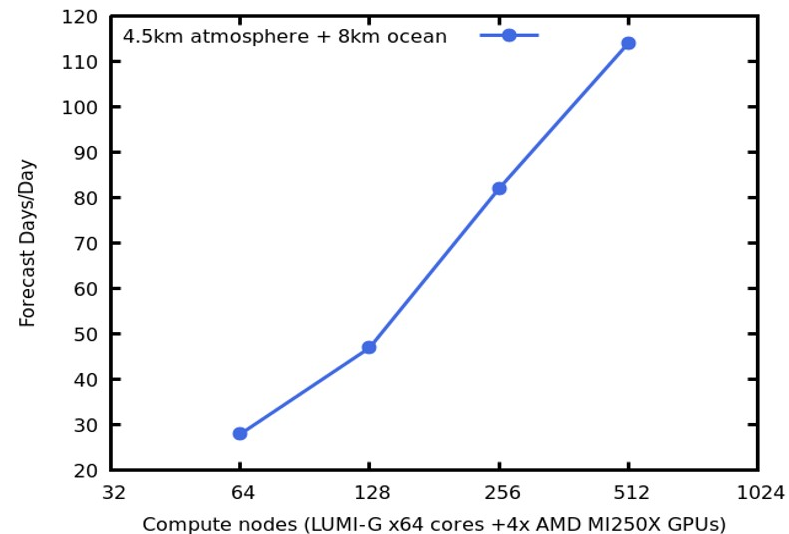
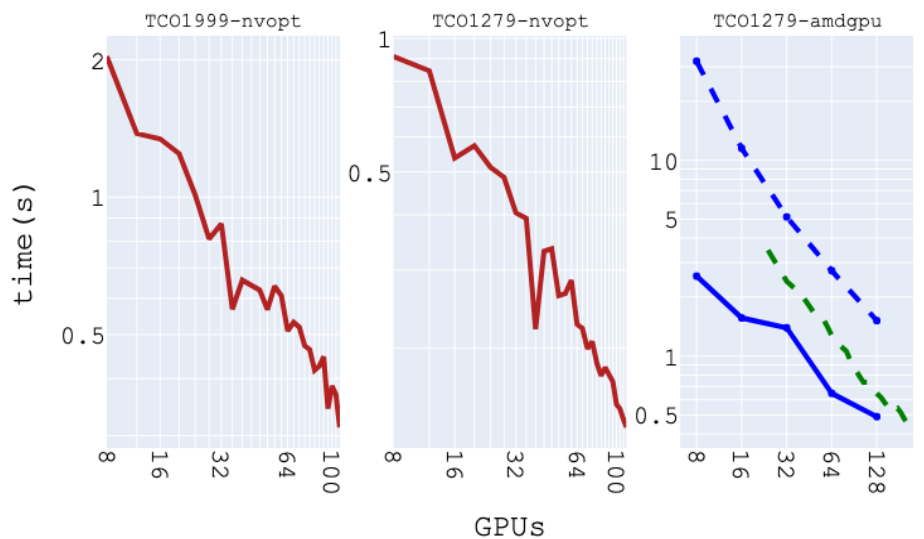
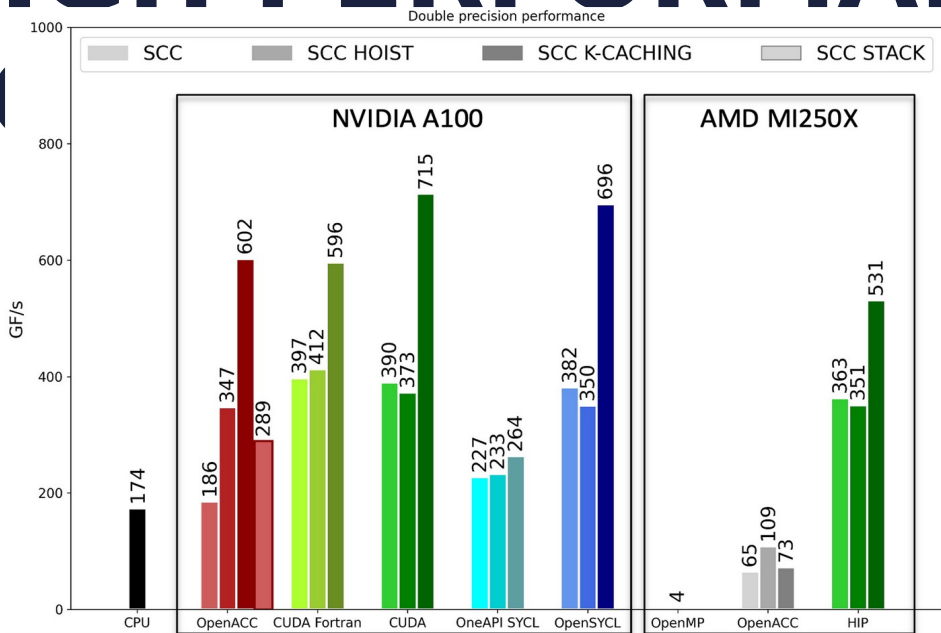
# Annex





