h3-Open-UTIL/MP:
a general-purpose coupling library
bridging legacy HPC applications and the future

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with

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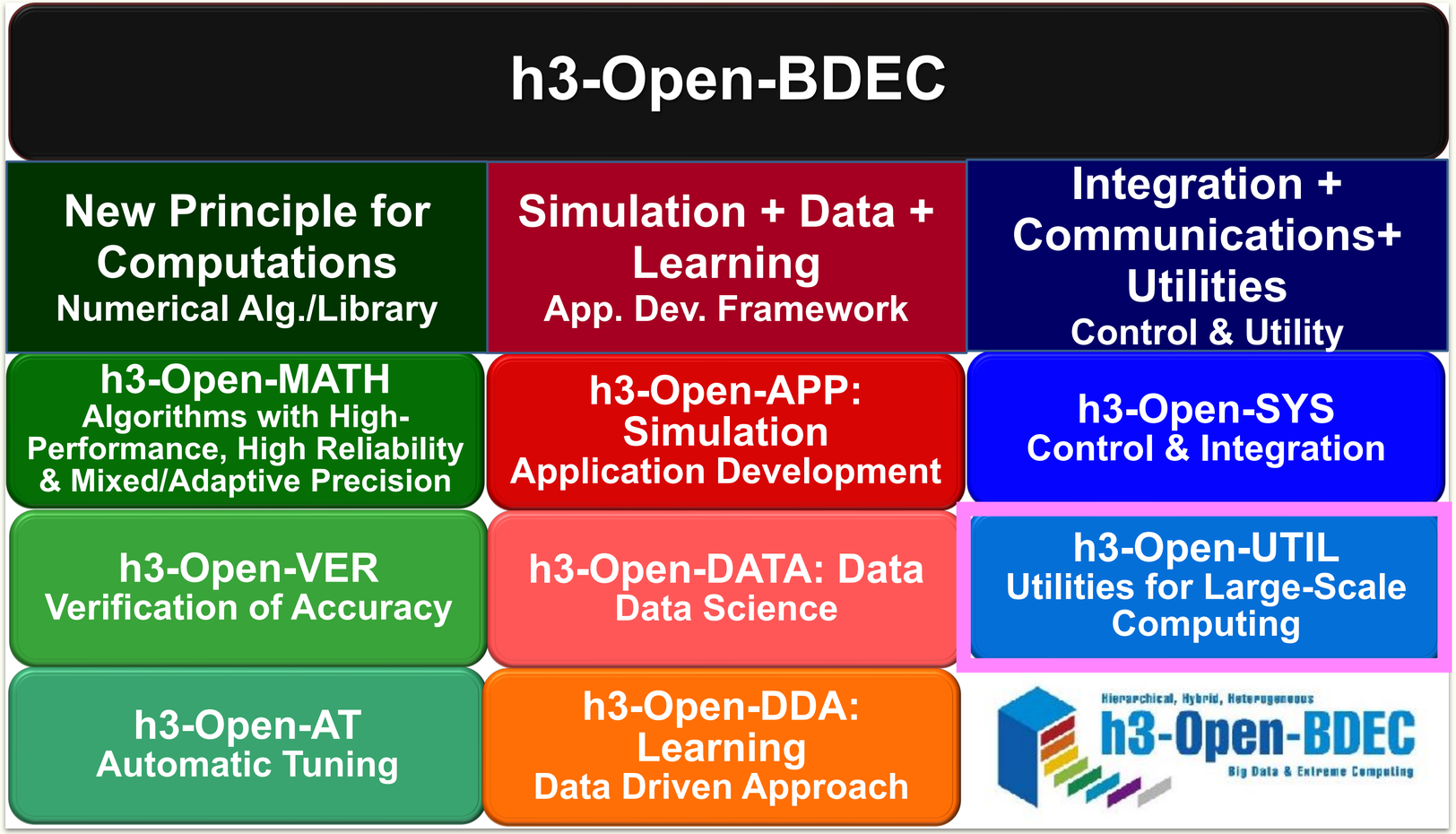
International Workshop on the Integration of (Simulation + Data + Learning) :
Towards Society 5.0 by h3-Open-BDEC
2021/12/3

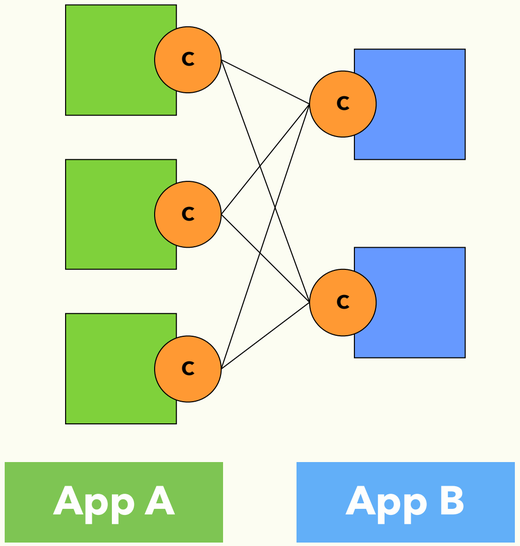
h3-Open-UTIL: Utilities for Large-Scale Computing

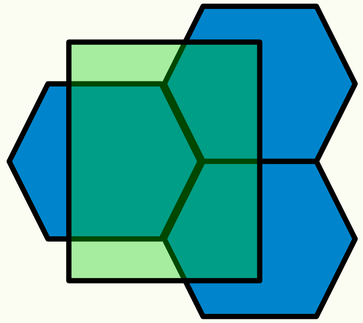


h3-Open-UTIL/MP: A general purpose coupling library

It manages...

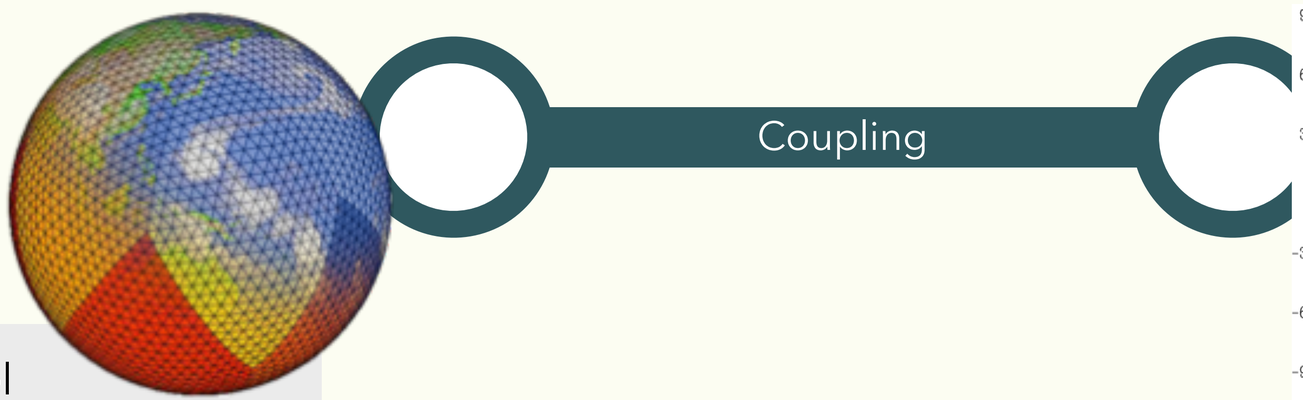
- Process groups: MPI communicator
- Data exchange rules
  - Process communication
  - Timing in the time integration of simulation
  - Spatial remapping between the different grid systems

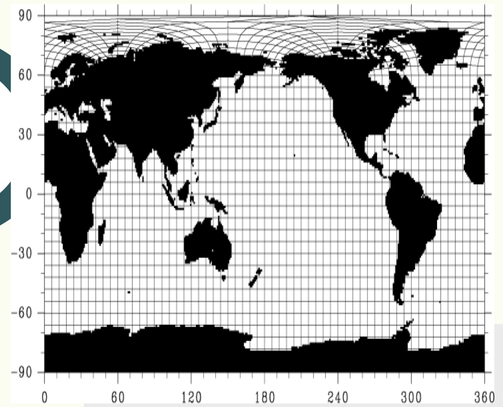




What ca we do with h3-Open-UTIL/MP?

