Development of Library for Future Meteorological/Climate Simulations: SCALE

RIKEN・AICS
Computational Climate System Research Team
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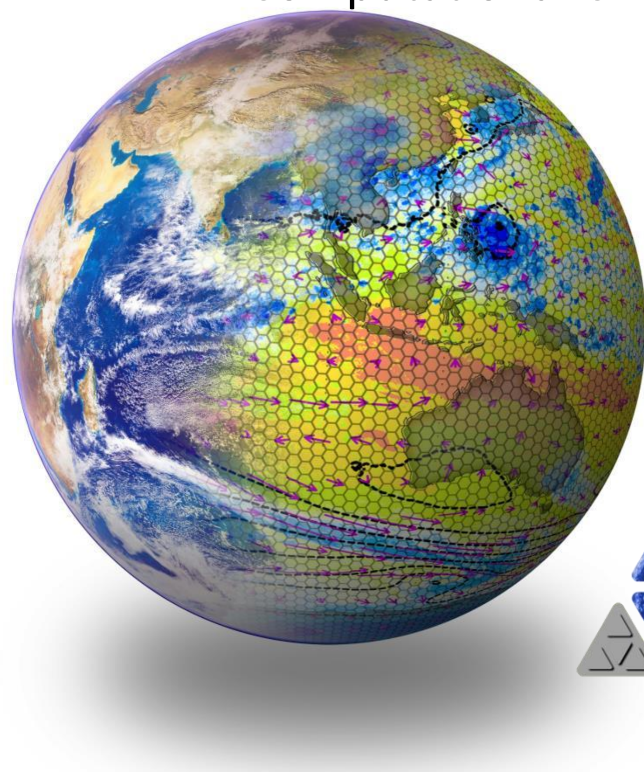
SCALE
Scalable Computing for Advanced Library and Environment



NICAM
Dynamical Core Package

Outline of my talk

- Introduction of SCALE, NICAM
  - What is NICAM/SCALE?
  - Example of large scale computation on K Computer:
    - SCALE: model-intercomparison, shallow cumulus
    - NICAM: Grand challenge like GCM simulation with very high resolution
- Possibility of collaboration
  - Infrastructure
  - Science

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Our main tools: SCALE+NICAM-DC

Physical process library
Reginoal dynamical core
Nishizawa et al. (2015,GMD)
Sato et al. (2015,PEPS)

Global dynamical core
Tomita et al.(2001,2002,JCP)
Tomita & Satoh (2004,FDR)

SCALE
Scalable Computing for Advanced Library and Environment

NICAM
Dynamical Core Package

To be merged!

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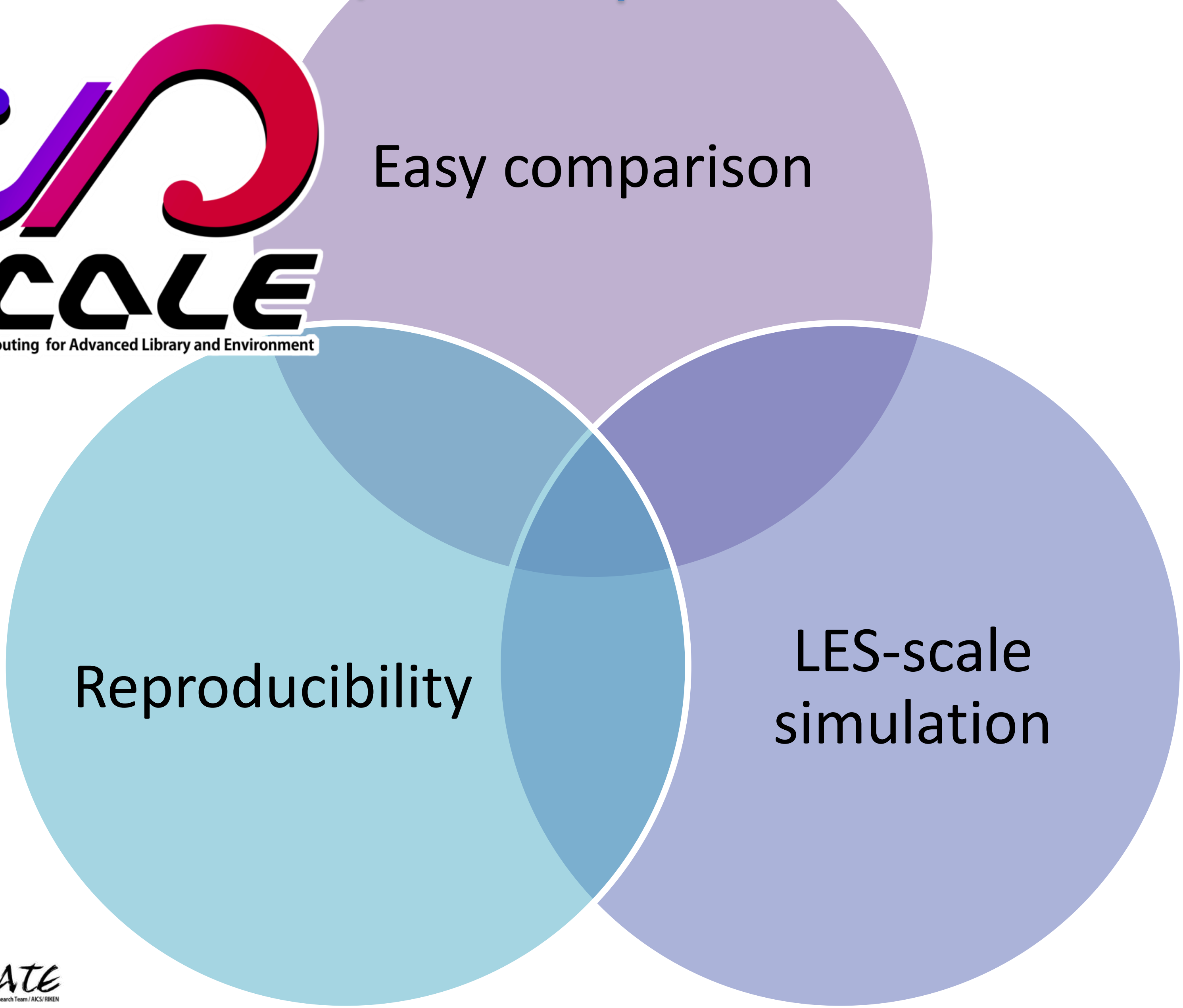
Our direction / concept of SCALE