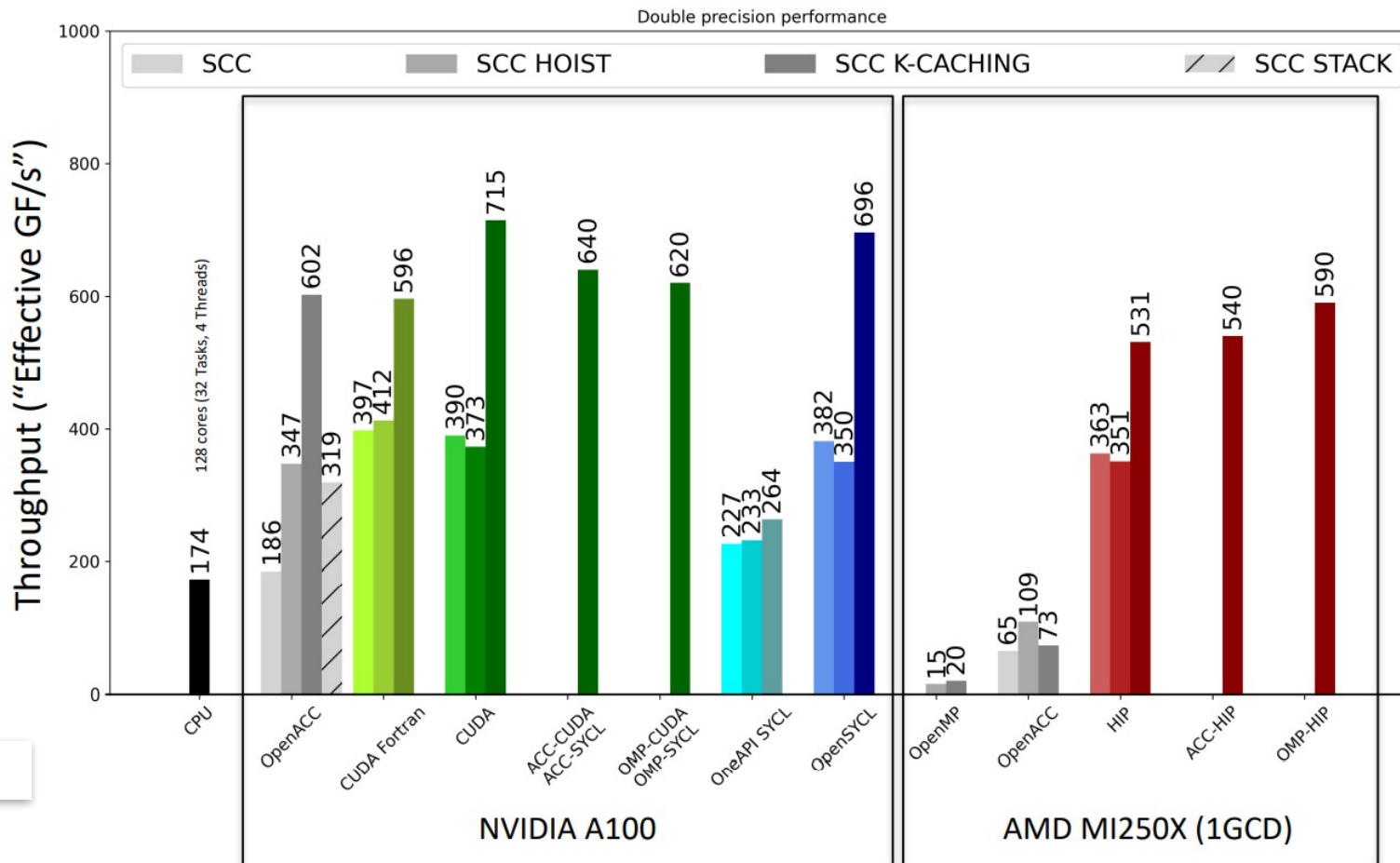
# HIGH PERFORMANCE

C



# IMPROVED GPU PERFORMANCE FOR SINGLE-COLUMN ALGORITHMS

- Adaptation via **source-to-source translation** using Loki
- Handling of **Fortran automatic arrays**: **recursive hoisting** or **pool allocator**
- **Speed-of-light implementation** of CLOUDSC in kernel languages (**CUDA, HIP, SYCL**)
- **Refactoring of Loki-SCC** recipe
- Ongoing refinement and development of new adaptation recipes for further performance improvements



# Compressed NetCDF for I/O and Inline Post-Processing

A decision was made to write out GFS.v16 forecast history files (atmf and sfcf) in netCDF format with compression. Parallel I/O was developed with updated netCDF and HDF libraries.

compression ratio:

Atmf 3d	5x	(33.6 GB to 6.7 GB),	lossy compression
sfc 2d	2.5x	(2.8 GB to 1.1 GB),	lossless compression

## Inline post-processing (post library)

- makes use of forecast data saved in memory for post processing, *reduces I/O activity, and speeds up the entire forecast system.*
- Since lossy compression is applied for writing out forecast history files, *inline post generates more accurate products* than the standalone offline post.

# WCROSS2 In Operation Since August 2023

## Locations

- Manassas, VA
- Phoenix, AZ

## Performance Requirements

- 99.9% Operational Use Time
- 99.0% On-time Product Generation
- 99.0% Development Use Time
- 99.0% System Availability

## Configuration

- Cray EX system
- **14.4 PetaFlops**
- Multi-tiered storage
  - 2 flash filesystems each with...
    - 614 TB usable storage
    - 300 GB/s bandwidth
  - 2 HDD filesystems each with...
    - 12.5 PB usable storage
    - 200 GB/s bandwidth
  - Total aggregate - 26.2PB at 1TB/s
- Lustre parallel filesystem
- PBSpro workload manager
- Eclflow scheduler

- Compute nodes
  - **3,060 nodes (60 spare)**
  - 3391,680 cores
    - **128 cores/node**
  - 1.3 PB of memory
    - 512 GB/node
- Pre/post-processing nodes
  - 132 nodes (4 spare)
  - 8,448 cores
    - 64 cores/node
  - 132 TB of memory
    - 1TB/node
- 200Gb/s Slingshot interconnect



# Met Office State of the Union

Summer 2022 – *ported* Gravity Wave miniapp to NVIDIA GPU  
Using NEMO openACC PSyclone transformation and **hand-written OpenACC**

1. Tested NVIDIA compiler
2. Tested changes to LFRic infrastructure
3. Demonstrated that it works
4. Demonstrated necessary changes to generated code

October 2023 – ported Gravity Wave miniapp to NVIDIA GPU  
Using 100% PSyclone generated OpenACC  
Performance (more to be done) and data movement  
Roll out to Gung Ho



## Physics

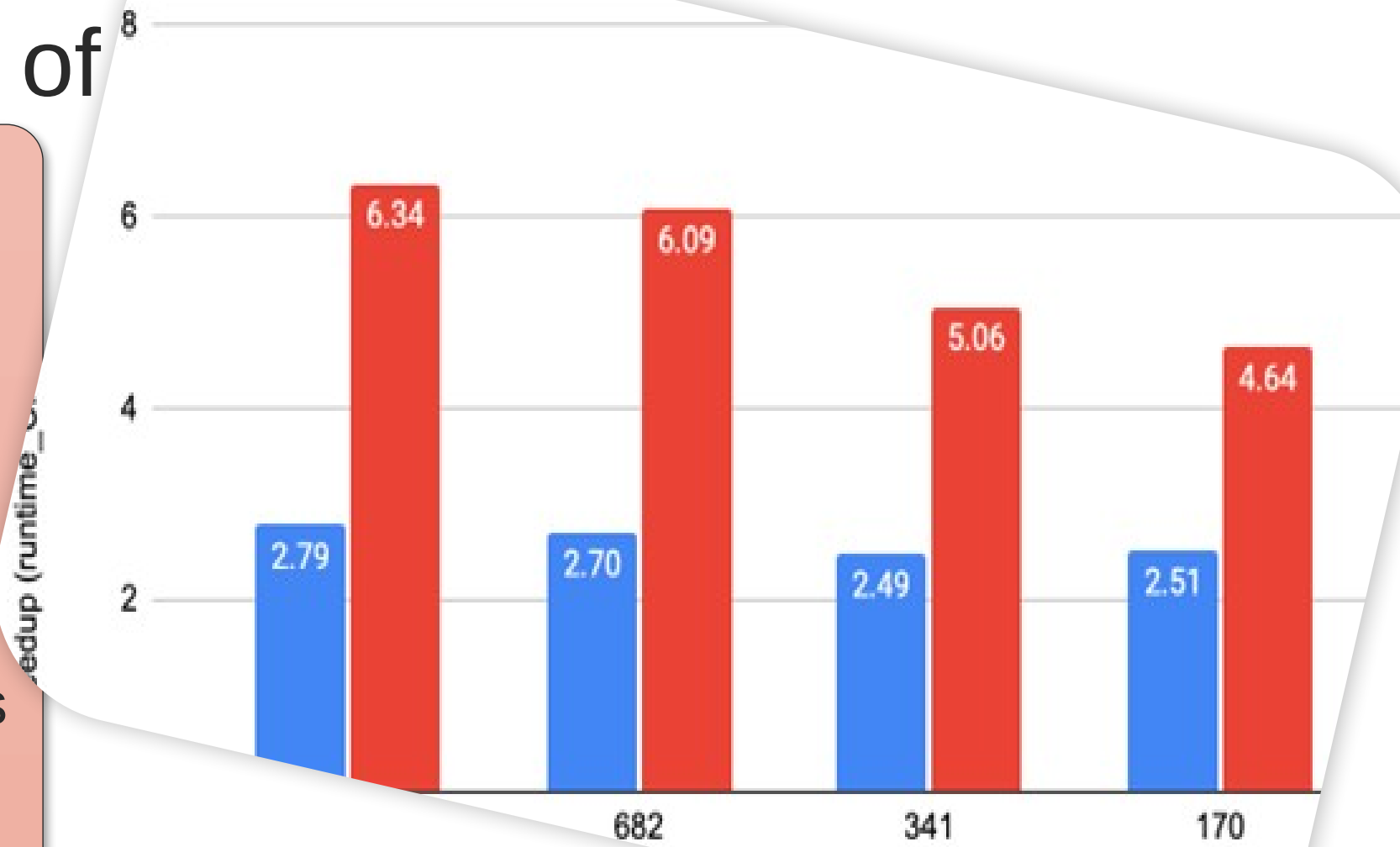
ORNL has worked with Socrates and Casim Refactor to organise memory and gather loops