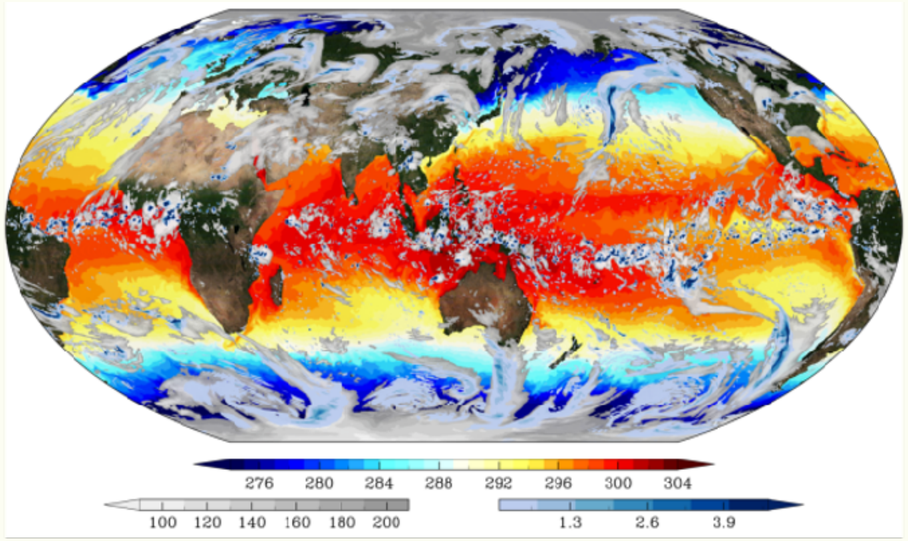
Multi Physics Coupling





Atmospheric model (NICAM)

- Developed by Meteorologist
- 20-years development
- 200k lines of Fortran code
- Icosahedral grid system
- 100-10000 processes

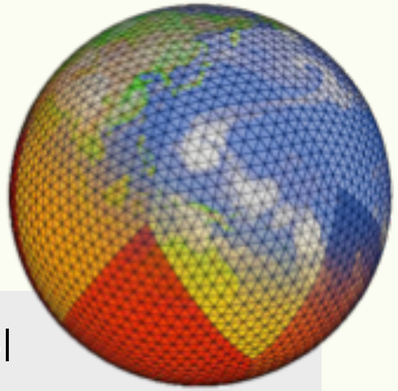


Picture from Miyakawa et al., 2017, GRL

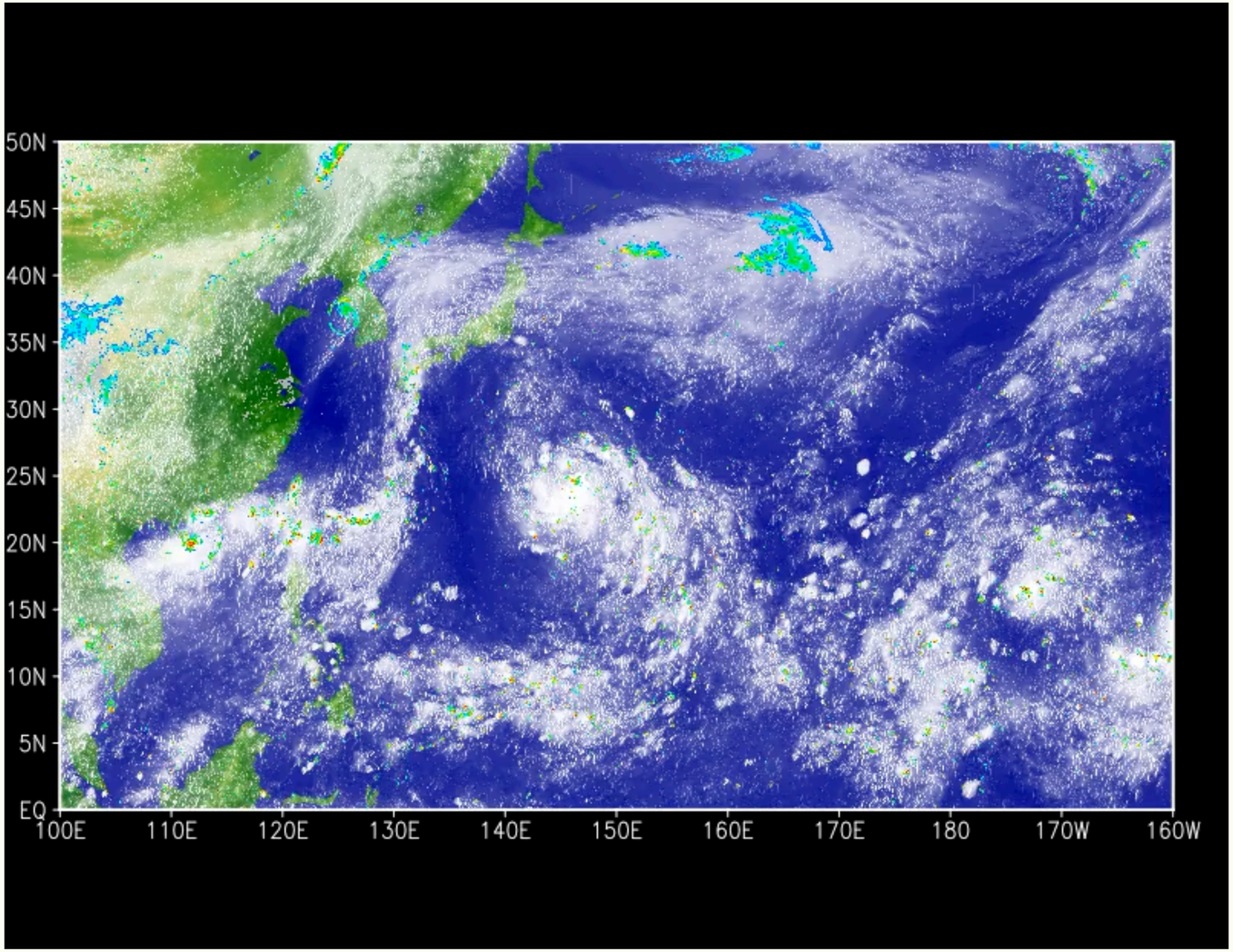
Ocean model (COCO)

- Developed by Oceanographer
- 20-years development
- 200k lines of Fortran code
- Tri-polar grid system
- 100-1000 processes

