Improvement of MPAS on the Integration Speed and the Accuracy

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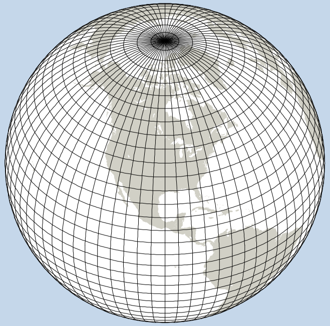
Contents

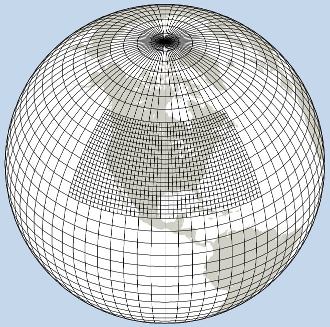
Introduction

- KISTI has been collaborating on a development of MPAS with NCAR MMM since 2014

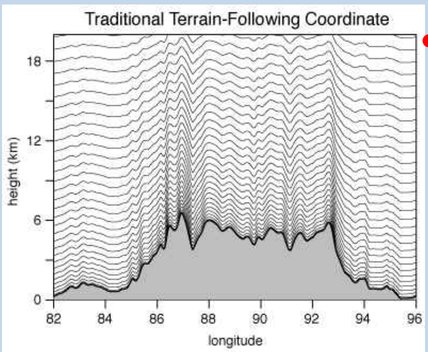
WRF



- Lat-Lon global grid
  - Anisotropic grid cells
  - Polar filtering required
  - Poor scaling on massively parallel computers



- Grid refinement through domain nesting
  - Flow distortions at nest boundaries

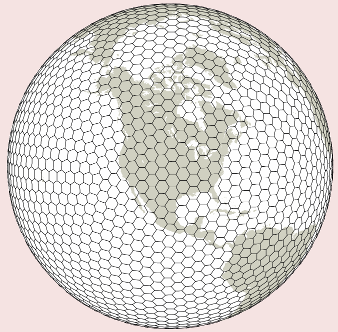


- Pressure-based terrain-following sigma vertical coordinate

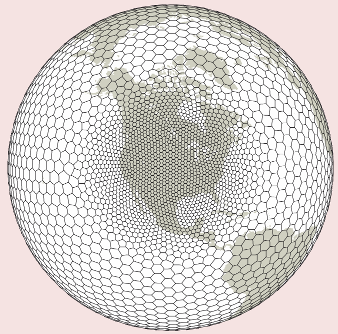
※ A hybrid sigma-pressure vertical coordinate is added in WRFV3.9

MPAS

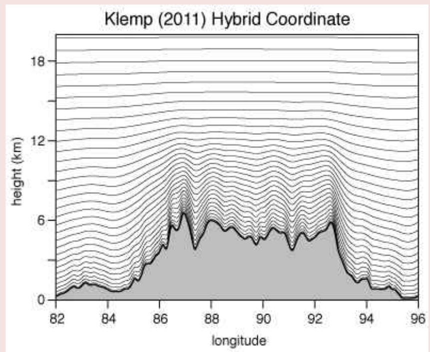
- Unstructured Voronoi (hexagonal) grid
  - Good scaling on massively parallel computers
  - No pole problems



- Smooth grid refinement on a conformal mesh
  - Increased accuracy and flexibility in varying resolution



- Height-based hybrid smoothed terrain-following vertical coordinate
  - Improved numerical accuracy



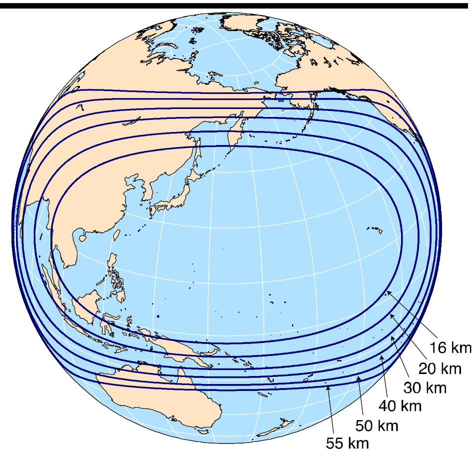
Park et al. (2015, KMS)

Introduction

- MPAS-TC (K-MPAS) which is suitable for typhoon forecast over the western Pacific has been developed through improving physics schemes and constructing appropriate variable resolution meshes.

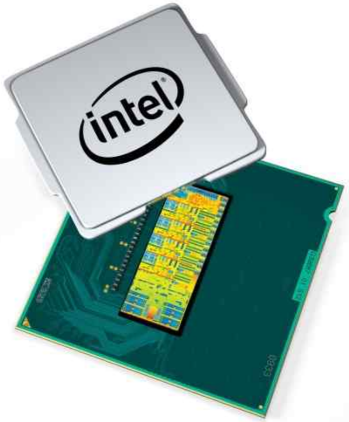
	MPAS(v5.2)	K-MPAS(v5.1)
Convection	Tiedtke scheme (Tiedtke, 1989; Zhang et al., 2011)	Tiedtke scheme - Optimization for the simulation of TCs
Surface flux	Monin-Obukhov (Fairall et al., 2003)	Monin-Obukhov - Improvement of surface flux (Davis, 2008) - False alarm in which strong typhoons were frequently occurred were reduced
1D ocean mixed-layer	X	O
GPU acceleration	X	O

- For the next steps, KISTI is making efforts to improve the integration speed and the accuracy of K-MPAS
  - Development of CPU-GPU heterogeneous code
  - Development of ensemble-based data assimilation system



15-60 km

CPU and Accelerator



- In the past, it was common to use CPU-based cluster system
- Recently, CPU and accelerator can be used together to improve the computing performance