Add OpenACC directives

Summit P9 vs V100

<https://doi.org/10.1145/3468267.3470612>

W. Zhang is visiting HQ this month



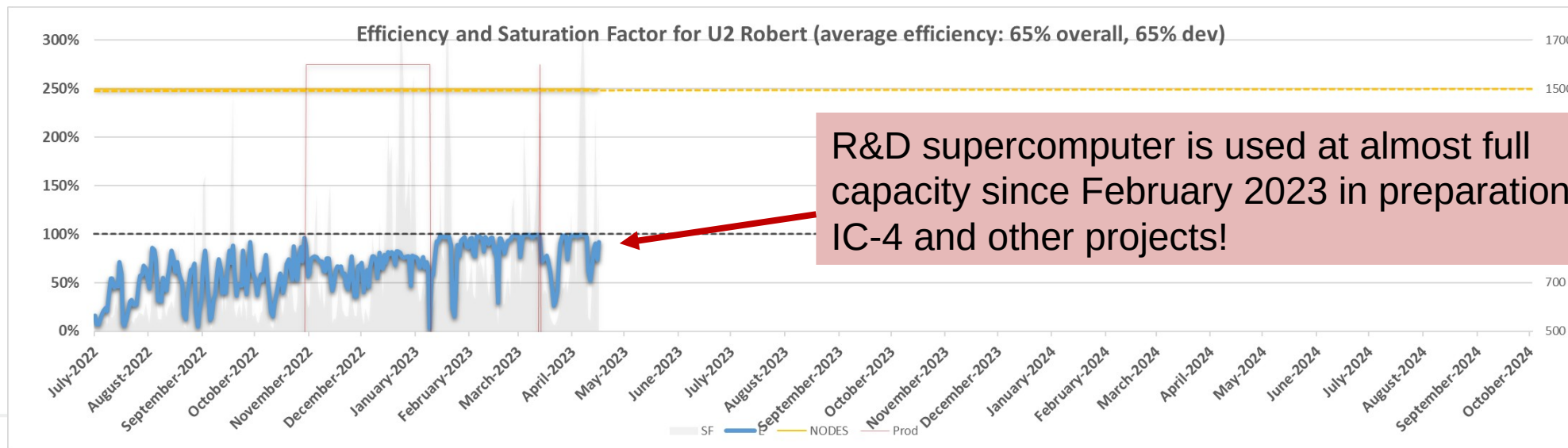
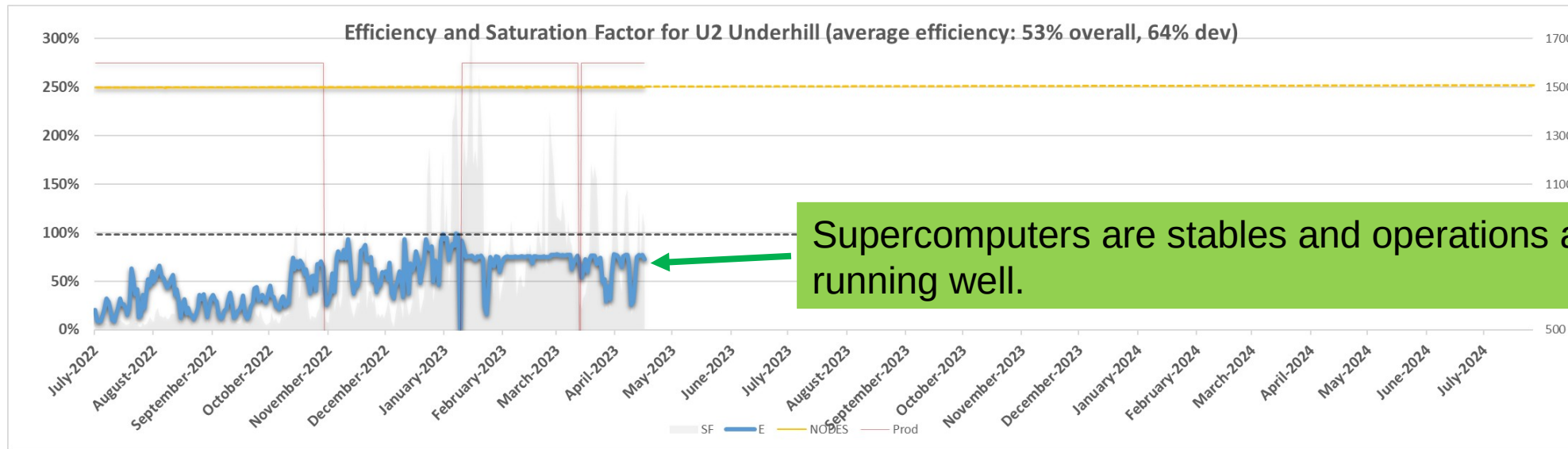
## STFC

1. Strip out OpenACC directives and regen with PScyclone (Socrates works)
2. Developing OpenMP offload

# High Performance Computing (HPC)

System	HPC Upgrade 1		HPC Upgrade 2 (2.5X)	
<b>Status</b>				
<b>Operational</b>	January 21, 2020		June 28, 2022	
<b>Top 500 Entry</b>	107 (06/2020)	115 (06/2020)	69 (06/2022)	70 (06/2022)
<b>Top 500 Rank</b>	249 (11/2022)	269 (11/2022)	76 (11/2022)	77 (11/2022)
<b>Specifications</b>				
<b>Name</b>	<b>Banting</b>	<b>Daley</b>	<b>Underhill</b>	<b>Robert</b>
<b>Manufacturer</b>	Cray/HPE XC50	Cray/HPE XC50	Lenovo ThinkSystem	Lenovo ThinkSystem
<b>Compute nodes</b>	1,266	1,266	1,494	1,494
<b>Cores</b>	53,200	53,200	148,320	148,320
<b>Site Storage</b>	71 PB		188 PB	
<b>Performance (Pflops/s)</b>				
<b>Rmax</b>	2.68	2.60	7.76	7.76
<b>Rpeak</b>	4.09	4.09	10.92	10.92

# Efficiency and Saturation Factor for U2





# Global Cloud Resolving Atmospheric Modeling on Exascale Computers

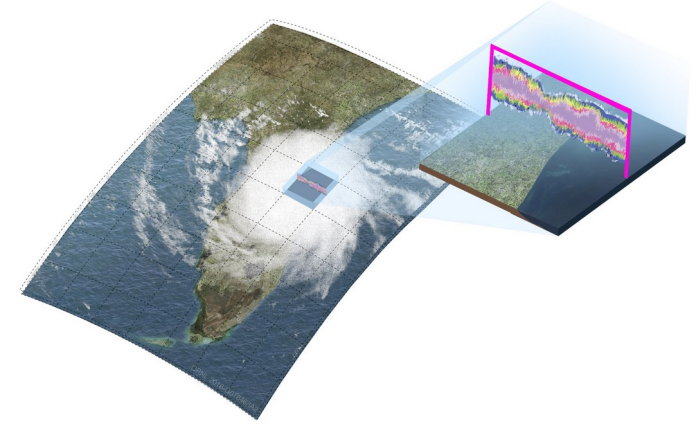
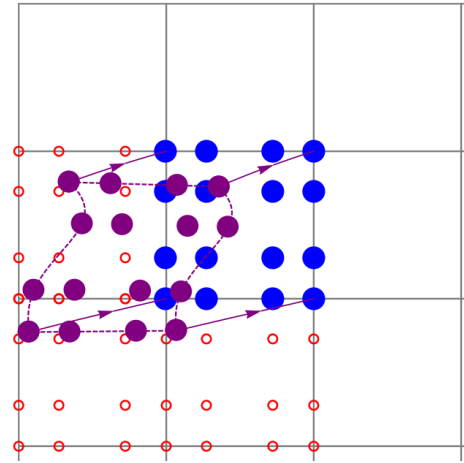
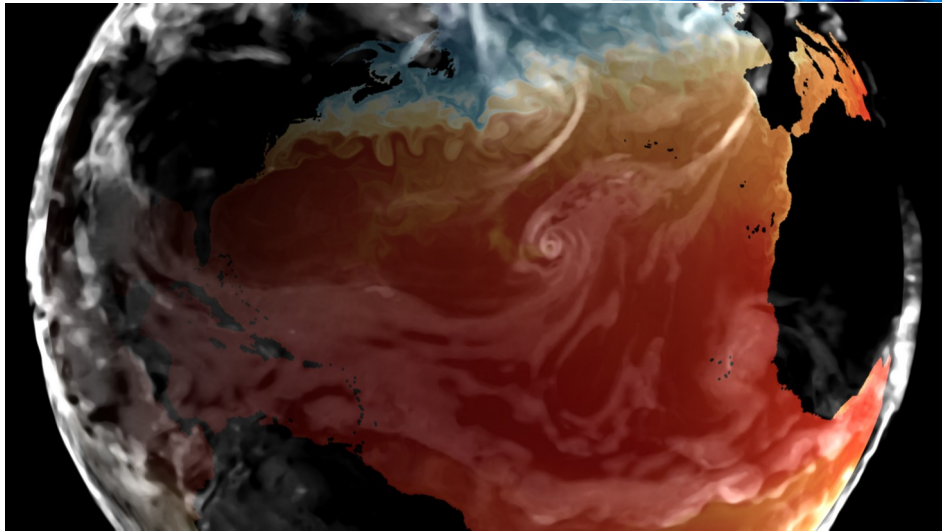
Mark Taylor (SNL), Luca Bertagna (SNL), Andrew Bradley (SNL), Peter Caldwell (LLNL), Aaron Donahue (LLNL), Oksana Guba (SNL), Noel Keen (LBNL), Sarat Sreepathi (ORNL), Trey White (HPE)