①Easy model comparison

Model inter-comparison is a key in evaluation of the reliability of the meteorological numerical simulations.

Why model intercomparison is needed?

Estimation of uncertainty of meteorological simulation

- The model is not always based on first-principle.
- The model includes many empirical rules / hypotheses
- The model has many tunable switches, (in physical parameterization)

Difficulty in validation of simulations

- limitation of observations (coverage, resolution, quantity)
- paleo/future climate, or other planets

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But,, problem?

Inter-model comparisons

total performance

Intra-model comparison

individual schemes

We want to have just one model including all key components.

=> If so, Intra-model comparison is possible?

- Cloud microphysics, cumulus parameterization, radiation process, turbulence, and so on.
- dynamical cores, e.g.,
    - discretization schemes
    - order of accuracy of difference scheme
    - implicit and explicit temporal integration schemes
- In addition,
    - tunable parameters
    - precision of floating point

<u>The difference of model results are easily understood.</u>

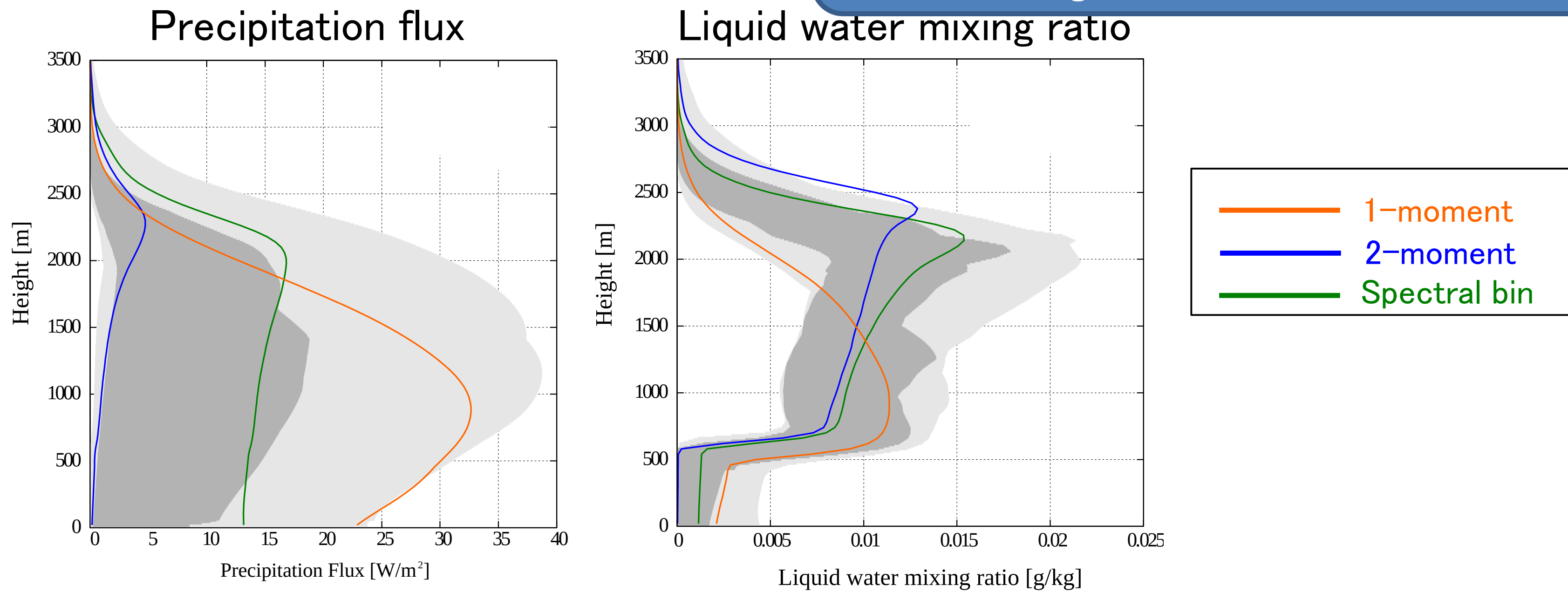
<u>1. From which does the difference come?</u>

<u>2. What is a key for representation of target phenomena?</u>

Example : Intra model comparison

Shallow cloud simulation :
The results spreads depending on the model setting

RICO experiment (van Zanten et al. 2011)



We can conclude (very very roughly) that
these differences are strongly depending on the cloud−microphysical schemes.
<u>1−moment:</u> The faster precipitation drop : due to saturation adjustment and quick autoconversion.
<u>2−moment:</u> The small an slow precipitation : due to in growth of huge droplet.