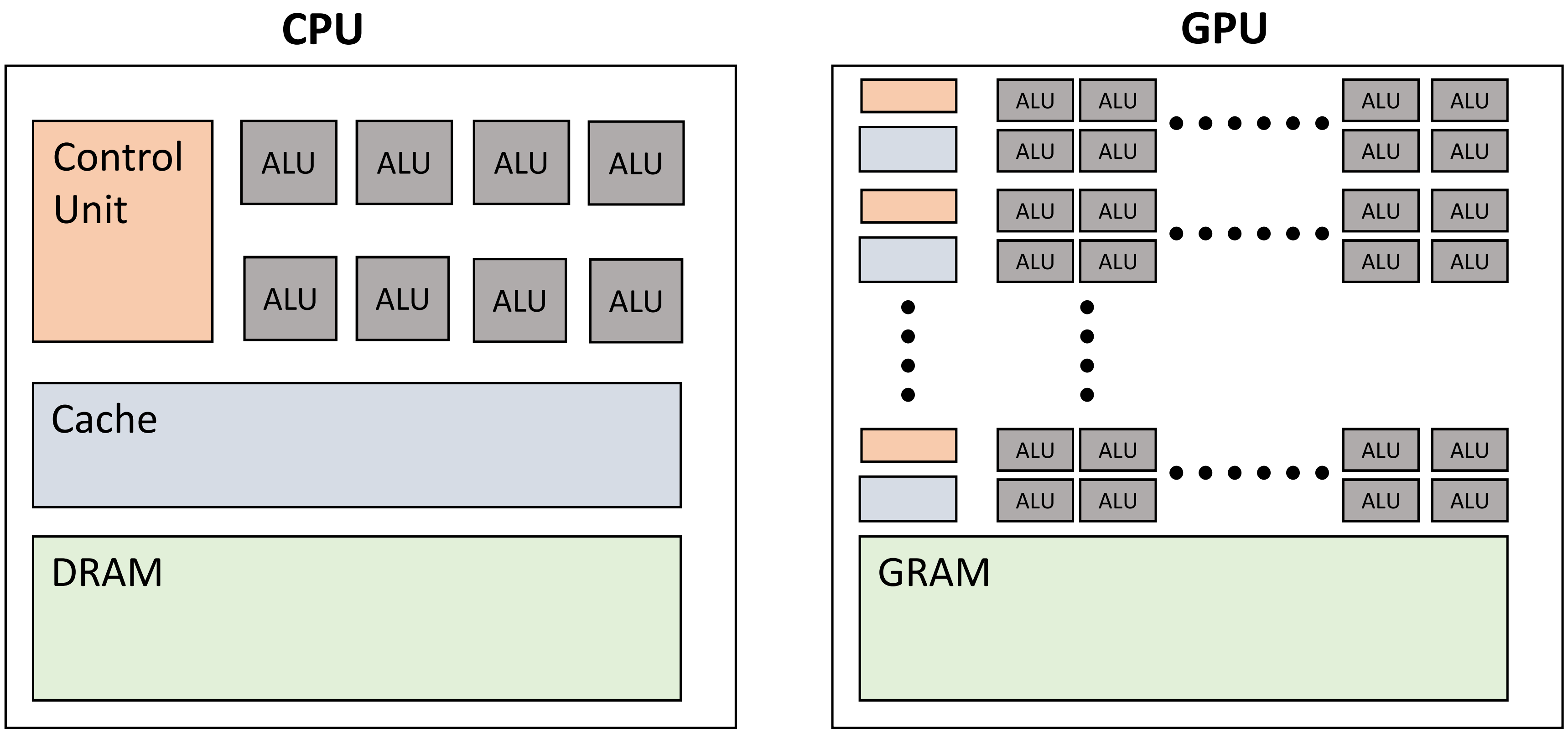
intel inside Xeon

NVIDIA TESLA

AMD FIREPRO

intel inside Xeon Phi

GPU Accelerator



- **Multi core CPU**
- **Few very complex core**
- **Single thread performance optimization**

- **Many core GPU**
- **Thousands of simpler cores**
- **Thousands of concurrent hardware threads**

From http://www.electronicspecifier.com/communications/vivante-es-design-magazine-gpus-the-next-must-have

How to use GPU for General Purpose

CUDA -Fortran, C, C++, Python

OpenCL -C, C++

OpenACC -Fortran, C, C++

```
!$acc data create(n0sfac) &
!$acc   pcopy(qrs,rslope,rslopeb,rslope2,rslope3,vt,den,denfac,t)
!$acc kernels
      do i = its, ite
        do k = kts, kte
          supcol = t0c-t(i,k)
          n0sfac(i,k) = max(min(exp(alpha*supcol),n0smax/n0s),1.)

                  . . . . . . . . . . . .

          vt(i,k,1) = pvtr*rslopeb(i,k,1)*denfac(i,k)
        enddo
      enddo
!$acc end kernels
!$acc end data
```

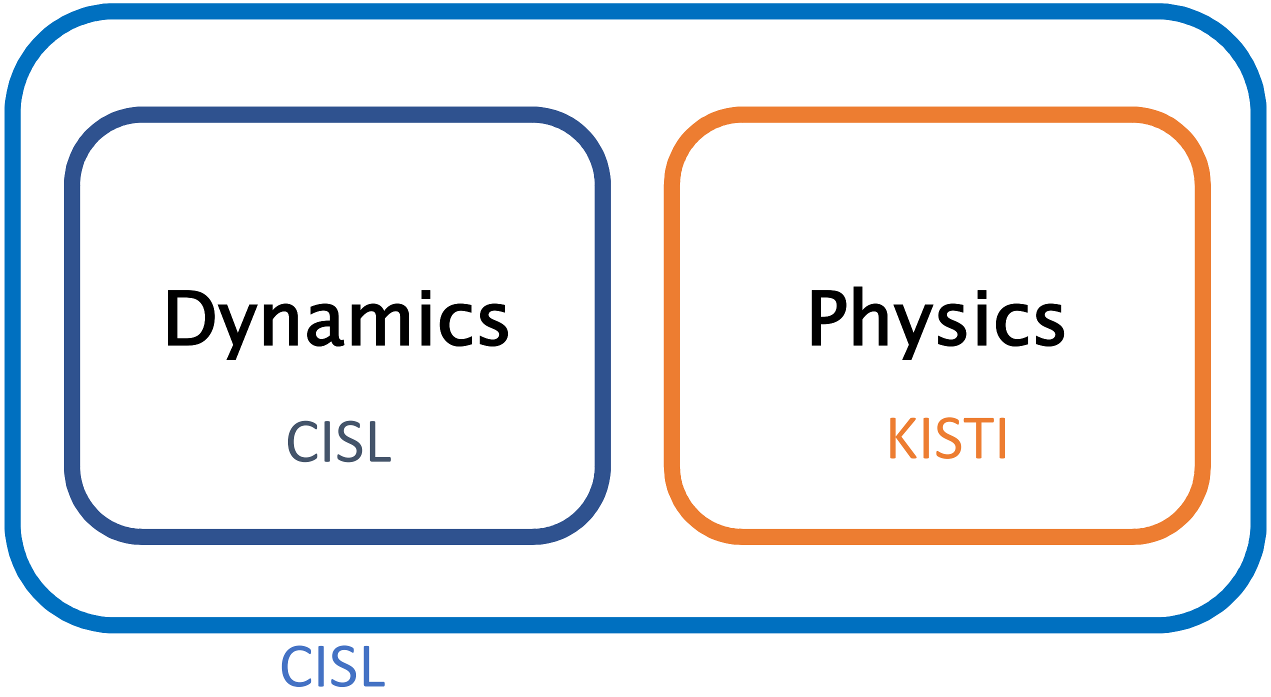
ex) Microphysics scheme in MPAS (i.e., WSM6) with OpenACC directives

- “More Science, Less Programming”
- OpenACC is a directive-based programming model
- Easy, Simple, Powerful

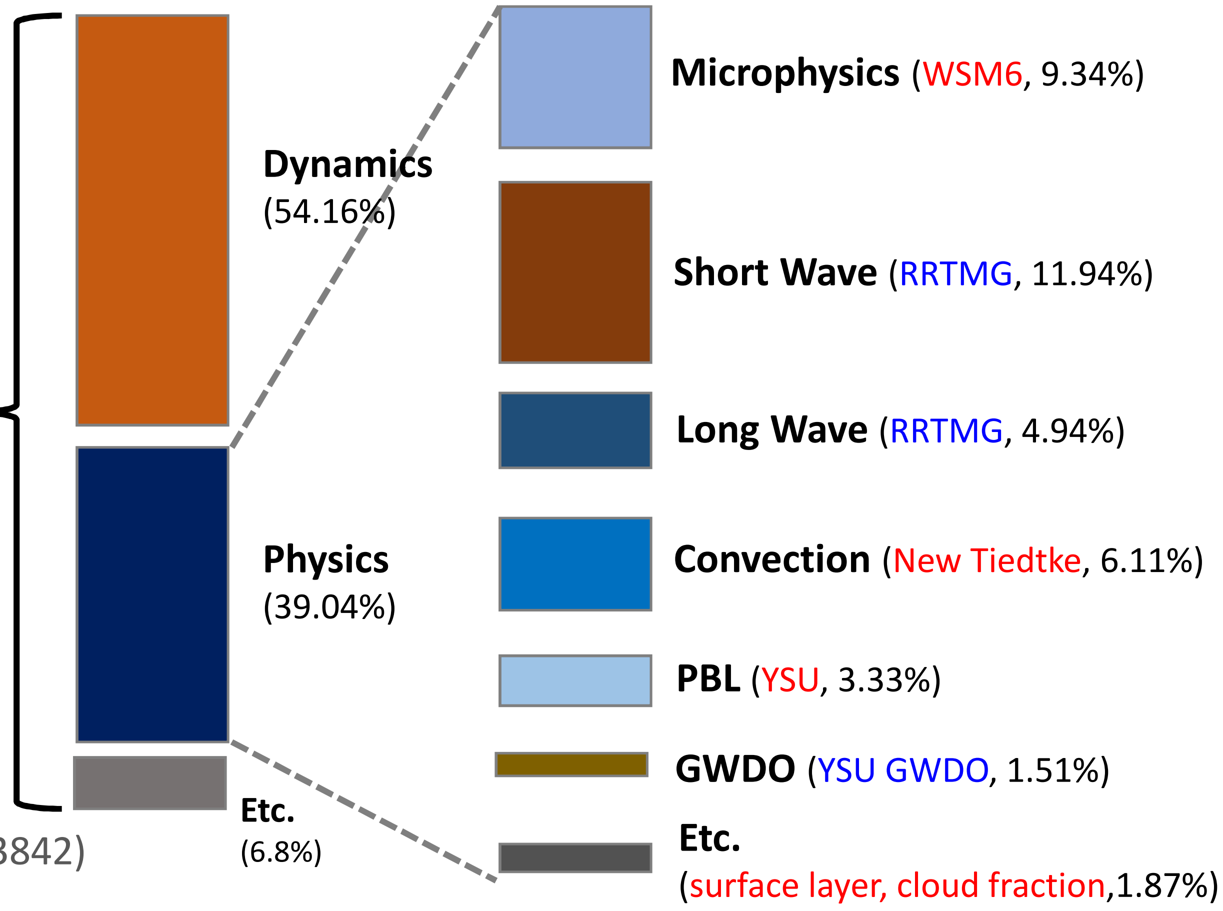
GCC · CRAY · PORTLAND GROUP · OpenACC Directives for Accelerators