A practical case: Atmospheric model NICAM

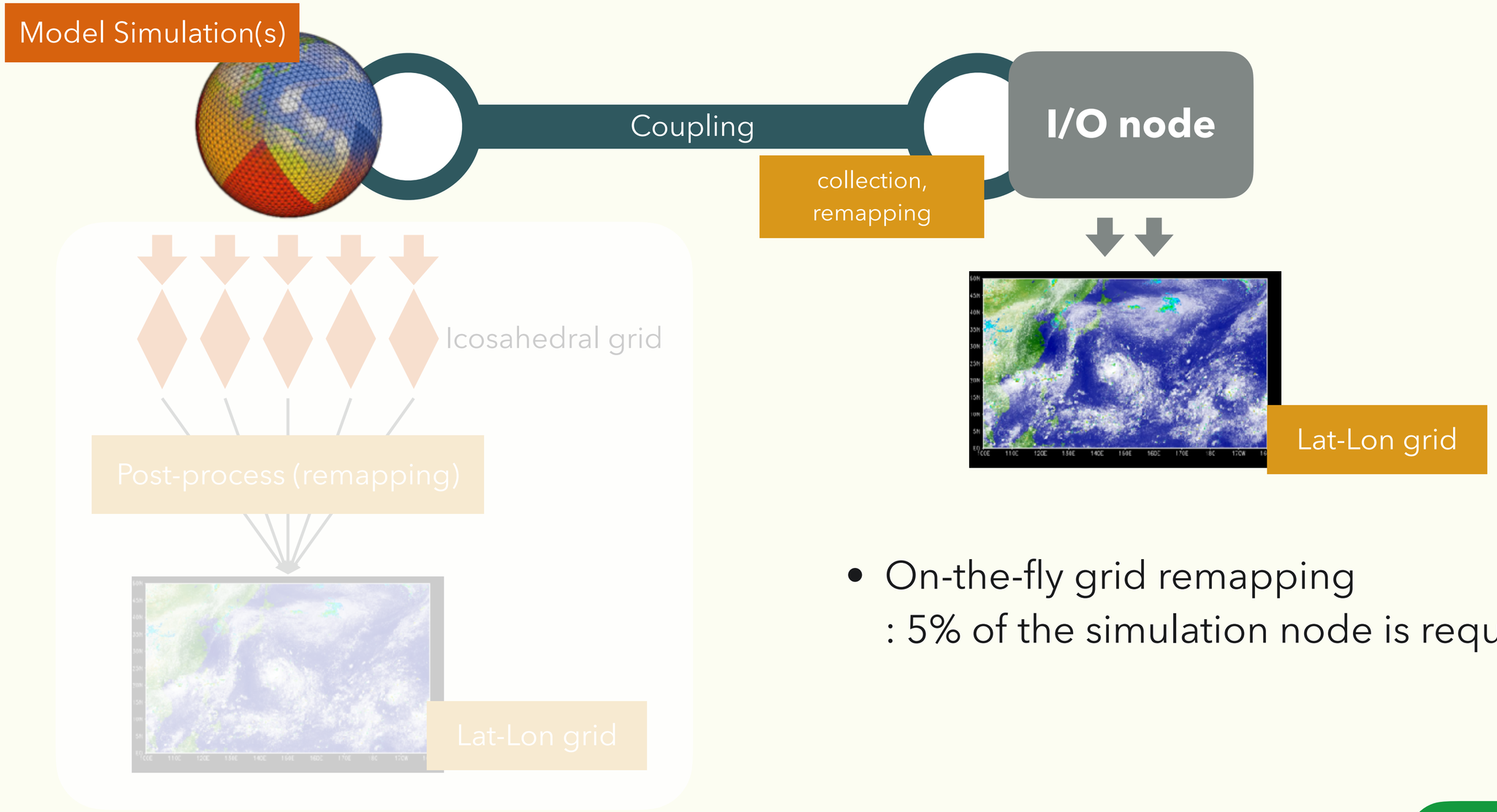


Atmospheric model (NICAM)



- h3-Open-UTIL/MP is a general purpose coupling library
  : not only for climate applications

I/O Node Coupling

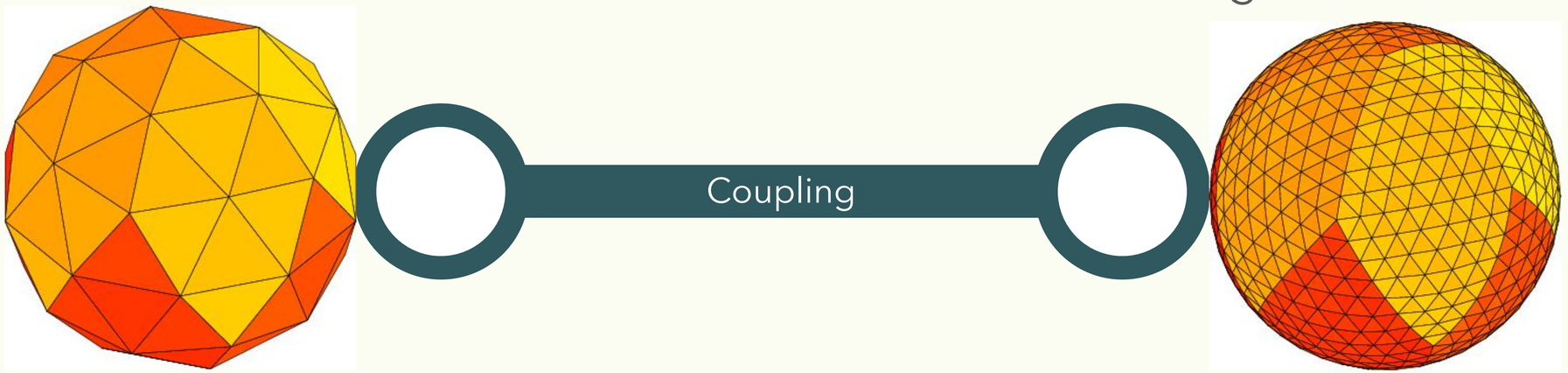


- On-the-fly grid remapping
  : 5% of the simulation node is required

Multi Detailed-level Coupling

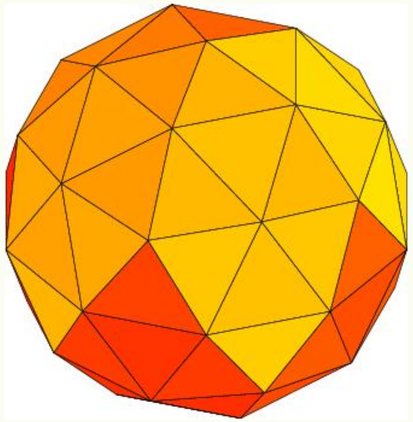
Low detailed level

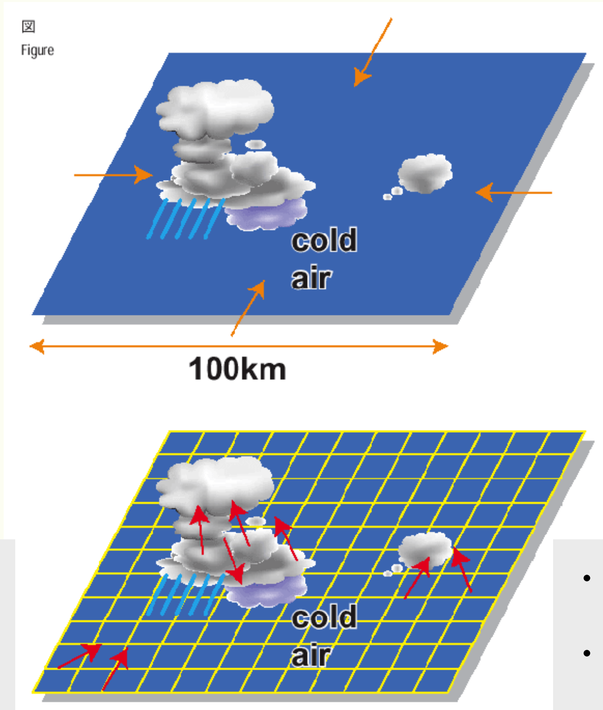
High detailed level



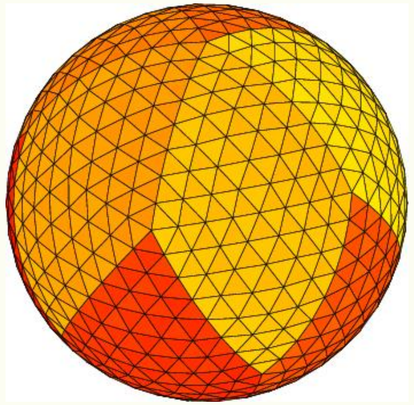
The process components (solvers) are resolution-dependent

Low-resolution
Atmospheric model





High-resolution
Atmospheric model



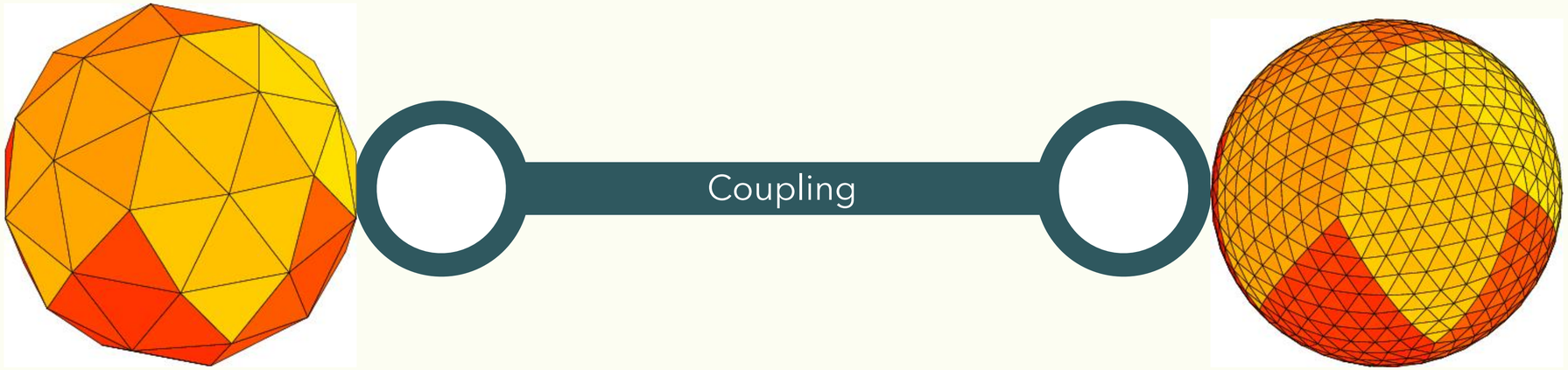
- Clouds and convections are parameterized
- Poor to reproduce heavy rainfall
- Climatology is well-tuned to the real world
- Light workload

- Clouds and convections are solved more explicitly
- Reproduce detailed meteorological phenomena
- There is non-negligible climatological biases
- Heavy workload (more than x1000!)