<u>Sato et al. 2015: Impacts of cloud microphysics on trade wind cumulus: which cloud microphysics processes contribute to the diversity in a large eddy simulation? PEPS, 2:23.</u>

②Reproducibility/ traceability

Scientific products should be able to be reproduced for the later verification
=> Reliability.

Openness of code, setting, and results to anyone

- SCALE is available to anyone as an open source software.

Sharing know-how

- Predecessors' knowledges have often been unpublished. (tuning parameter
  reasonable limiter of filter etc.)
- In our policy, we publish all knowledge of those, e.g., How does tune the parameter tuning, and how does set limiter.

③ High resolution computation : e.g. LES-scale simulations

Several added values are expected
in high-resolution simulations (e.g. LES)

If more fundamental physical principles can be used, uncertainty can be expected to be reduced.

- cumulus parameterization -> cloud microphysics
- RANS -> LES

Better representation of extreme detail

- finer topography / surface conditions
- less spatial averaging

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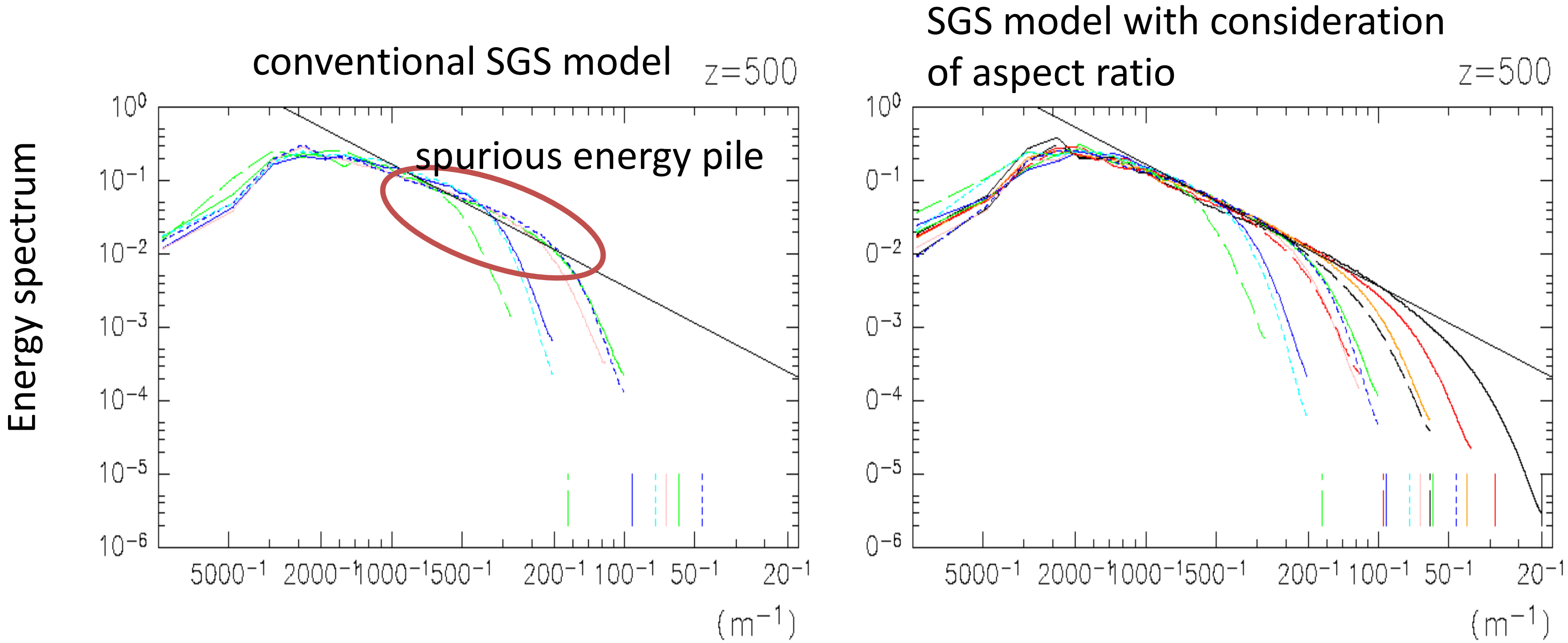
Example : Validation of large grid aspect ratio (dx/dz) in LES

Unstable PBL turbulence experiment



conventional SGS model: spurious energy pile due to small mixing length
large aspect ratio: artificial large skewness at the top of the PBL