Development of CPU-GPU heterogeneous code

- For the development of MPAS hybrid code, we have discussed with NCAR CISL since December in 2015.



MPAS Physics Execution Time on CPU

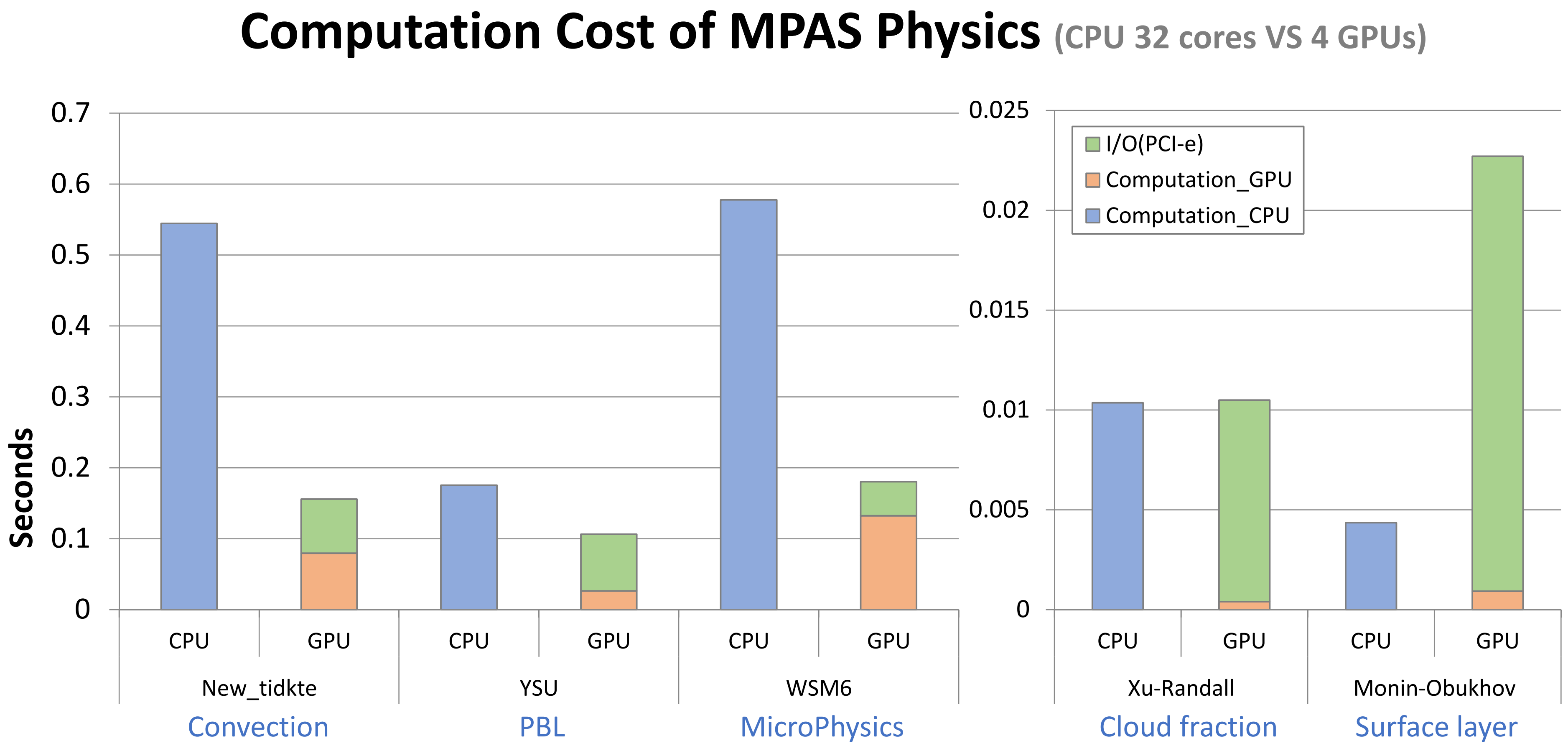


- 60km resolution (# of cells: 163842)
- 41 vertical layers
- dt=180s
- 1 day forecast

RED : Ported on GPU

BLUE : Plan to port on GPU

GPU Acceleration Performance



PGI-17.5, 60km resolution (# of cells: 163842), 41 vertical layers, dt=180s, 1 day forecast
Haswell E5-2698 v3 @ 2.30GHz, dual socket 16-core
NVIDIA Tesla P100

Performance of K-MPAS for TC track forecast

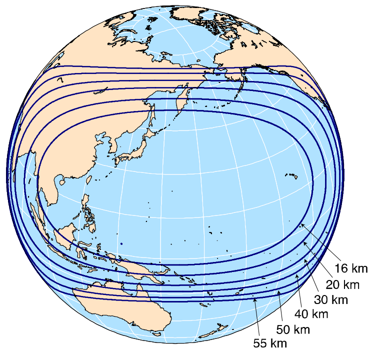
- 2016 Typhoon track forecast (12 cases)