WGNE Update

Contact: Sarat Sreepathi (ORNL), [sarat@ornl.gov](mailto:sarat@ornl.gov)

- DOE's Exascale Energy Earth System Model (E3SM) project
- SCREAM: Simple Cloud Resolving E3SM Atmosphere Model
- Porting SCREAM to Exascale machines:
  - Rewrite from scratch C++/Kokkos
  - Fortran vs C++ performance
  - Scaling to exascale



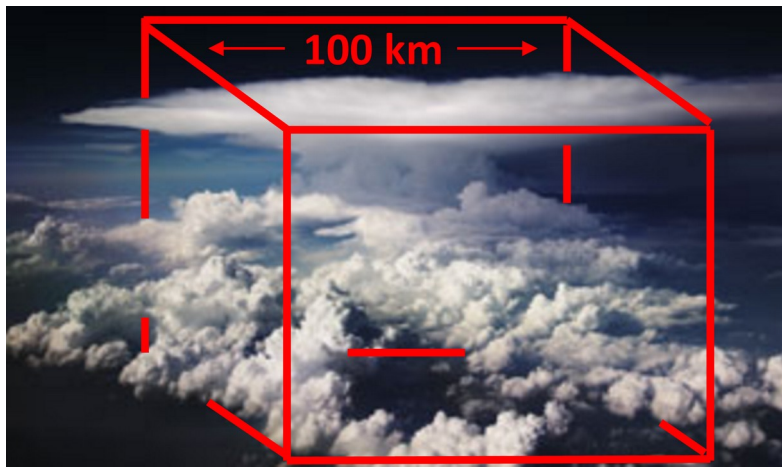


- **BER-ESMD: E3SM Project**
- ~50 FTEs, 8 labs + Universities
- Energy Exascale Earth System Model
- DOE-SC science mission: Energy & water issues looking out 40 years
- Ensure E3SM will run well on upcoming DOE exascale computers
- <https://github.com/E3SM-Project>

- **ASCR/BER SciDAC**
- ~10 FTEs over multiple projects
- Large focus on new algorithms

- **ASCR ECP Project**
- ~10 FTEs
- E3SM-MMF: "superparameterization"

# Cloud Resolving Atmosphere Model

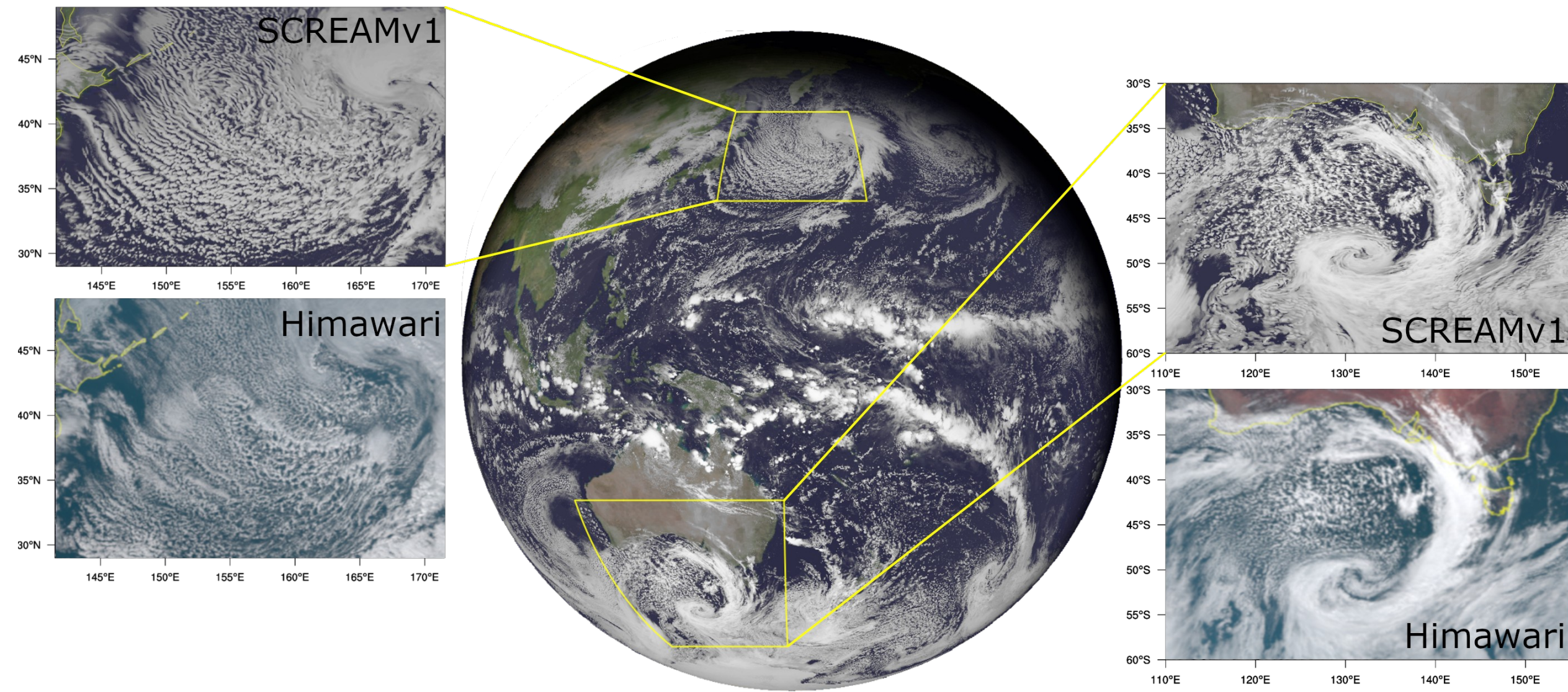


- Cloud-resolving simulations (with 3 km) avoid the need for convection parameterizations, which are the main source of climate change uncertainty (Sherwood et al., Nature 2014)
- Resolved convection will substantially reduce major systematic errors in precipitation because of its more realistic and explicit treatment of convective storms.
- Improve our ability to assess regional impacts of climate change on the water cycle that directly affect multiple sectors of the US and global economies, especially agriculture and energy production.



*Movie: Precipitation (colors) and integrated water vapor (gray) for an atmospheric river from E3SM's DYAMOND2 simulation. By Paul Ullrich/UC Davis*



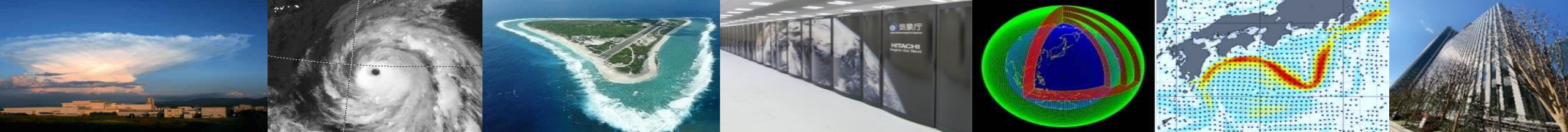


- Ability to capture cloud structures is impressive
- Example: cold air outbreaks, extra-tropical cyclones are well-represented
- Fig: 2d into a SCREAM DYAMOND simulation (January 22, 2020 at 2:00:00 UTC). Himawari visible satellite image and shortwave cloud radiative effect from SCREAMv0.