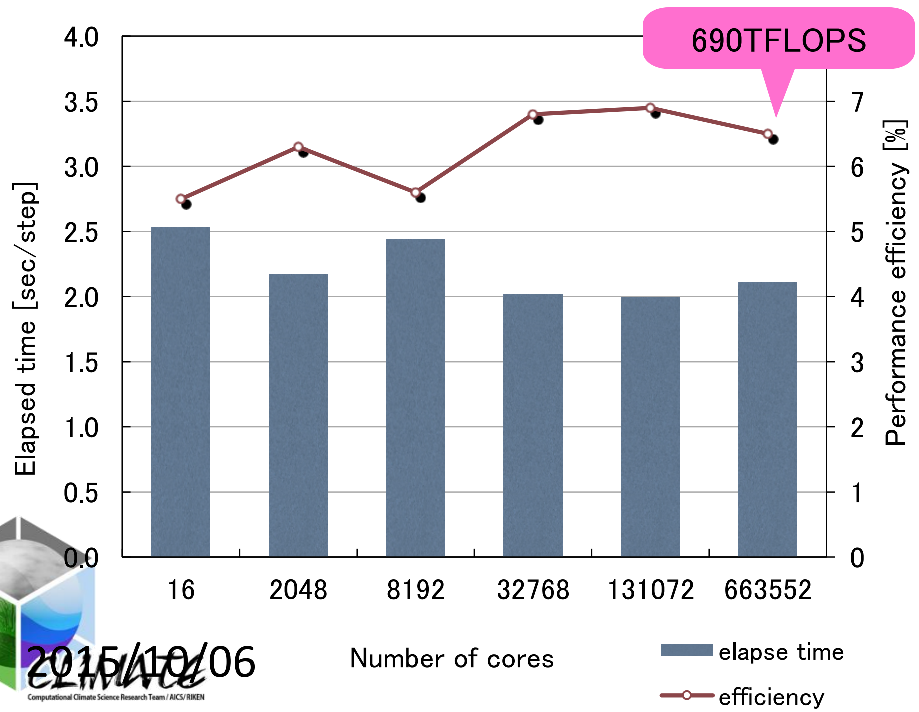
Nishizawa et al. 2015: Influence of grid aspect ratio on planetary boundary layer turbulence in large-eddy simulations, GMD, 8, 6021-6094.

Computational performance

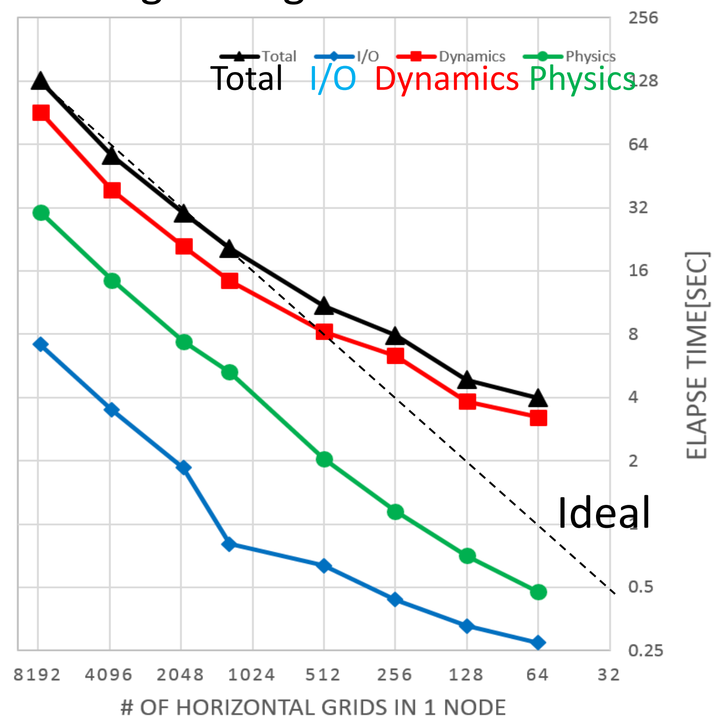
performance @ K computer

- above 10% of peak performance (dynamical core)
  - 5~8% for full simulation (including I/O)
- Almost perfect weak scaling up to full system (663,552 cores)
- good strong scaling

Weak scaling



Strong scaling



Future Issues to HPC

Still, validity of parameterization should be continued

- How does assumption of parameterizations affects results?
- Easy framework for this is needed.

Computational efficiency should be pursued

- efficient use of computational resource(week/strong scaling)
- Currently, a key issue is still bandwidth in DC.

Data explosion should be considered

- better data handling in pre/post processes
- Analysis also should be in parallel.