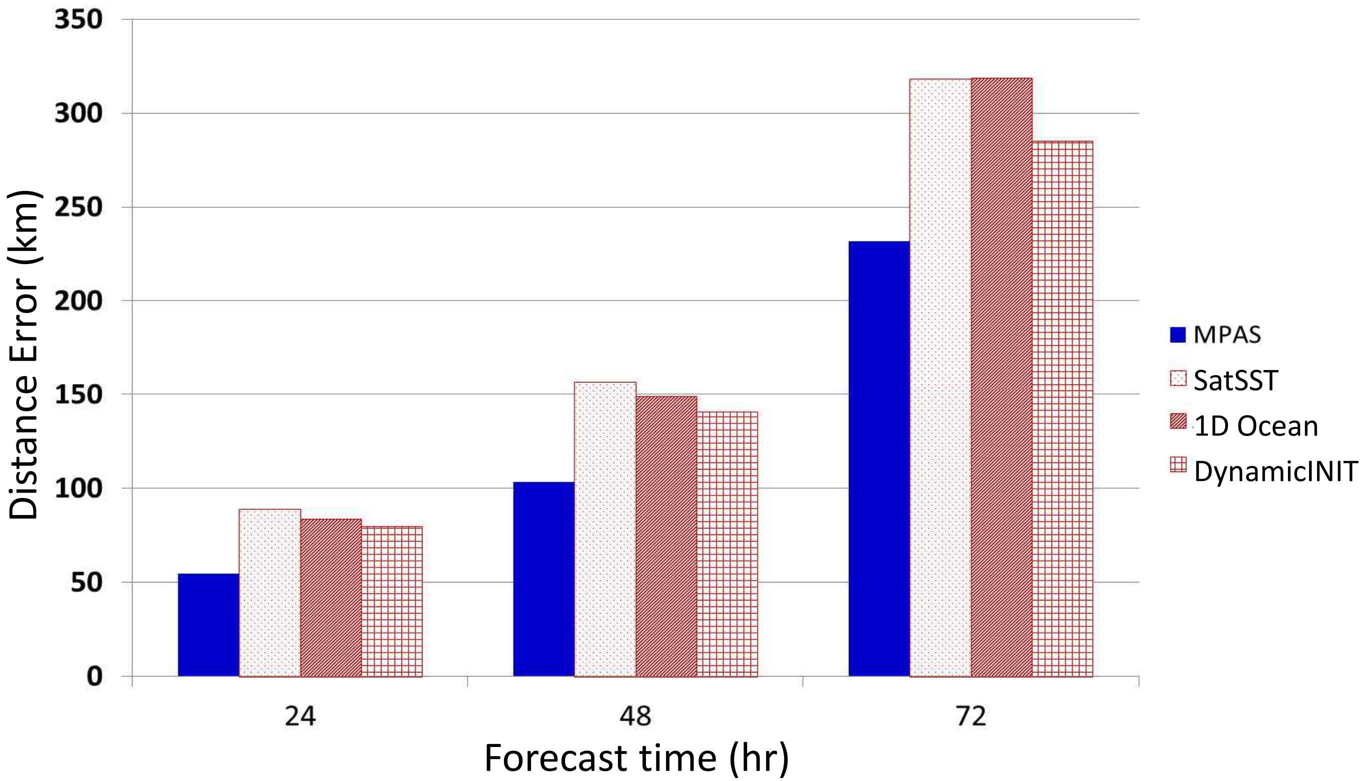
WRF-based TC forecast models of KISTI

Model	Feature
SatSST	SST is updated by using satellite observation
1D Ocean	1D ocean model is coupled to WRF
DynamicINIT	Dynamic initialization of TC is applied

VS

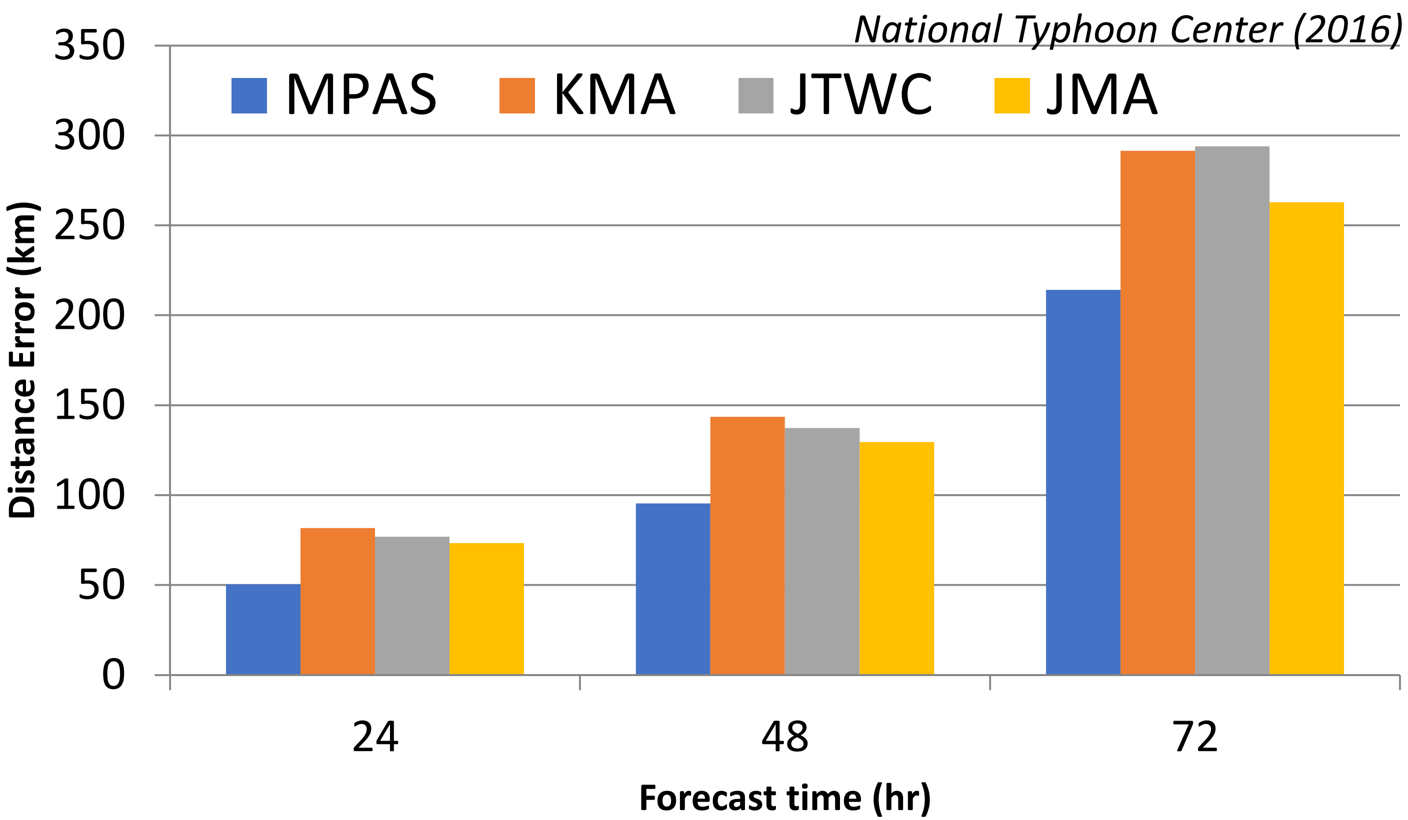
K-MPAS





Performance of K-MPAS for TC track forecast

- 2016 Typhoon track forecast (12 cases)

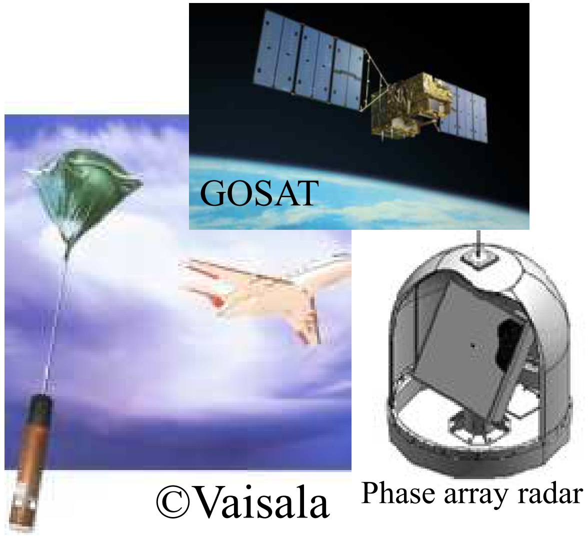


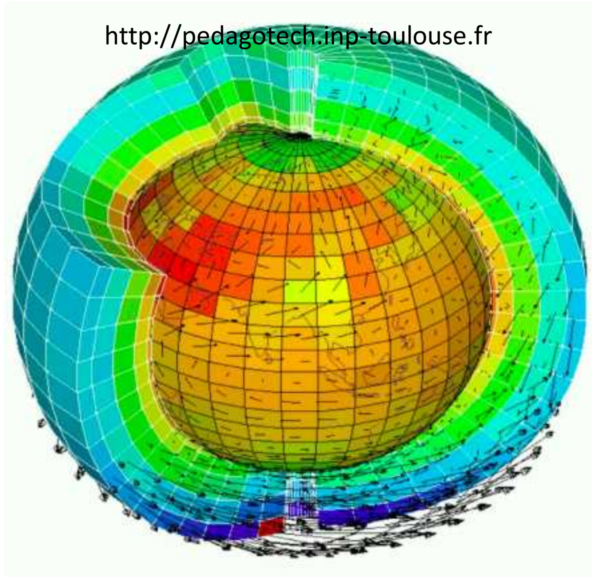
- K-MPAS shows a good performance for the TC track forecast
- Data assimilation has not been applied to the MPAS yet.