Multi Detailed-level Coupling (low->high)

Low-resolution
Atmospheric model

High-resolution
Atmospheric model



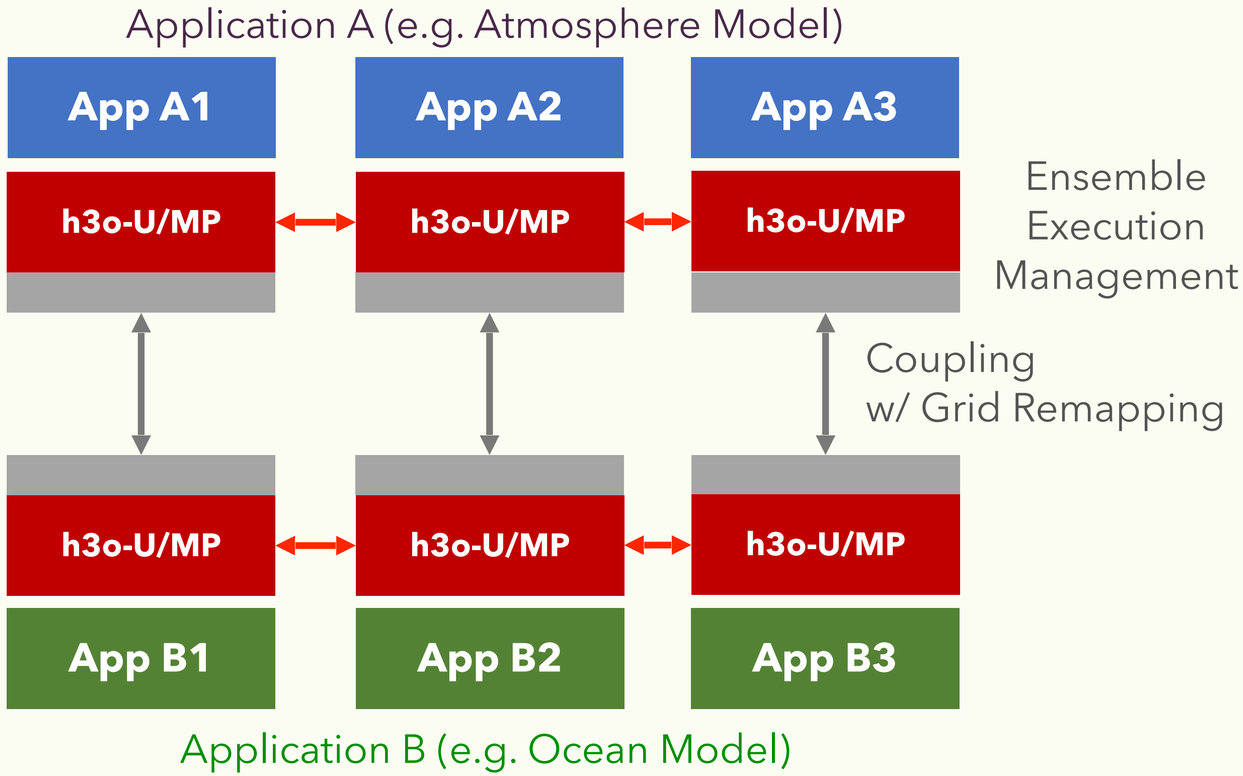
Faster simulation time

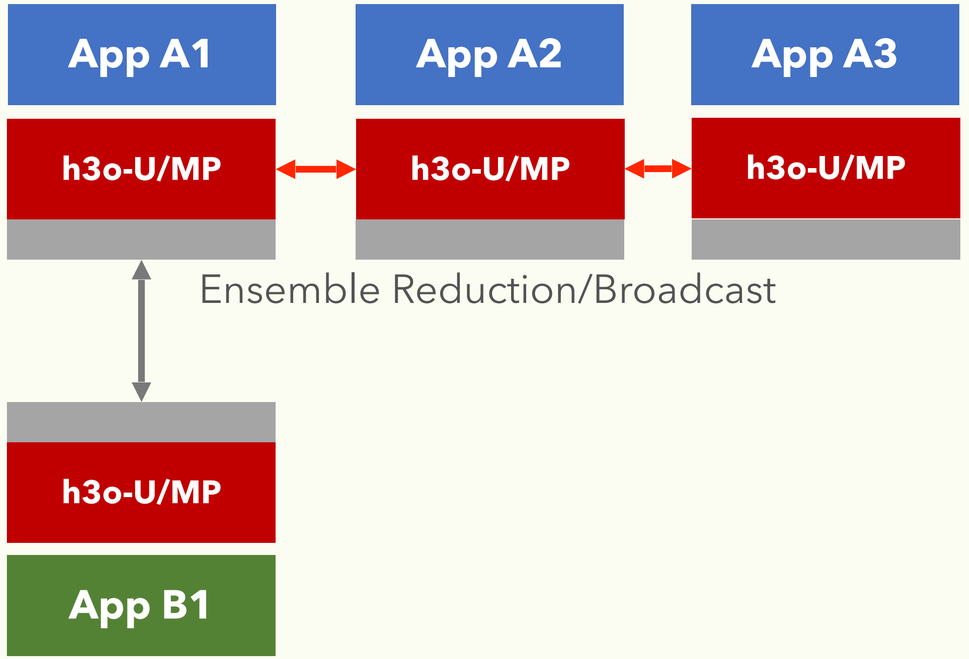
Good at detailed local weather

Nudging large-scale (low-wavenumber) states

- If low-res simulations have some additional value in climatological reproducibility, it can be helpful for covering the weakness of high-res simulations

Ensemble Coupling





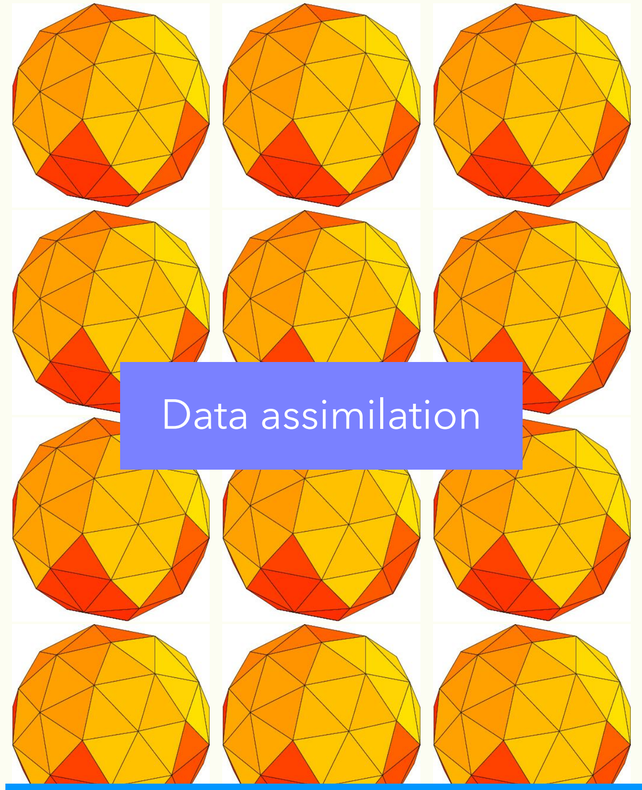
M x (A + B) execution

$\overline{\text{(M x A)}}$ + B execution

Challenges on Wisteria/BDEC-01(1)