Current SCALE: if you are interested…

Dynamics

- Governing equations :
  3-dimensional fully compressible
- Grid system :
  Arakawa-C type
- Temporal integration :
  HEVE, HEVI, HIVI
- Temporal difference :
  3 steps Runge-Kutta scheme
- Spatial difference :
  4th order central difference
- Topography :
  Terrain-following
- Positive definitive :
  FCT scheme

Other

- Offline/Online nesting system
- LETKF assimilation system

Physical schemes

- Cloud microphysics :
  Kessler (Kessler, 1969)
  1-moment bulk (Tomita et al., 2008)
  2-moment bulk (Seiki and Nakajima, 2014)
  1-moment bin (Suzuki et al., 2010)
  super droplet method (Shima et al., 2009, *experimental*)
- Turbulence :
  Smagorinsky SGS (Brown et al. 1994, Scotti et al. 1993)
  MYNN level 2.5 (Nakanishi and Niino 2004)
- Cumulus parameterization :
  Kain-Fritsch (*in preparation*)
- Radiation :
  MSTRN-X (Sekiguchi and Nakajima, 2008)
- Aerosol microphysics:
  3-moment bulk (Kajino et al., 2013, *experimental*)
- Surface flux:
  Louis-type (Uno et al. 1995)
  Beljaars-type (Beljaars and Holtslag 1994, Wilson 2001)
- Land :
  Slab model with a bucket model
- Ocean :
  Slab ocean model
- Urban :
  Single-layer urban canopy model (Kusaka et al., 2001)

NiCAM

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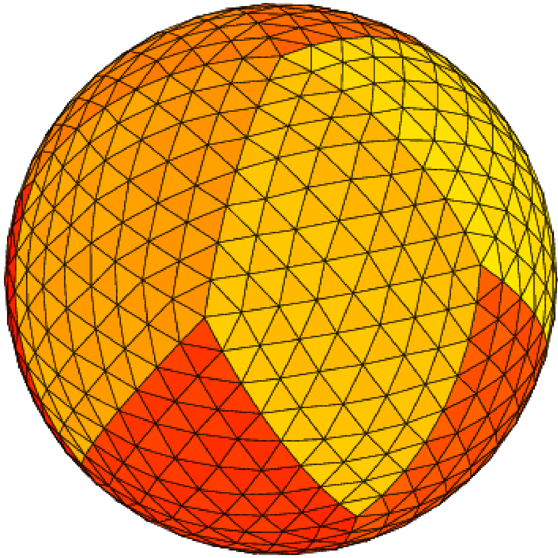
Challenge! (explicit expression of cloud)

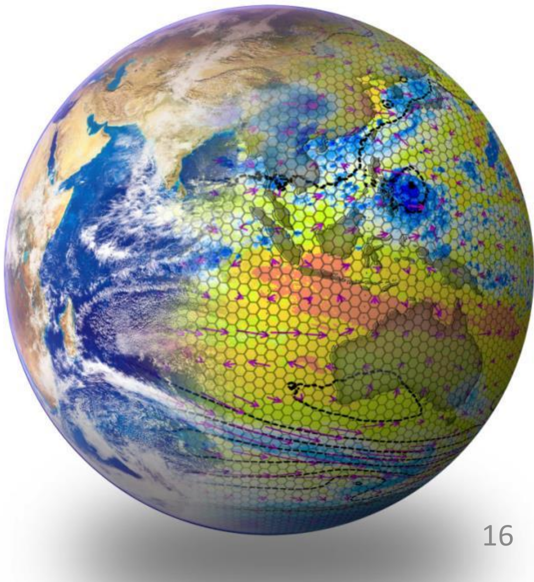
Our research community (NICAM research community)' approach:
Resolve the cloud system & related process over the globe

NICAM development : ~2000
still development is continuing!

Conceptual development philosophy

- **Explicit resolving the cloud itself**
  - Use of Icosahedral grid
    - To get a quasi-homogeneous grid for computational efficiency
  - nohydrostatic DC
    - To resolve cloud scale (deep convection, shallow cloud etc.)
  - Sophistication of cloud expression:
    - To avoid the ambiguity of cumulus parameterization and understand the cloud dynamics





Recent results on K computer (two landmark works)

Super-high simulation : sub-km grid spaceing (Miyamoto et al. 2013, 2014 GRL, ASL) : capability computing
Many ensembles by GCRM: MJO predictability (Miyakawa et al. 2014 Nature comm.) : capacity computing

Grand Challenge on K computer!