Data assimilation

- *A statistical combination of observations and short-range forecasts*
  - "Using all the available information, to determine as accurately as possible the state of the atmospheric (or oceanic) flow" *- Talagrand (1997)*

Observation + **Model**





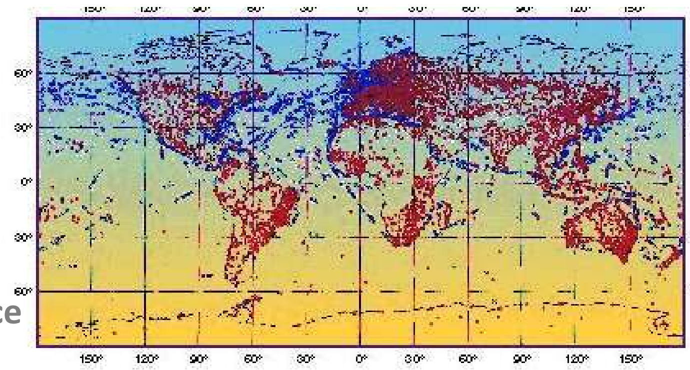
- We usually utilize two independent information of observation and model forecast to obtain the best estimate of the true state of the nature.

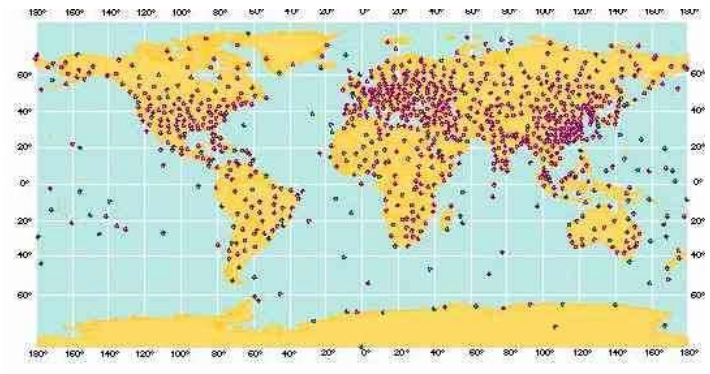
Sources of information – Observations

- Ground-based measurements

https://www.wmo.int/pages/prog/www/OSY/Gos-components.html

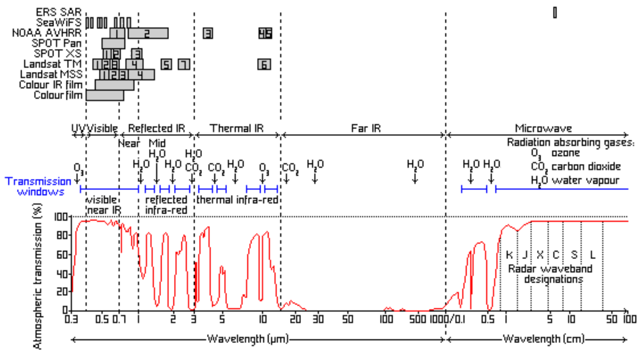
surface

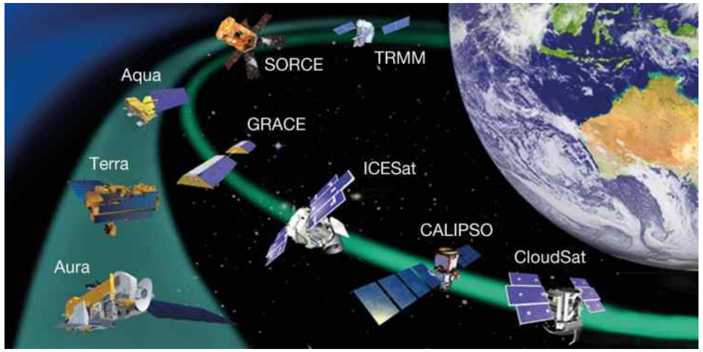




Upper-air

- Remote sensing data from the satellites

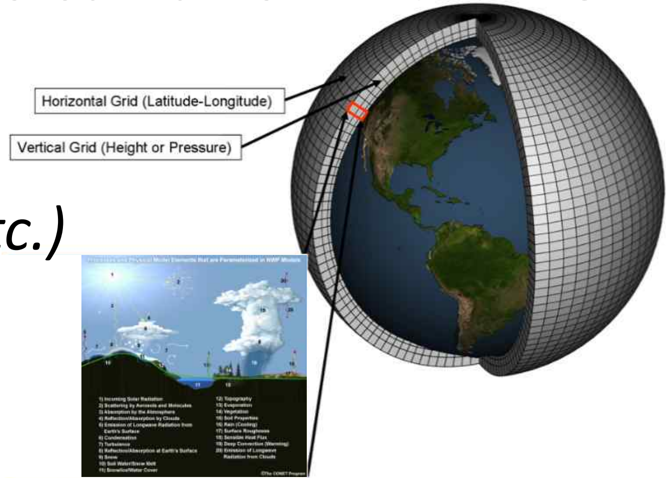




- Observations provide information with instrumental errors
- The information is limited in time and space

Sources of information – Numerical models

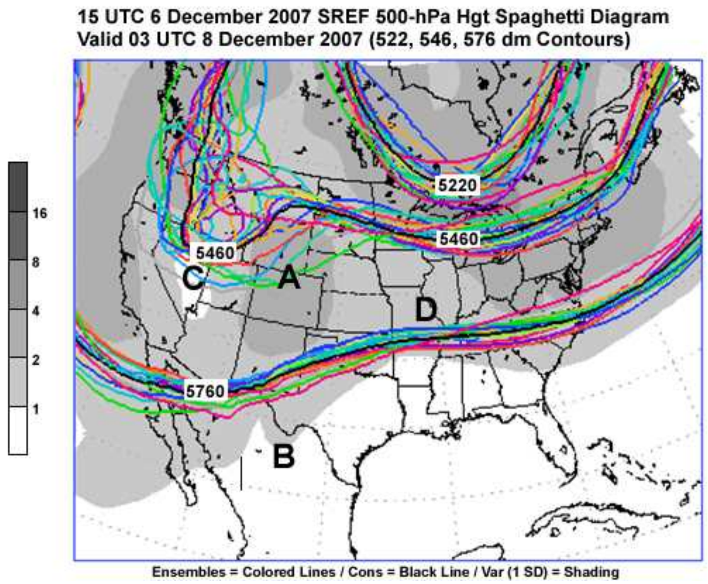
- Partial differential equations of physical laws w.r.t. time
  - $x_n = \boldsymbol{M}(x_{n-1})$
    - *x*: a state of variables
      (e.g. wind, temperature, humidity, etc.)
    - *n*: time index
    - ***M***: nonlinear numerical model
  - Discretization of the equations for the model grids

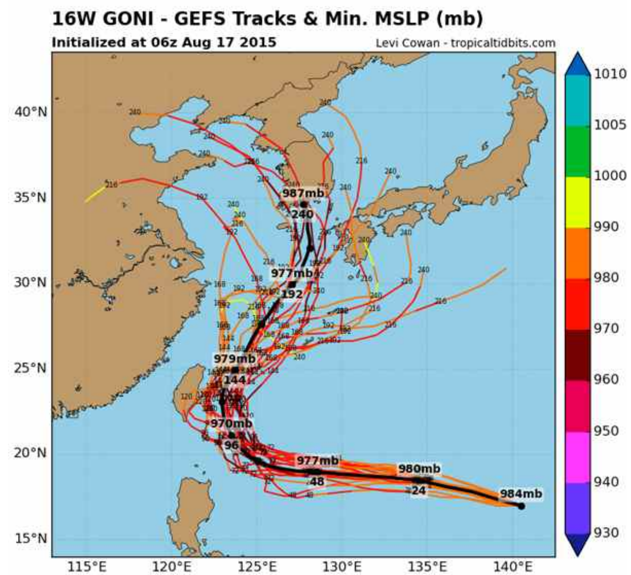


➔ *Limited accuracy of the model* ***M*** *(e.g. sub-grid phenomena)*

➔ *errors of initial data* (x_{n-1}) can grow quickly due to chaotic nature of the atmosphere (even when the model is perfect!)