Multi Detailed-level＋Ensemble coupling

Low-resolution Ensemble

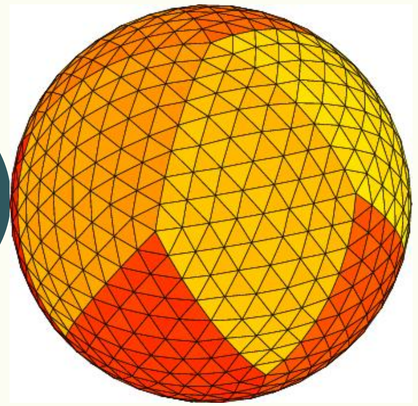


Data assimilation

Good at large-scale atmospheric state and climatology

Coupling

High-resolution



Good at detailed local weather

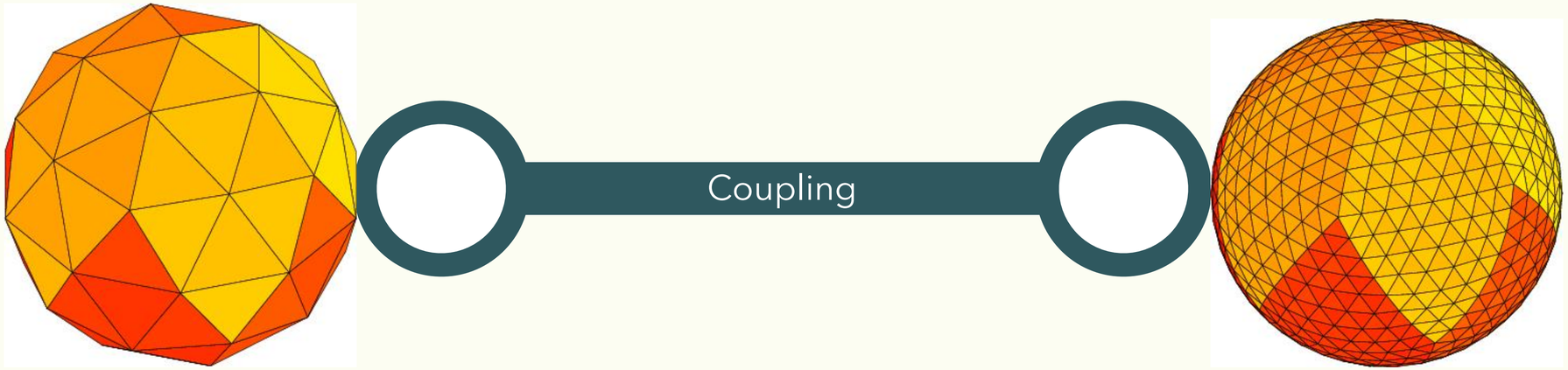
Nudging large-scale (low-wavenumber) states

Faster than high-resolution ensemble data assimilation!

Multi Detailed-level Coupling (high->low)

Low-resolution
Atmospheric model

High-resolution
Atmospheric model



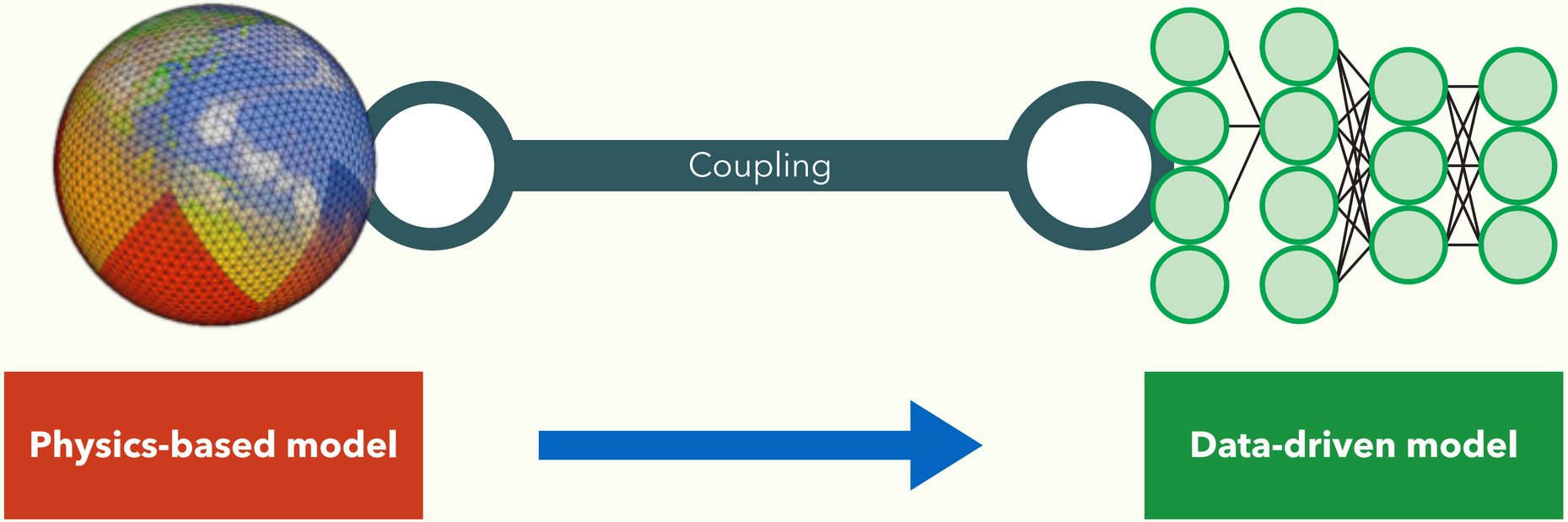
Light workload
Suitable to long-term simulation

Good at detailed local weather

Can we use the results of high-resolution simulations to further reduce uncertainty?

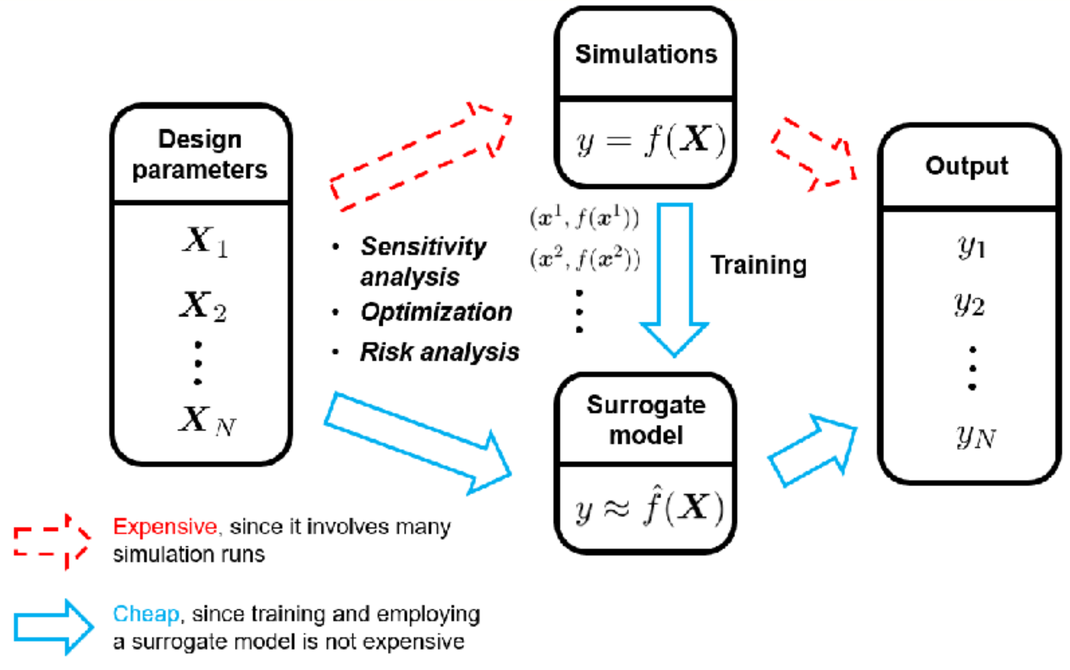
→Let's train parameterized component models!