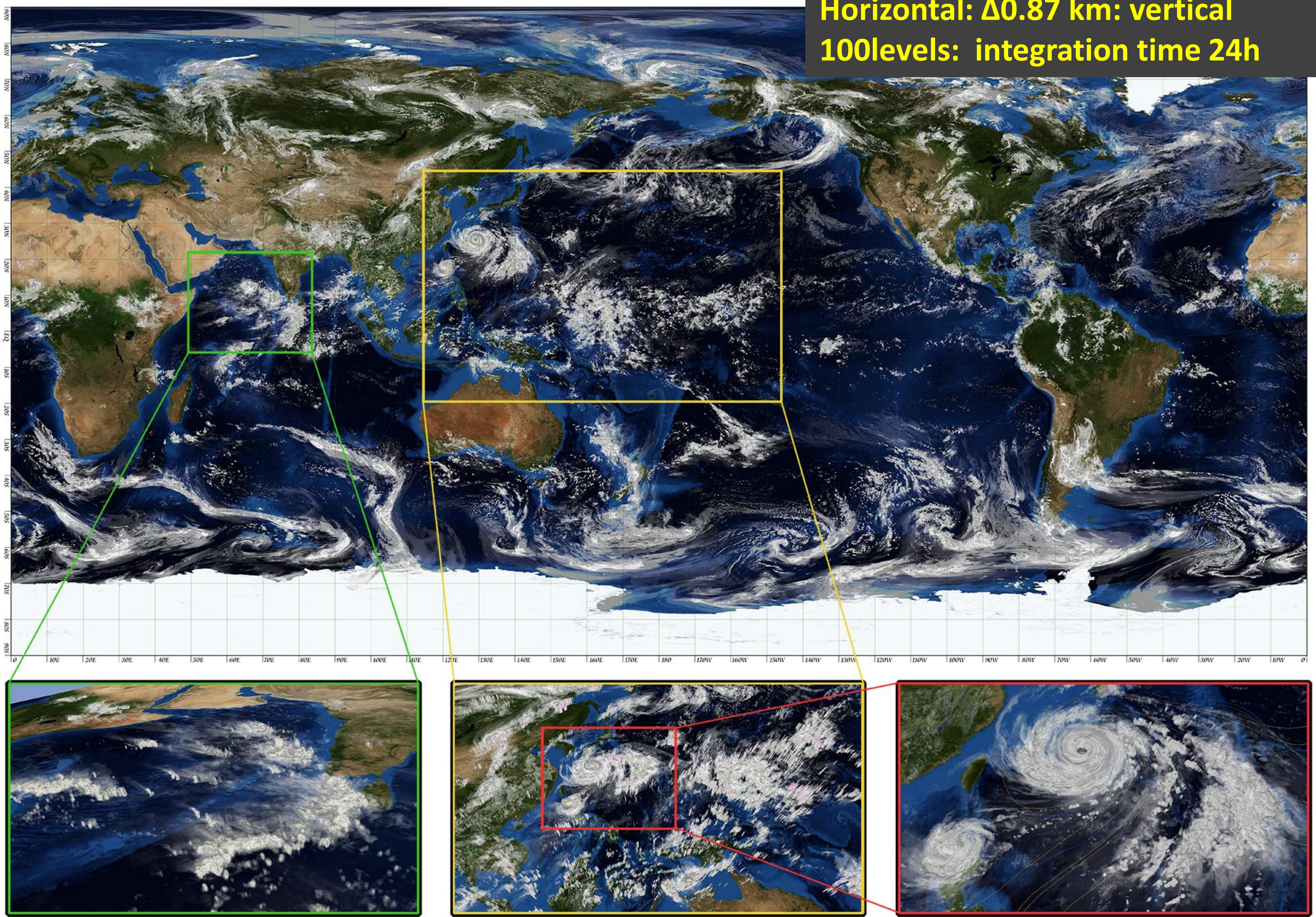
- Horizontally 860m resolution, vertically 100 levels
  - Use of ¼~full system of K-computer
  - First ever simulation with sub km horizontal grid AGCM.
- Purpose
  - One reference solution to coarser grid simulation.
    - How is the convergence?!
  - Computationally, check the scalability at the use of full resource.
- Scientific scope:
  - How is Global “picture” of deep convections?

Why challenging? What is a challenge?

Even current High-end machine, sub-km GCM may be a demonstration simulation:
However, next generation HPC enable us to integrate the long time simulation.

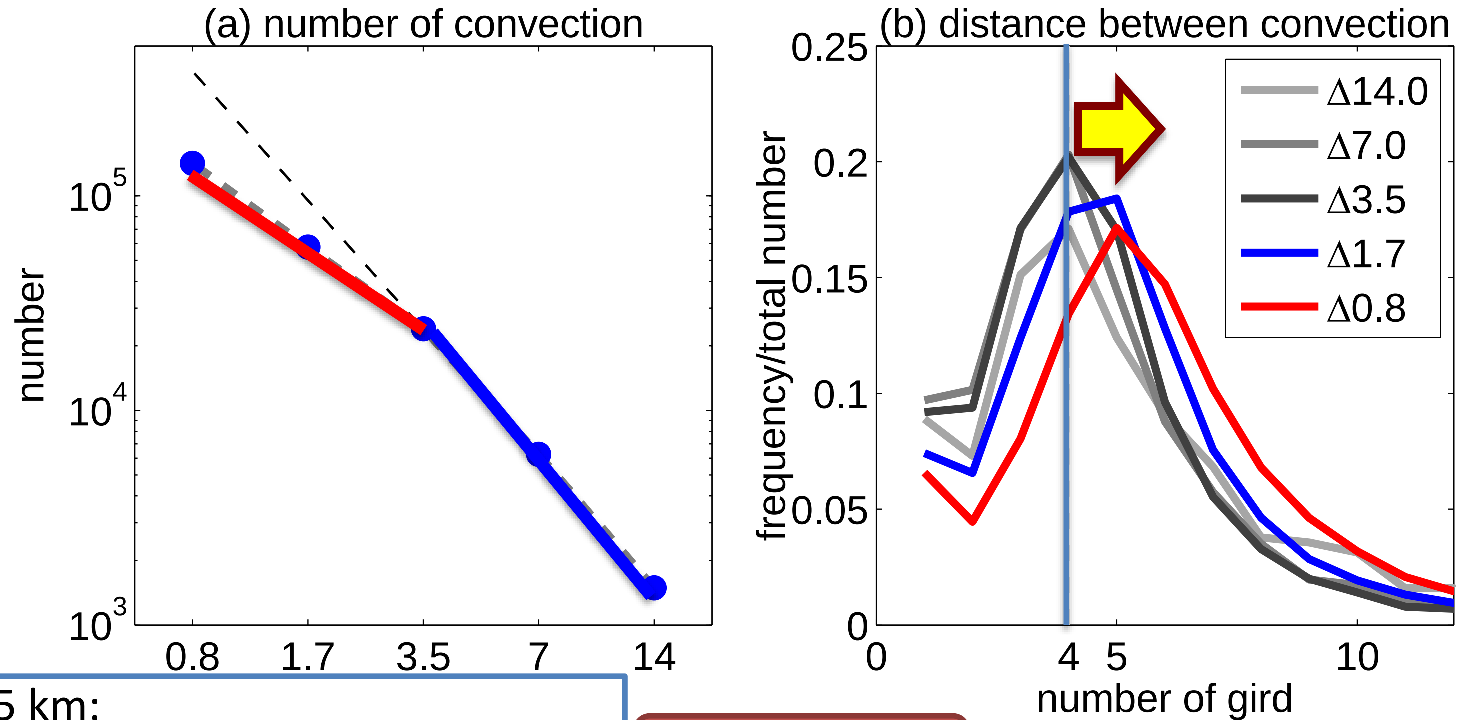
A snapshot of sub-km AGCM (NICAM)