Ensemble-based data assimilation system





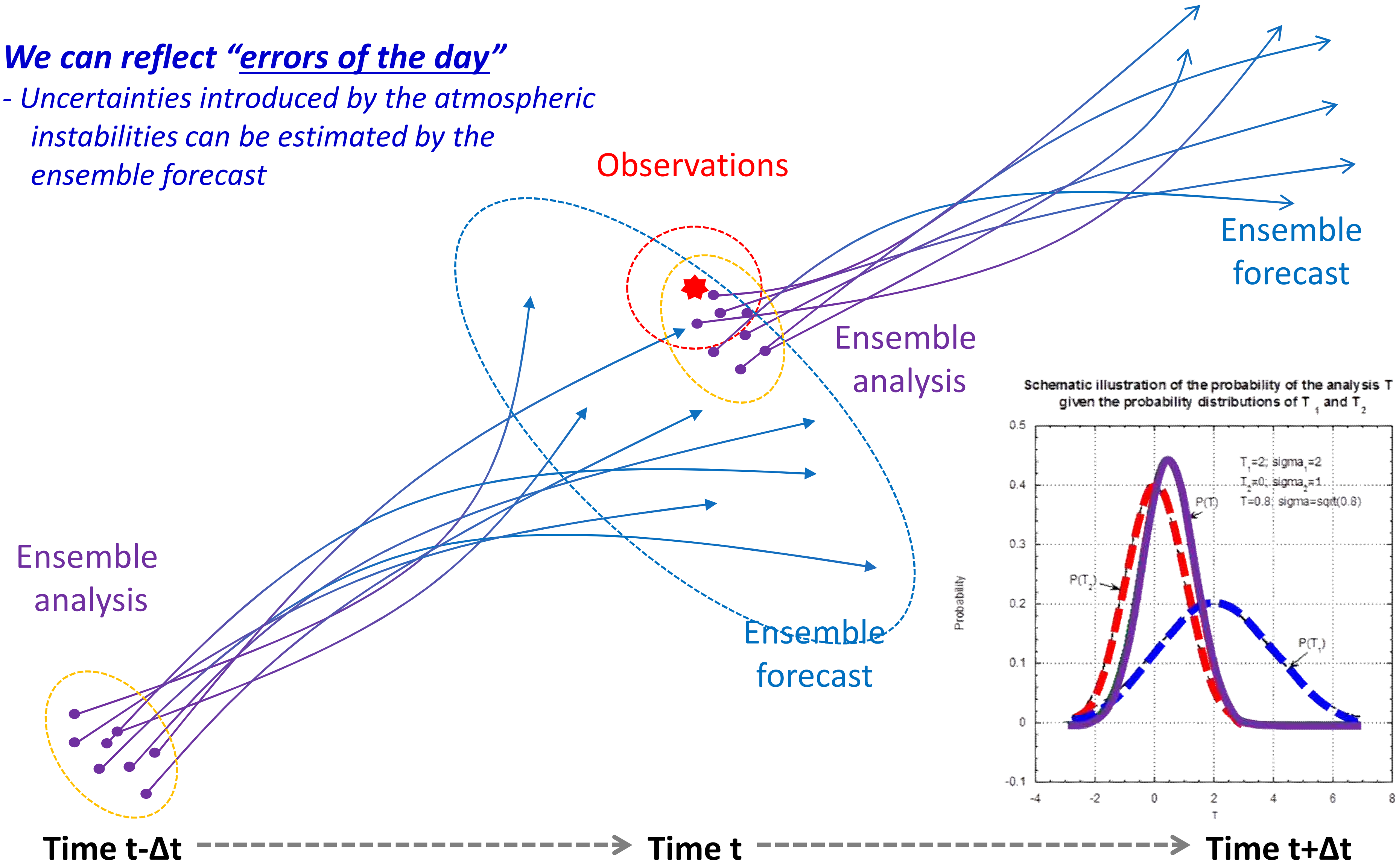
- Success of data assimilation strongly depends on how accurate we can estimate errors of the information.
    - Model error is much more complicated and difficult to estimate than observation error because it highly depends on *atmospheric instability*, observation density, etc.
    - Especially for the extreme weather, it is essential to estimate *real-time forecast error* as accurate as possible

➔ In such cases, ensemble data assimilation (EnKF) is certainly advantageous to a variational DA (VAR) because EnKF considers "errors of the day" while VAR uses static forecast error estimates.

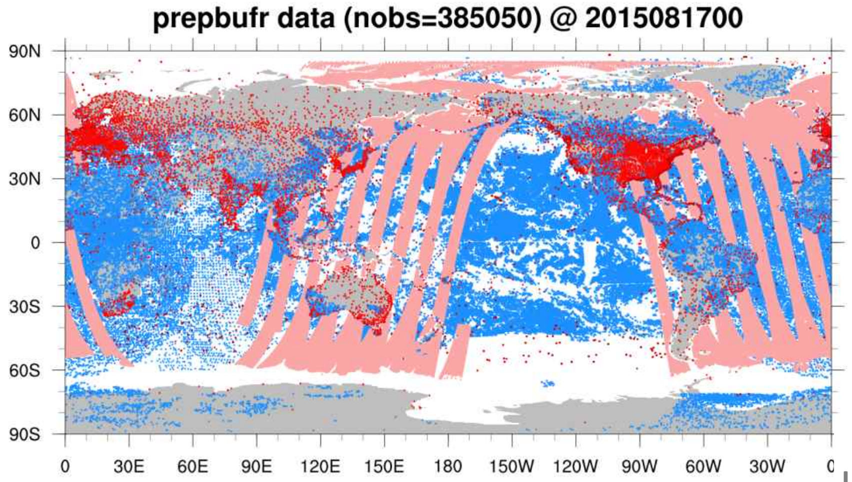
EnKF data assimilation

We can reflect "<u>errors of the day</u>"

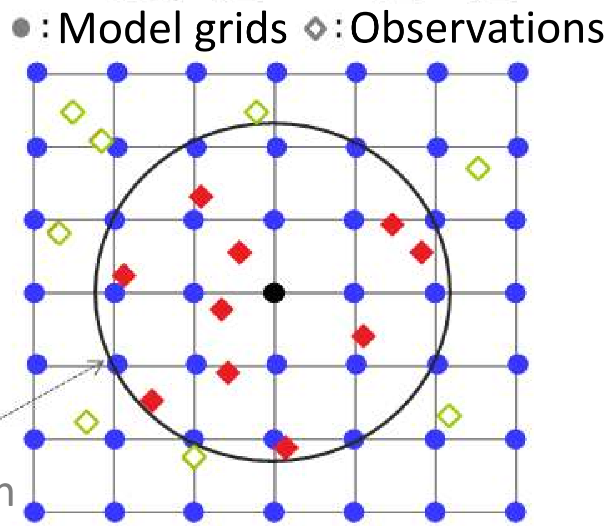
- Uncertainties introduced by the atmospheric instabilities can be estimated by the ensemble forecast