# Summary

- SCREAM: E3SM atmosphere model rewritten in C++/Kokkos for performance portability
- Competitive with Fortran code on CPUs
- Running well on NVIDIA and AMD GPUs (and hopefully soon Intel GPUs)
- Achieved a longstanding goal of  $> 1$  SYPD at cloud resolving resolutions on Frontier
- 2023-2024: Running some of the first decadal length cloud resolving simulations



# HPC readiness: input from JMA

Japan Meteorological Agency

# Highlights

- GSM (JMA Global Spectral Model) preparing for future HPCs
  - Improvement of grid decomposition (as reported in WGNE 37)
  - Flexible array structure suitable for both CPU and GPU
  - Reduced precision in MPI communication and its evaluation
- GPU porting of ASUCA (JMA regional NWP model)
- MRI.COM (MRI/JMA ocean model) preparing for future HPCs
  - Single precision in SOM advection
  - GPU porting

## Array Structure of each model

GSM: (i, k, j) ordering

ASUCA: (k, i, j) ordering

MRI.COM: (i, j, k) ordering

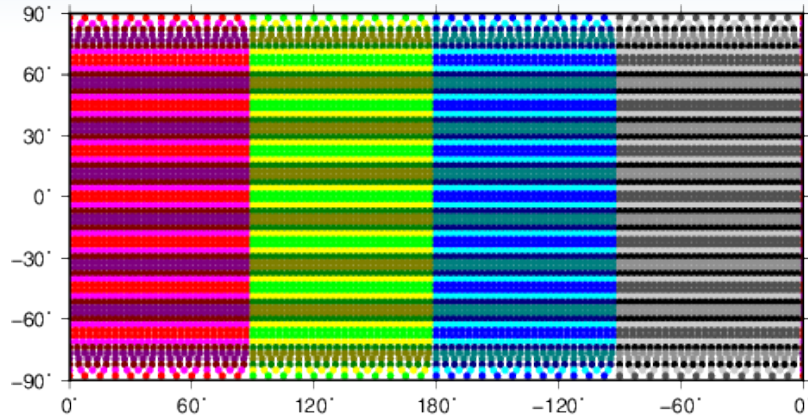
(i, j, k) : (x, y, z) directions



# Improvement of grid decomposition : a T163 16MPI case

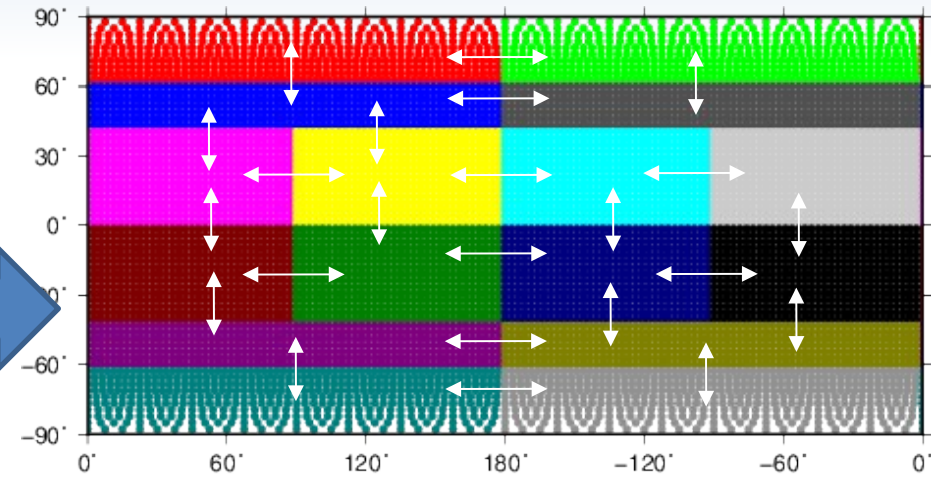
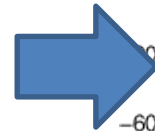
## Current decomposition (two grid stages)

For parameterization, I/O and spectral transform



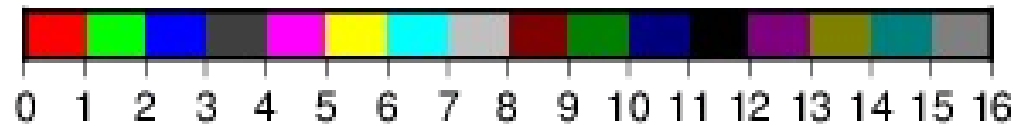
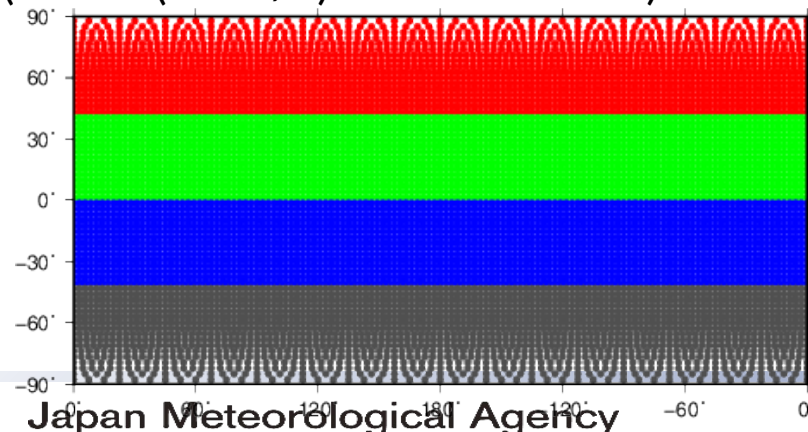
Transpose (with all-to-all MPI communication) required every time step

## New decomposition (unified grid stage)



Only halo communication for SL advection

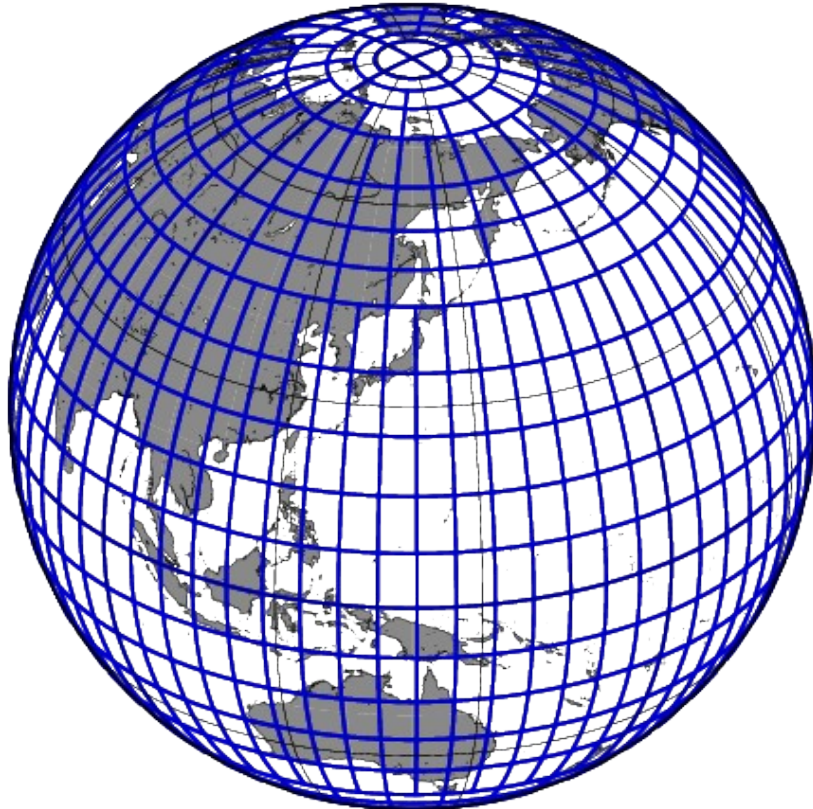
For SL advection  
(first to (Kmax/4)th vertical levels)



MPI rank

# Improvement of grid decomposition: Tq959 960MPI case

Tq959L128 960mpi



- Pros.
  - Suitable for both derivative stencils in gridspace and spectral transform.
    - also preparation for grid-spectral hybrid approach
  - Only halo communication (no all-to-all communication) required for Semi-Lagrangian advection
- Cons.
  - Load-balance of computation in physics parameterizations gets worse (however, pros. overweigh in high-resolution runs)

# Single precision in MPI communication for GSM

- GSM: A semi-implicit semi-Lagrangian global model with a spectral method
  - Its computational performance strongly depends on MPI communication.
  - Single-precision rather than double-precision in MPI comm. is an effective way to reduce amount of the communication, hence, to improve the computational performance
    - Less risks than full single precision calculation
    - Also a step for the single precision GSM
- Impacts of single precision only in MPI communication on computational costs and forecasts are tested preliminarily.