Multi Approach Coupling

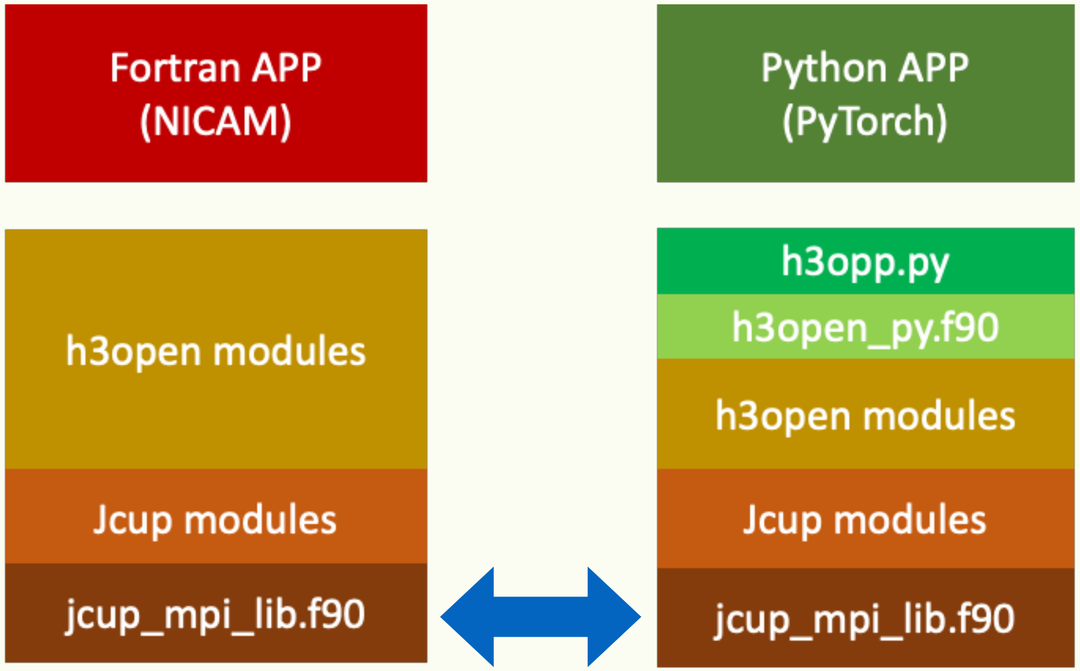


- Provide teaching data on-the-fly
- Plug-in to target component of the application
  - To make the surrogate model in the component-level
  - Gradual transition from physics-based models/legacy application

Multi Approach Coupling



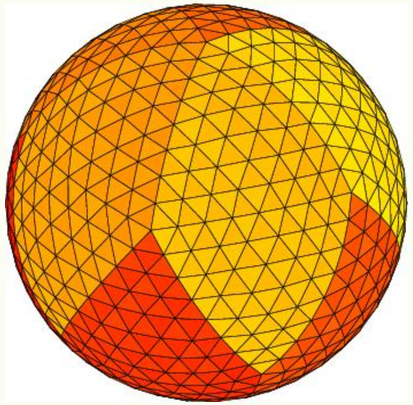
by Shuai Guo https://towardsdatascience.com/



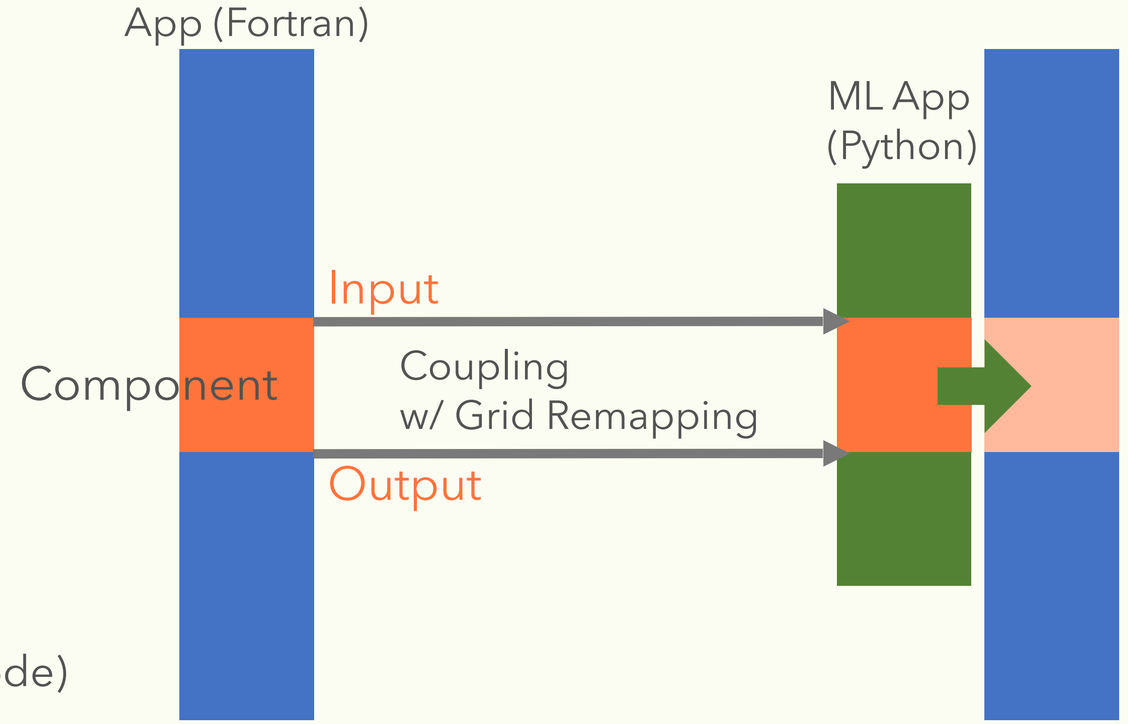
- Coupling with a legacy fortran application and a modern python ML library

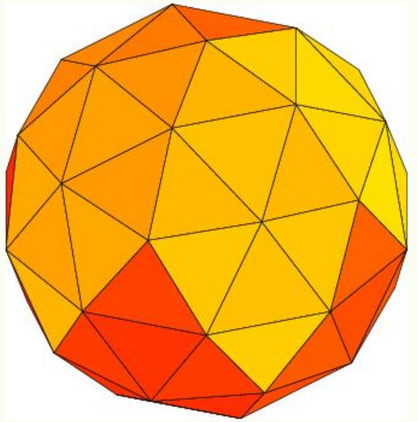
Challenges on Wisteria/BDEC-01(2)

Multi Detailed-level＋Multi Approach



High Resolution
Atmospheric Model
(Convection-Resolving Mode)

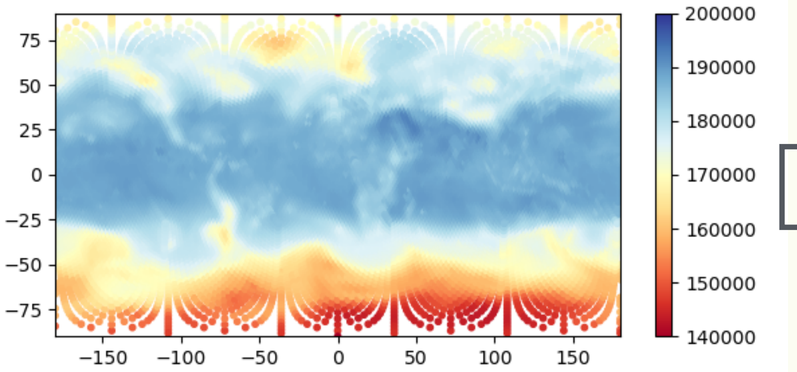




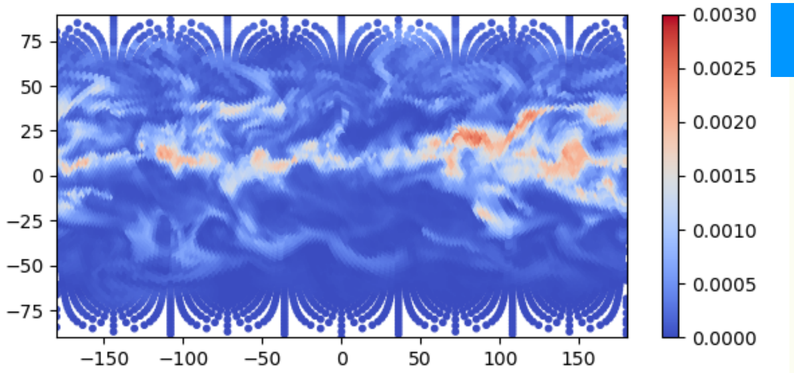
Low Resolution
Atmospheric Model
(Convection-Parameterization Mode)