Local Ensemble Transform Kalman Filter (Hunt et al. 2007)



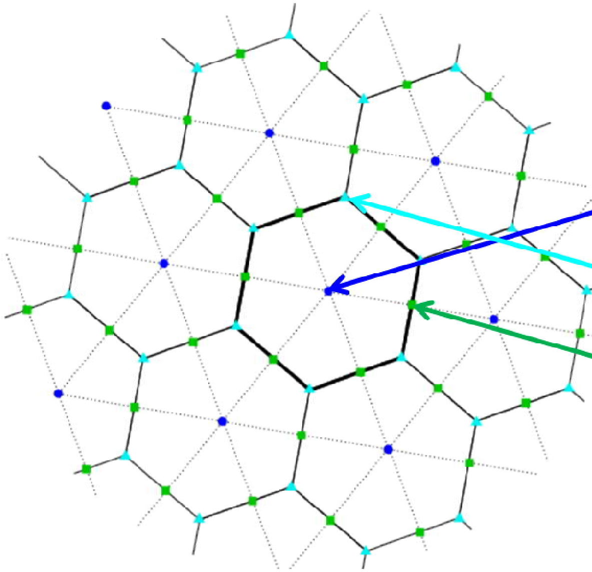
# of model grids : $O(10^6$-$10^7)$



- Forecast of numerical model should be transformed to the observation space *globally*.
  - Observation operator (spatial interpolation and variable transformation)
- For an analysis at one point, LETKF uses only neighborhood information within a local region, which is a part of "***embarrassingly parallel***".

Special treatment of LETKF for MPAS

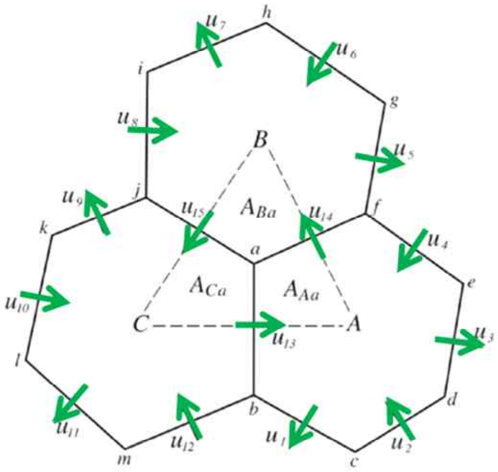
- Defining feature of MPAS



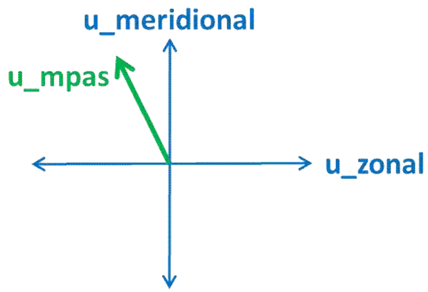
(ref. MPAS tutorial)

Fields in MPAS-Atmosphere may be defined at

- **Cell** locations (blue circles) - the generating points of the Voronoi mesh
- **Vertex** locations (cyan triangles) - the corners of primal mesh cells
- **Edge** locations (green squares) - the points where the dual mesh edges intersect the primal mesh edges

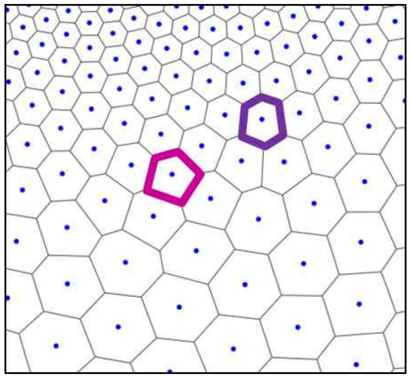


u_mpas



Observation data provides information of u_zonal and u_meridional

In MPAS-A, these locations are used to implement a C-staggered grid based on the Voronoi tessellation: prognosed normal velocities are located at *edges*, and other prognosed quantities are nominally located at *cells*.

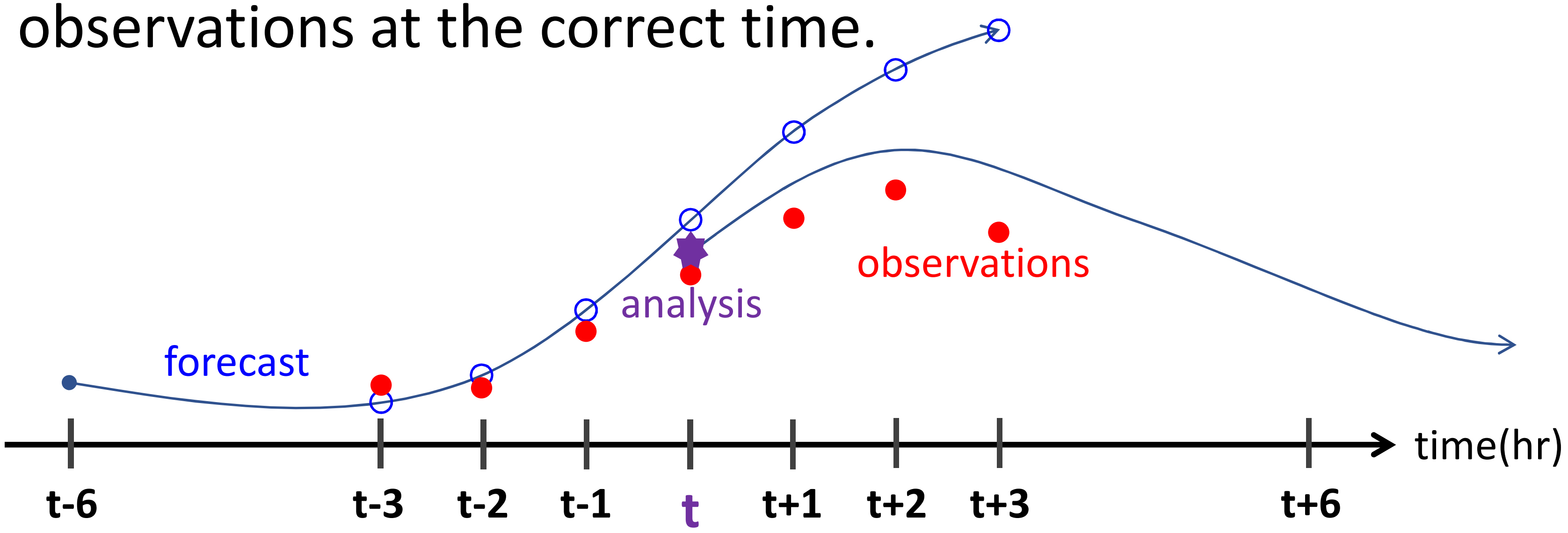


😐

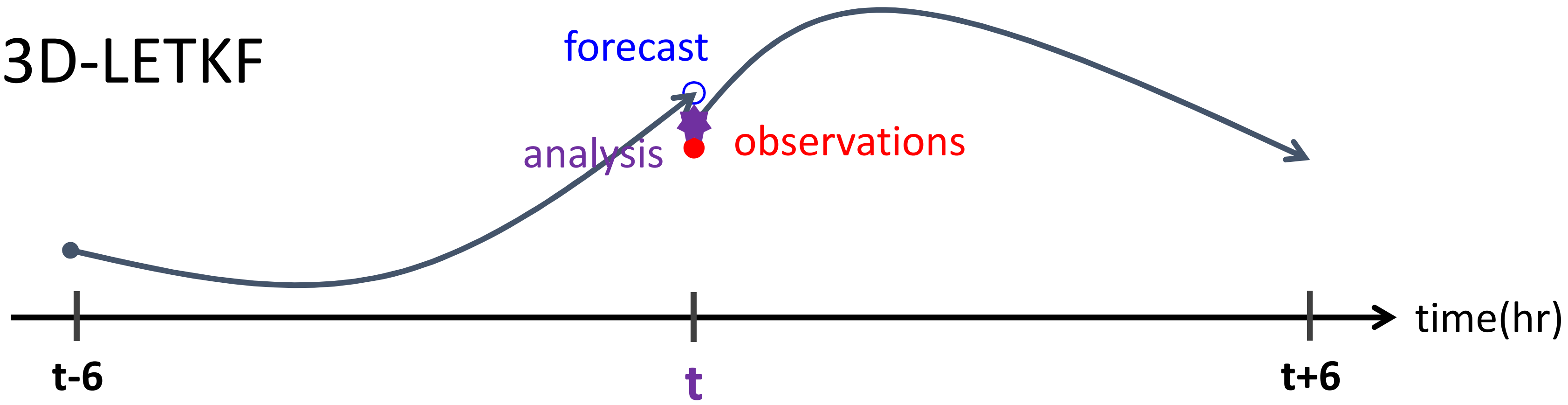
"I know many advantages of unstructured grid, but it makes implementation of LETKF more difficult!"