# GPU porting of ASUCA

- ASUCA: JMA's operational regional model (Ishida et al. 2022)
- Code characteristics:
  - (k,i,j) ordering ( Array(nz, nx, ny))
  - MPI-OpenMP hybrid parallelization
  - Subroutines are called in a horizontal loop
- Dynamics
  - MPI comm. necessary
  - Vertically dependent loops for a tri-diagonal matrix solver
- Physics
  - Parallel in the horizontal
  - Strong loop carried dependence in vertical

```
subroutine calculate
real(8): x(nz,nx,ny),y(nz,nx,ny)
real(8) :: s(nz)

!$OMP PARALLEL DO &
!$OMP& PRIVATE(s,...)
do j = 1, ny
do i = 1, nx
...
call cal_main( x(1,i,j), y(1,i,j), s(1),....)
```

# HPC readiness of MRI.COM

- MRI.COM : MRI Community Ocean Model (Sakamoto, et al. 2023)
  - A depth coordinate model that solves the primitive equations under hydrostatic and Boussinesq approximations
  - Used in ocean monitoring/forecasts, climate prediction, and research on coupled NWP as a feasibility study
  - (i,j,k) ordering array structure
- Adopt to future HPCs / speed up required
  - Time-to-solution is critical as an operational model
  - As a climate model, long term (>100 yrs) time integration for spin-up required
- Recent research topics of MRI.COM in the context of HPC readiness
  - Reduced precision in the SOM advection scheme
  - GPU porting

# GPU porting of MRI.COM

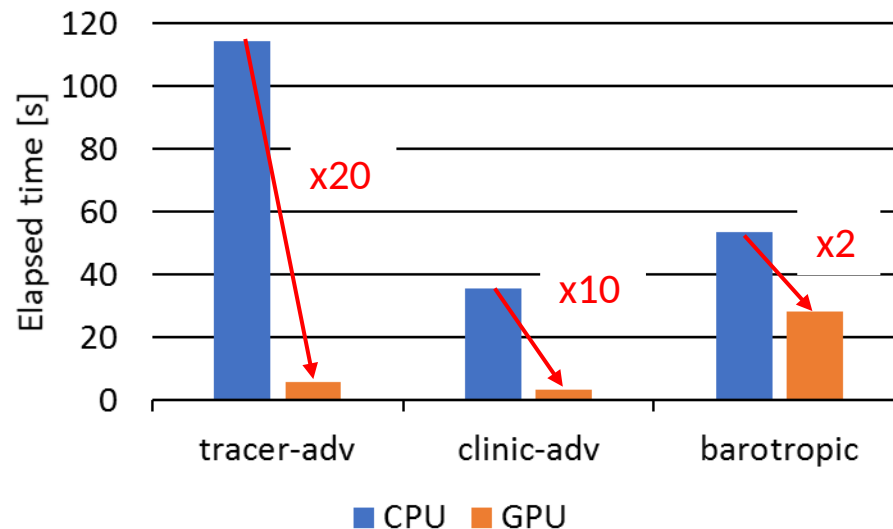
- GPU porting of MRI.COM was tested in a rectangular domain.
  - Horizontal grids :  $242 \times 202 \sim O(10^4)$ , Vertical layers : 40
    - Mimicked problem size per node for ocean part of JMA/MRI Coupled Prediction System
  - Focus on only calculation parts
    - Optimizing CPU <-> GPU data transfer and MPI parallelization will be next steps.
- High-cost processes are ported to GPU.
  - Dynamical process (particularly advection) for tracer variables
  - Momentum equations (barotropic and baroclinic components)
  - OpenACC directives are inserted in most loops of these processes.
  - Some loops are modified for 3-dimensional parallelization.
    - The original CPU-based codes consist of 2-dimensional parallelization with OpenMP.



# GPU porting of MRI.COM

- CPU: Intel Xeon Gold 6226 2.7GHz 12C/24T x2 with DDR4 memory (140GB/s)
- GPU: NVIDIA Tesla V100-PCIe-32GB x1 with HBM2 memory (900GB/s)
- Run 10-day (960-timestep) forecast to check the performance.

Acceleration of bottleneck processes (calculation parts only)



tracer-adv	Advection of tracers with QUICK scheme (3-dimensional)
clinic-adv	Advection of baroclinic components (3-dimensional)
barotropic	Time integration of barotropic components (2-dimensional)

- All of these processes are accelerated by GPU.
  - In particular, the processes parallelized in 3-dimensional are accelerated remarkably.
- Optimizing CPU <-> GPU data transfer is ongoing. (e.g. reducing amount / frequency )

# References

- Ishida, J., K. Aranami, K. Kawano, K. Matsubayashi, Y. Kitamura, and C. Muroi, 2022: ASUCA: The JMA Operational Non-hydrostatic Model. J. Meteor. Soc. Japan, 100, 825-846.
- Sakamoto, K., H. Nakano, S. Urakawa, T. Toyoda Y. Kawakami, H. Tsujino, and Goro Yamanaka, 2023: Reference Manual for the Meteorological Research Institute Community Ocean Model version 5 (MRI.COMv5), TECHNICAL REPORTS OF THE METEOROLOGICAL RESEARCH INSTITUTE No.87.

# Mahalanobis distance - Globe

24h

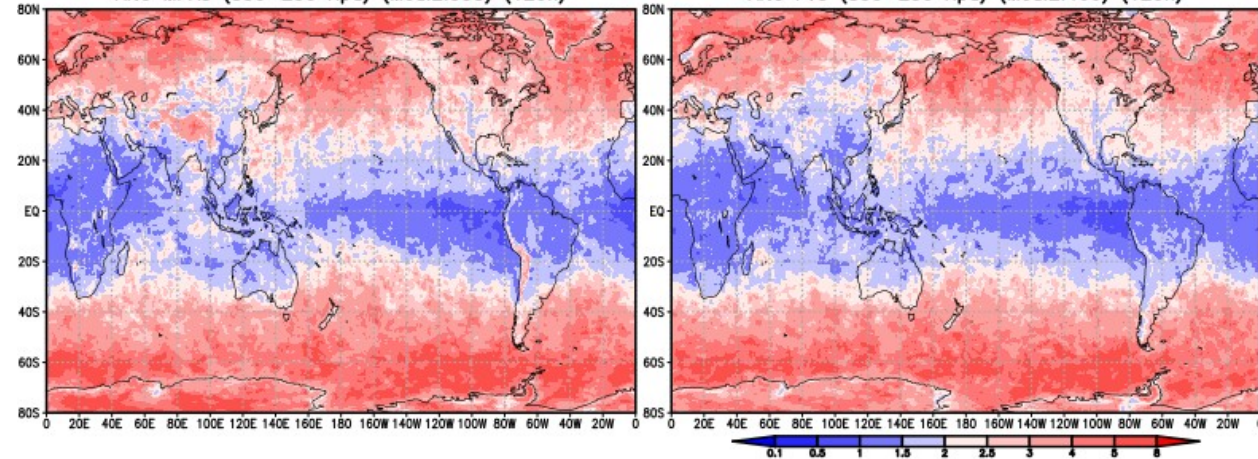
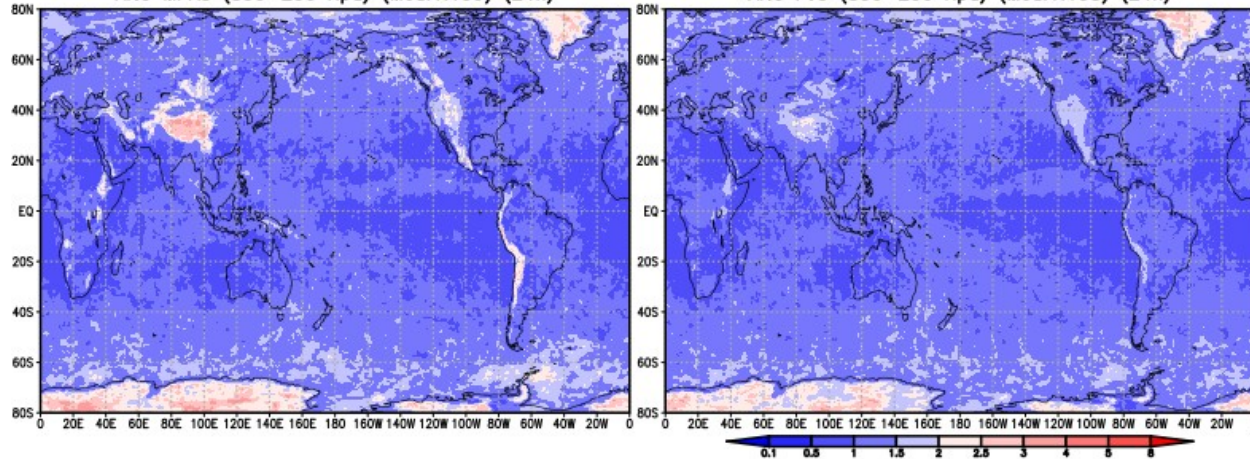
120h