- Extract input/output datasets of the cloud microphysics component from high-res simulation
- Transfer datasets from high-res to low-res with spatial remapping
- Train NN with the coarse-grained high-res input/output datasets
- Then, trained NN is used as a cloud component (surrogate model) in low-res simulation

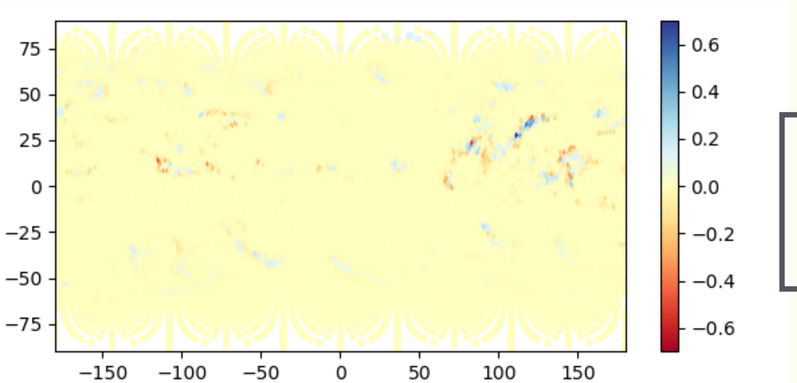
Temperature



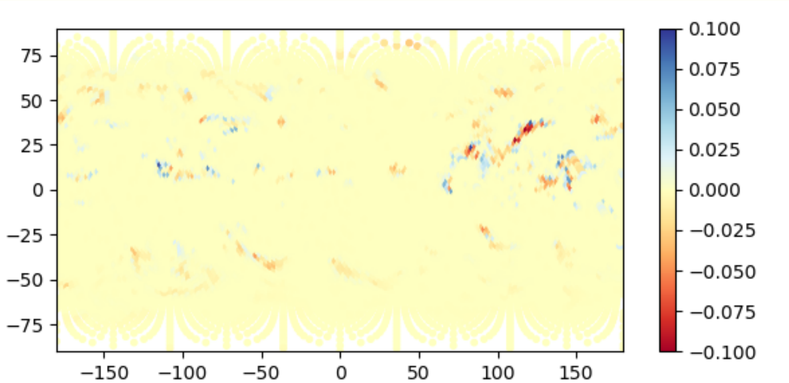
States

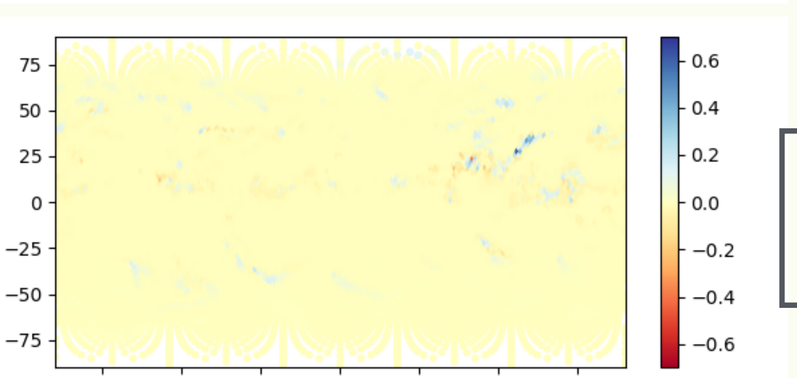


Water vapor

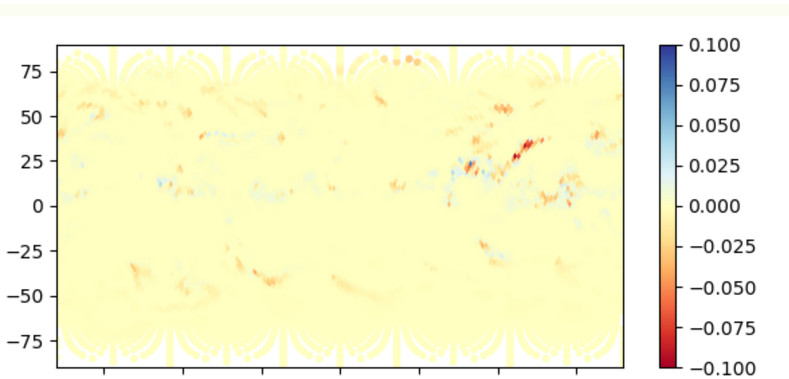


Tendency
(reference from high-res)



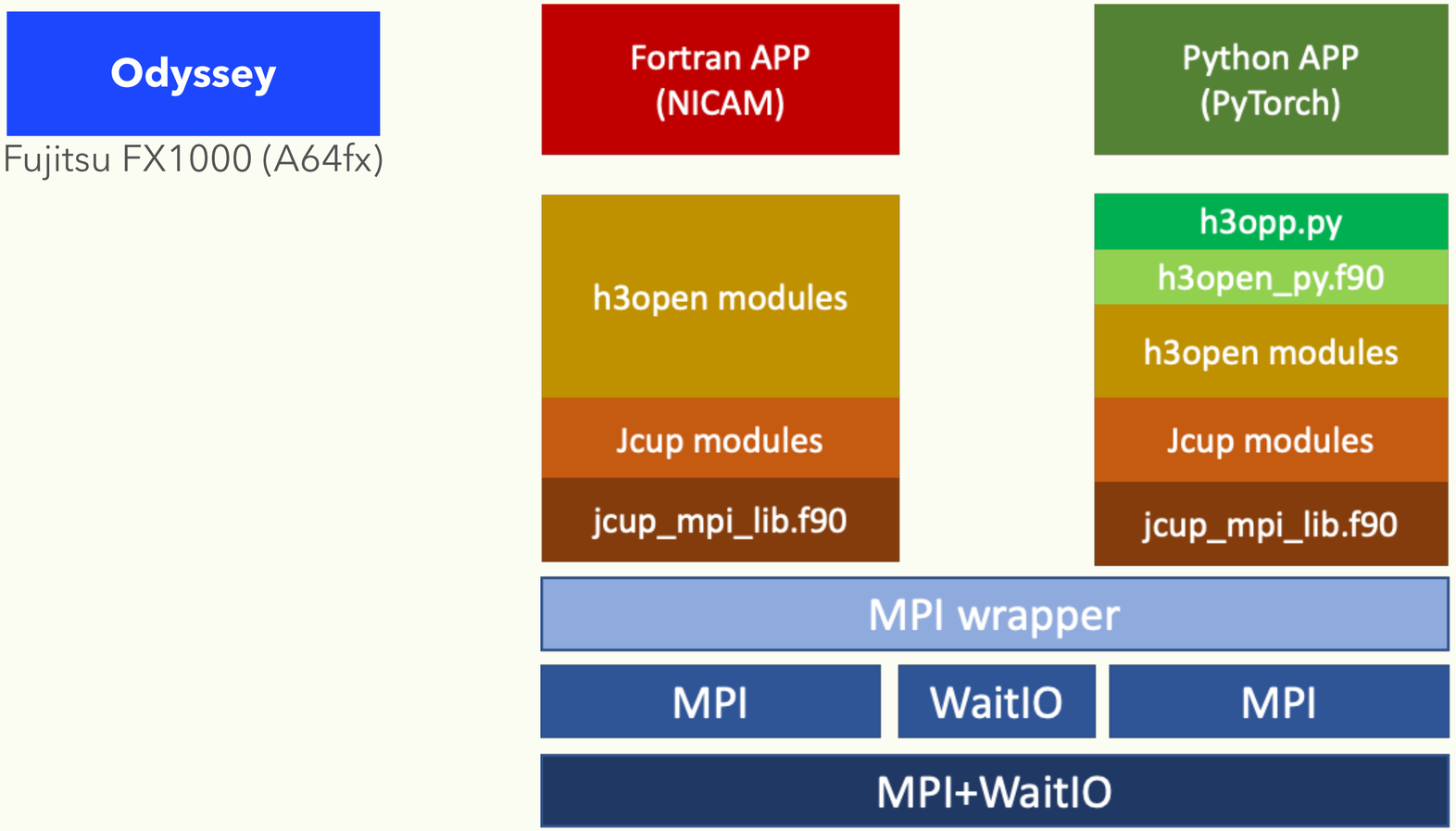


Tendency
(predicted by NN)