Horizontal: Δ0.87 km: vertical 100levels: integration time 24h



Convergence of 1. number of convection 2distance of neighboring convection

Miyamoto et al.2013 Geophys. Res. Lett.



Δx ≧ 3.5 km:

- # of conv.: increase by factor of 4
- Conv. distance between convection: 4 grids => unphysical?

Δx ≦ 1.7 km:

- # of conv.: decrease in increasing rate
- Conv. distance: >5 grids => close to the nature

conclusion

Convection features (structure, number, distance

<u>**change between Δ3.5 km ⇔ Δ1.7 km**</u>

- Δx should be 2.0～3.0 km to resolve convection in global models

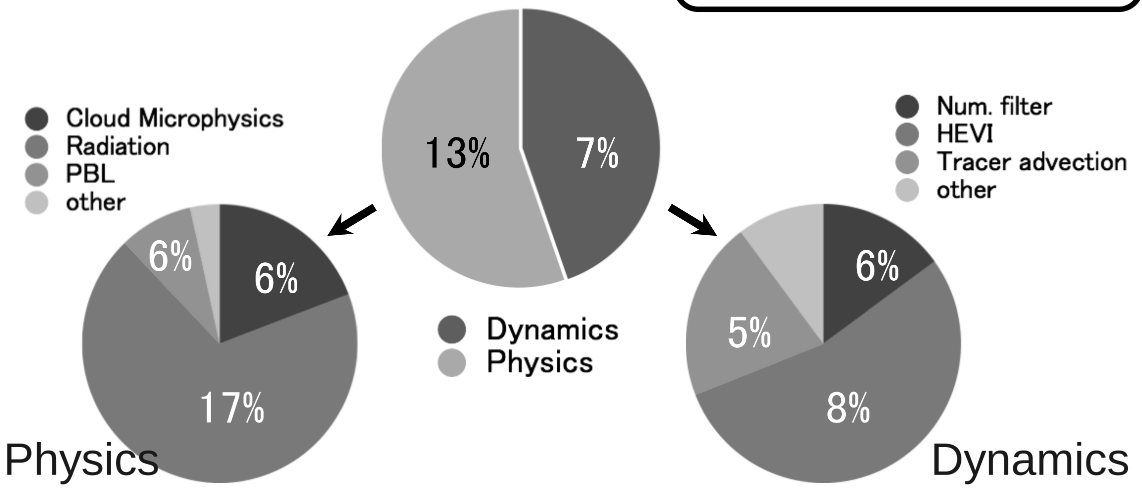
<u>Resolution of 2km is tipping point!</u>