ANO MPAS (850–250 Hpa) (Med:1.159) (24h)

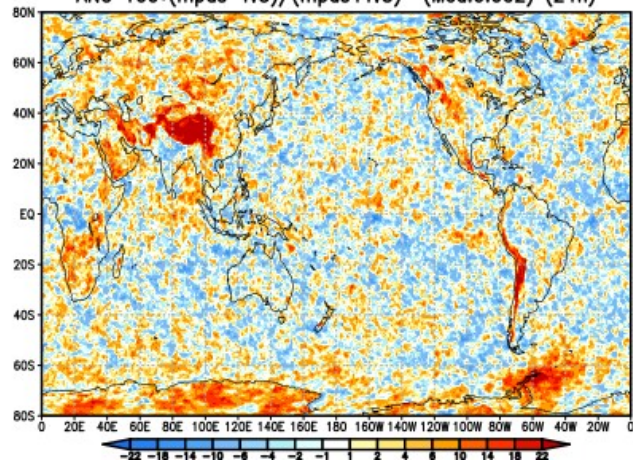
ANO FV3 (850–250 Hpa) (Med:1.138) (24h)

ANO MPAS (850–250 Hpa) (Med:2.558) (120h)

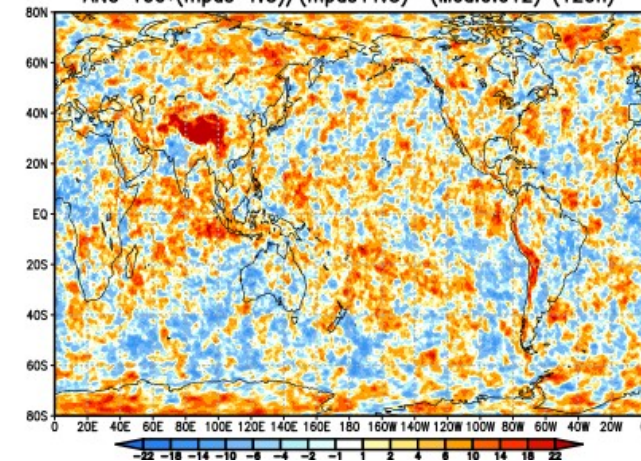
ANO FV3 (850–250 Hpa) (Med:2.466) (120h)



ANO  $100 \cdot (\text{mpas} - \text{fv3}) / (\text{mpas} + \text{fv3})$  (Med:0.002) (24h)



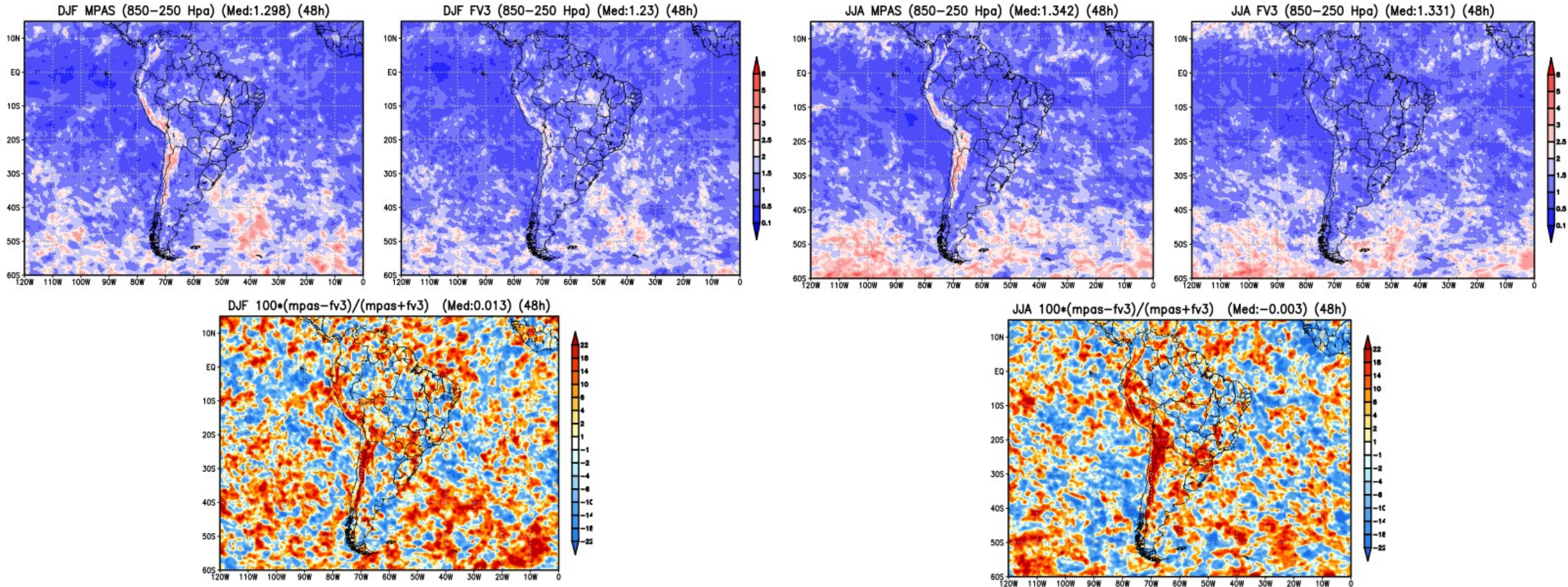
ANO  $100 \cdot (\text{mpas} - \text{fv3}) / (\text{mpas} + \text{fv3})$  (Med:0.012) (120h)