Challenges on Wisteria/BDEC-01(3)

Multi Detailed-level＋Multi Approach＋Multi HPC System



- Collaboration with h3-Open-SYS/WaitIO (Next presentation)
- The application is unaware of whether the coupler is using MPI communication or WaitIO

Summary

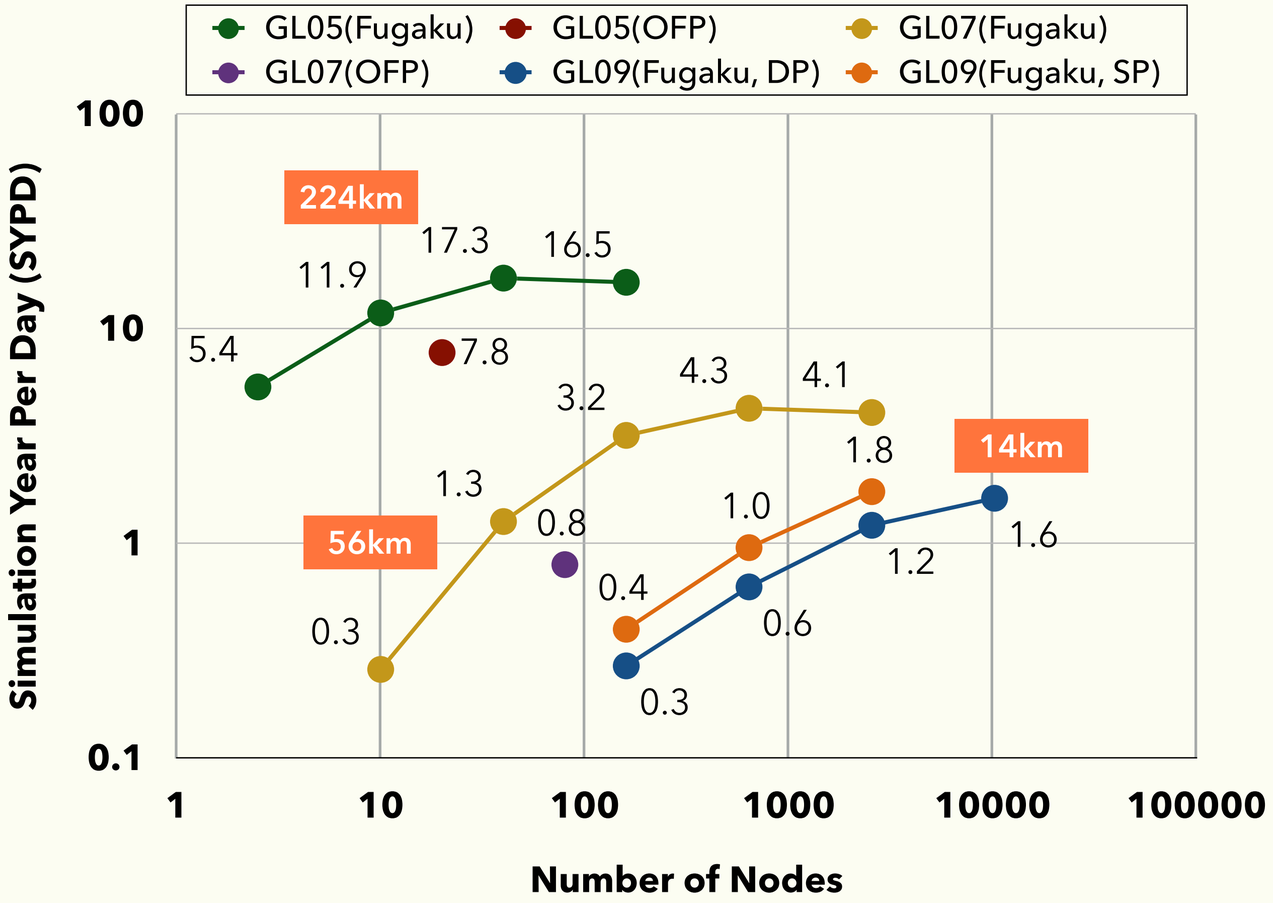
A General purpose coupling library h3-Open-UTIL/MP enables;

- multi-physics coupling, simulation-IO coupling, ensemble coupling, multi detailed-level coupling, multi approach coupling
- legacy applications to integrate HPC + AI (S+L) step-by-step

- By using **h3-Open-SYS/WaitIO** together, users will be able to perform calculations using heterogeneous supercomputers easily

backup

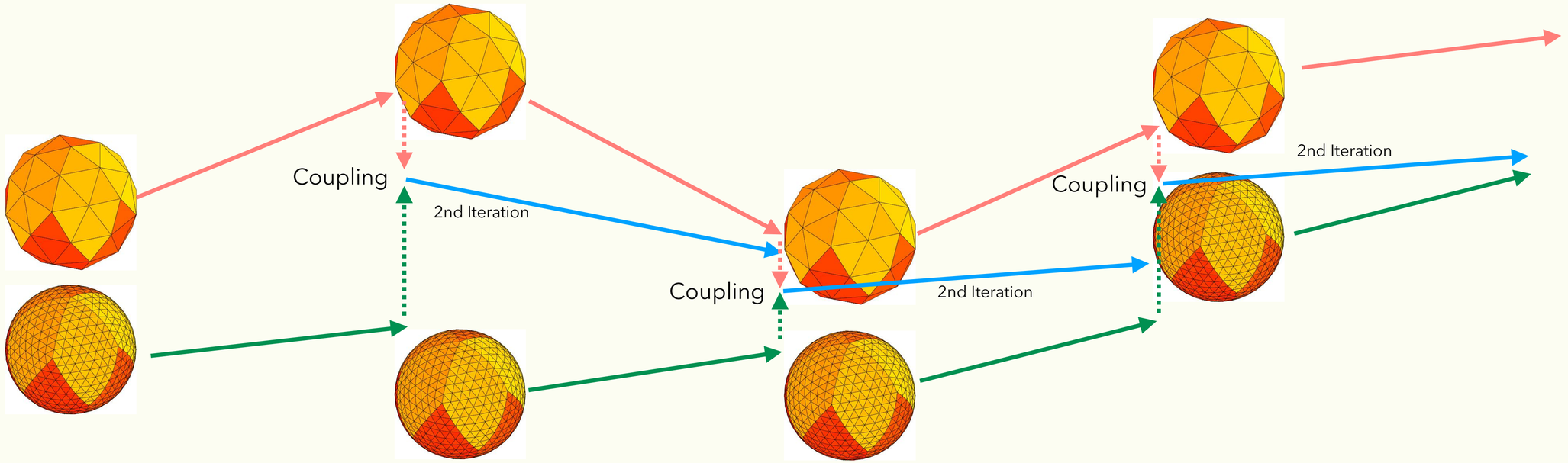
A strong-scaling problem in the high resolution climate simulations



- Doubling the horizontal resolution increases the problem size by 8 times (4 times in the spatial direction and 2 times in the time direction)
- Process division is only in the spatial direction
- Difficult to extend simulation time for high-resolution climate simulation effectively, no matter how many processes are available

Toward breaking the wall of the high resolution climate simulations

ML-based Approximate computing + Parallel in Space&Time



- Poor convergence when PinST is performed using models with significantly different levels of detail
- Improving accuracy of low resolution models using AI