Efficiency of NICAM on K Computer

H. Yashiro
(RIKEN/AICS)

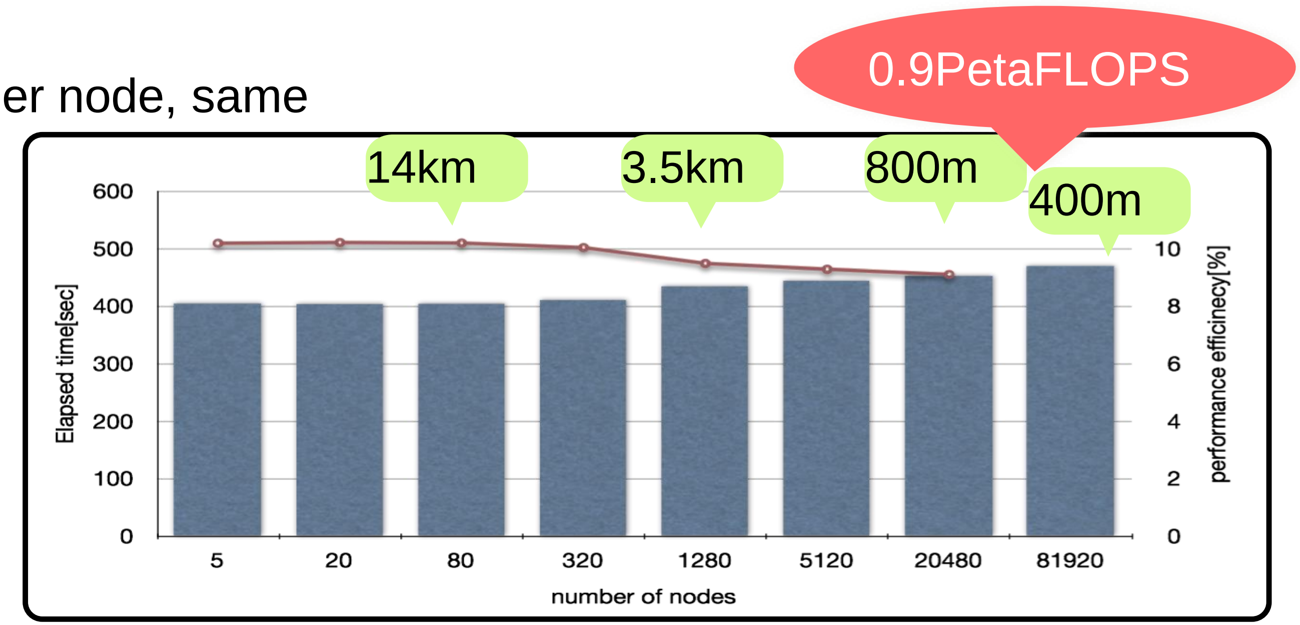
Performance efficiency

- Just after porting from ES : ~4%
- Cache optimization to stencil operators : ~5%
- Cleaning the time-wasting codes : ~7%
- Modify conditional branches, refactoring : **~10%**



Weak scaling test

- Same problem size per node, same steps
- Good scalability



Where shall we go after this?

1. Higher resolution
2. Much more ensembles
3. More Sophisticated physics

Ultimately, one direction,…, and challenging issue is higher resolution.

GCRM => GLES?!

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AGCM milestone from GCRM to GLES?!(roughly estimate)

Assumption: sustained peformance 10% (we wish)

Resolution Grid interval/ level	Total FLOP for 1day simulation	Machine	efficiency (%)	Elapse time for 1day simulation	Elapse time for 1 month simulation	What's resolved? What is meaningful for scientific advance?
3.5km/L40	[illegible]	131TFLOPS (ES2)	15%	3.2hour	4day	Meso-scale convection system. Cold pool dynamics
800m/L100	36800P	10PFLOPS (K computer)	10%	10hours	12.5days	Convection resolving?
400m/L100	295000P	1EFLOPS	10%	50min	24days	Definitely convection resolving(expected)
200m/L100	2360E					Breakthrough does not exits. But good expression of deep cloud
100m/L100	18880E					Insufficient for LES
50m/L200	302Z	100EFLOPS	10%	50min	24hour	Global LES???

We are here

Exa scale era

Tentative goal?

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Possible Collaboration issue

~ along introduction of our team mission~

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Direction of our research in AICS in next 5 years (Candidates of colabolation)

- **Infrastructure:**
  - **Extension of basic library SCALE :**
    - **User friendly library**
      - **How does standard interface determine?**
        - » **Exchange of subroutine level is very useful for model inter or intra comparison.**
      - **E.g. CBLEAM activity in Japan (initiated by AICS our team)**
    - **Massive parallel analysis routines for acceleration of scientific output, social outcome**
      - Not only acceleration of simulation itself but also acceleration of analysis phase:
      - Adding them to SCALE
    - **Easy programing and high performance computing:**
      - DSL(Domain Specific Language)? e.g. stencil DSL?

Direction of our research in AICS in next 5 years (Candidates of colabolation)

- **Science:**
  - **<u>BIG DATA assimilation:</u>**
    - **Now, developing….**
      - **NICAM + LETKF (with DA research team & post K priority subject)**
        - **Many satellite data is available.**
        - **One goal : Reanalysis data by cloud resolving model**
      - **SCALE+LETKF(with DA research team)**
        - **PA data provides tremendous information in time and space.**
        - **We are tackling to each cumulus with 30min lead time**
  - **<u>Reginal Climate assesement! : downscale to city level</u>**
    - **Disaster prevention and mitigation, adaptation**
      - Multi-model ensemble (SCALE can do it!) drastically reduce the uncertainties for the future climate assessment in the regional model
      - Model bias reduction by data assimilation
        - e.g. Determination of unknown parameters
  - **<u>Planetary science</u>**
    - **Generalization of earth knowledge**
  - **Theoretical issuu**
    - **Moist LES theory**

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NICAM870m/L96 animation

NICAM 870 m - 96 levels

Real Case Simulation: 25 - 26, Aug., 2012

SPIRE field-3: Study of extended-range predictability using GCSRAM

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風龍：本名吉田龍二、理研AICS複合系気候科学チーム所属、博士（理学）

2011年彗星のごとく現れ、京を用いた計算の可視化において、数々の名作を生み出してきた。2014年学位取得後、その技にますますの磨きがかかり、業界（？）でも引く手あまた。今後の活躍（**研究も？**）が期待される若手のホープである。

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