# Mahalanobis distance - South America and oceans

## 48h forecast length

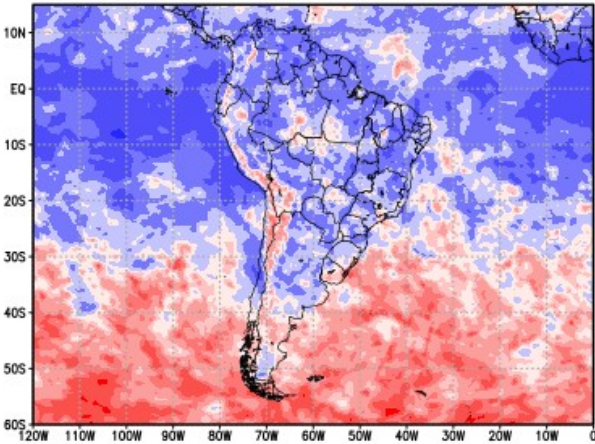




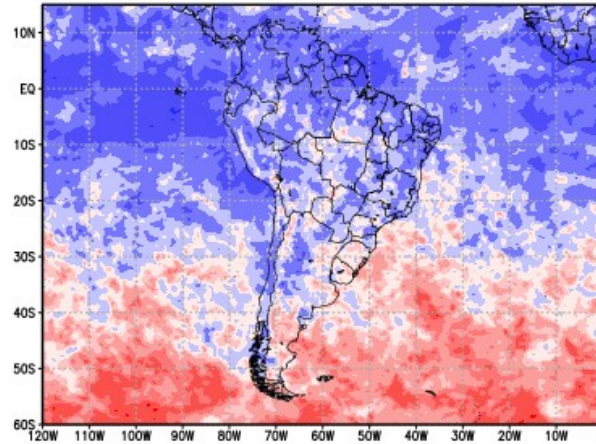
# Mahalanobis distance - South America and oceans

## 120h forecast length

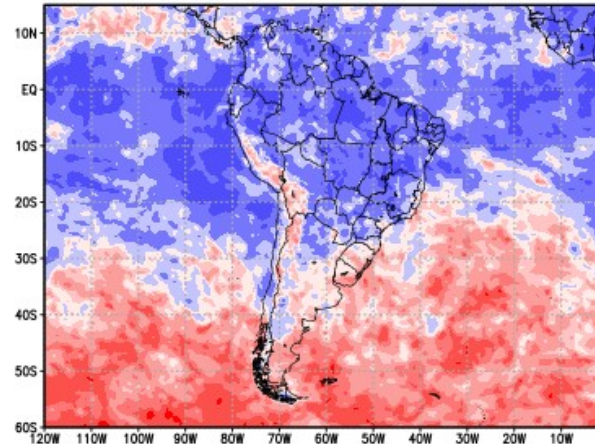
DJF MPAS (850–250 Hpa) (Med:2.112) (120h)



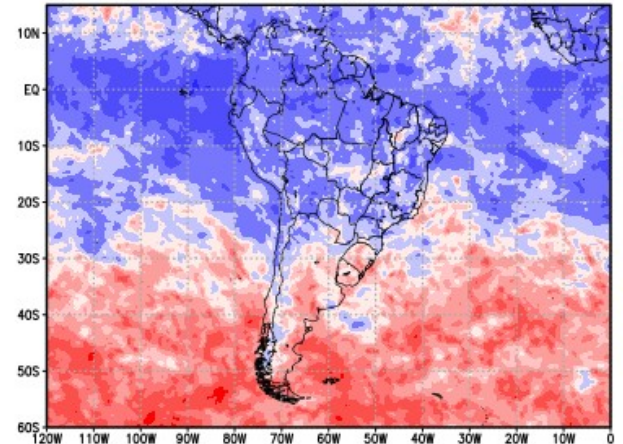
DJF FV3 (850–250 Hpa) (Med:1.965) (120h)



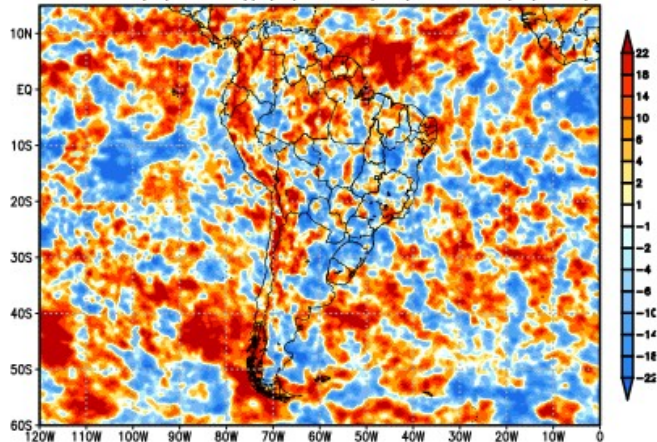
JJA MPAS (850–250 Hpa) (Med:2.194) (120h)



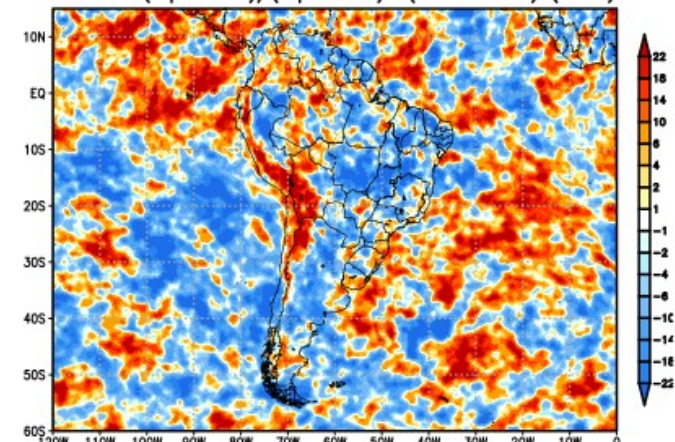
JJA FV3 (850–250 Hpa) (Med:2.231) (120h)



DJF  $100 \cdot (\text{mpas} - \text{fv3}) / (\text{mpas} + \text{fv3})$  (Med:0.024) (120h)



JJA  $100 \cdot (\text{mpas} - \text{fv3}) / (\text{mpas} + \text{fv3})$  (Med:-0.008) (120h)



## Precipi mean intensity computed over the global domain, in mm/day

Time integration	IMERG	MPAS	ShiELD	Diff MPAS	Diff ShiELD	Diff perc. MPAS (%)	Diff perc. ShiELD (%)
36h	3,19928	3,09617	3,47084	-0,10311	0,27156	-3,223	8,488
60h	3,20317	3,17713	3,52475	-0,02604	0,32158	-0,813	10,039
84h	3,19727	3,23611	3,61322	0,03884	0,41595	1,215	13,010
108h	3,17839	3,27442	3,65614	0,09603	0,47775	3,021	15,031
132h	3,20712	3,31056	3,68918	0,10344	0,48206	3,225	15,031
156h	3,20342	3,34213	3,72282	0,13871	0,5194	4,330	16,214
180h	3,20599	3,35401	3,75819	0,14802	0,5522	4,617	17,224
204h	3,20136	3,37975	3,77914	0,17839	0,57778	5,572	18,048
228h	3,18150	3,38142	3,81426	0,19992	0,63276	6,284	19,889



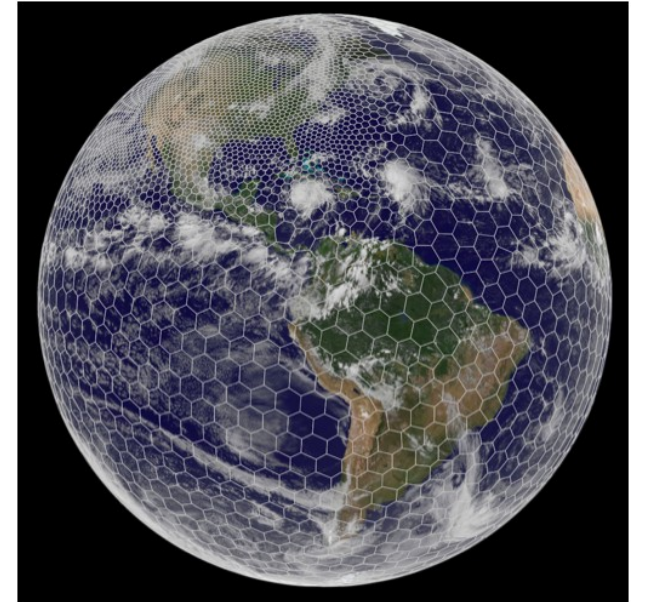
# Model for Ocean-land-Atmosphere prediction



**MONAN's** dynamical core

**MPAS**

Model for Prediction Across Scales



# Thank you



WORLD  
METEOROLOGICAL  
ORGANIZATION



[wmo.int](http://wmo.int)