4-dimensional LETKF

- As a density of observations gets finer in time and space, DA system needs to reflect the background and the observations at the correct time.

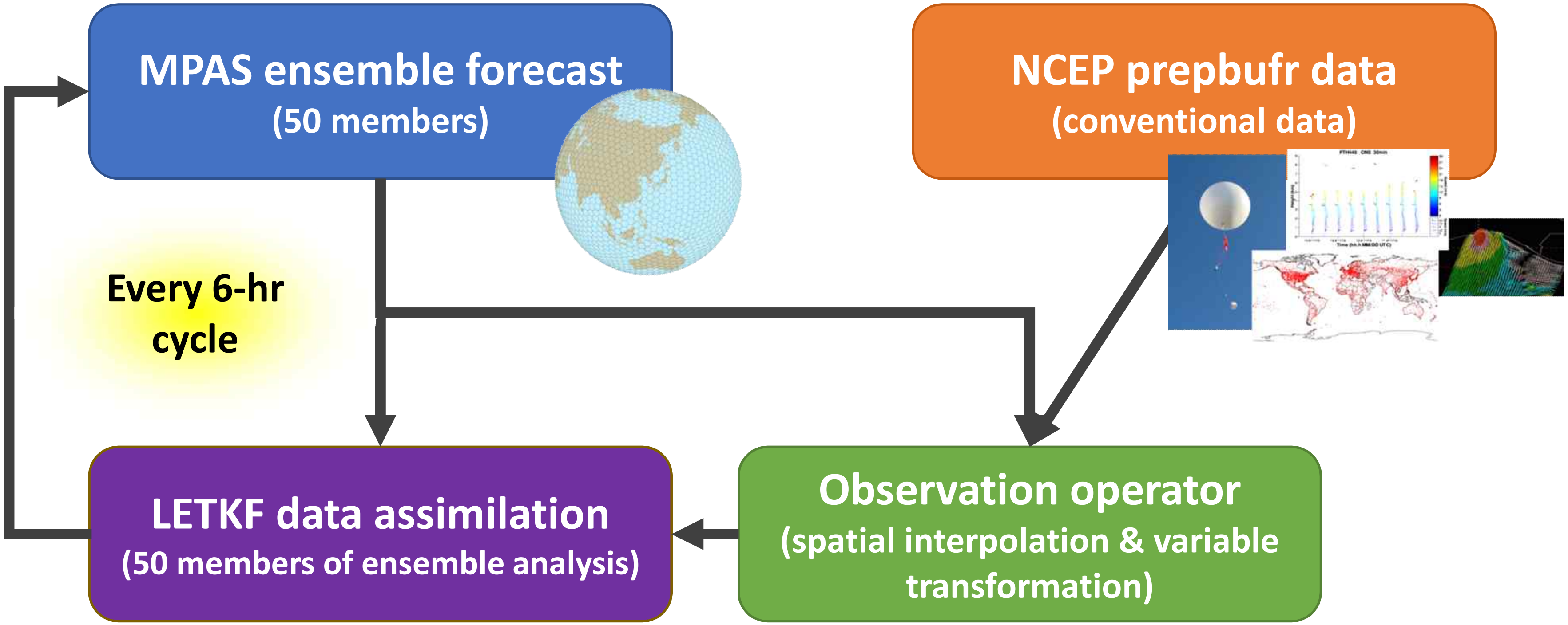


- 3D-LETKF

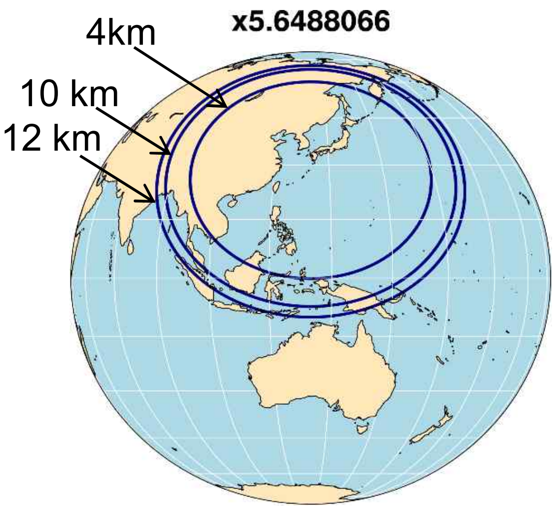


MPAS-LETKF @ KISTI

- Current system can assimilate NCEP prepbufr conventional data.
- Now, we're working on radiance data assimilation with AMSU-A, which requires variable transformation in the observation operator (RTTOV v. 11.0).



Scalability test – Model configuration and Test plan



3-15 km mesh

<u>Numerics</u>
- Model top ~ 30 km
- Model levels ~ 56 levels
- Mesh size ~ 6,488,066 cells

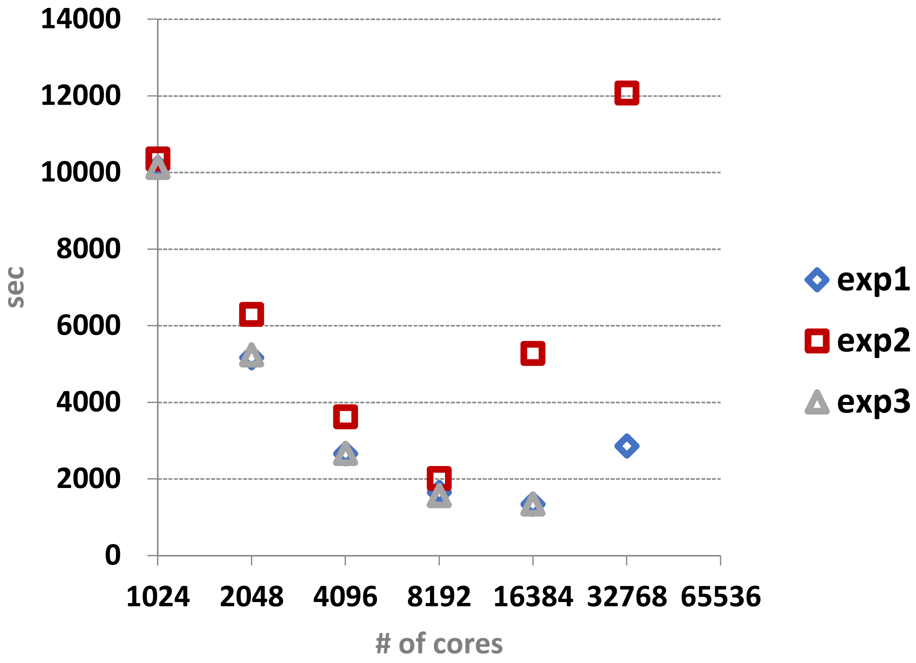
<u>Physics</u>
- Surface Layer : Monin-Obukov
- PBL : YSU
- Land Surface Model : NOAH 4-layers
- Convection : Tiedtke
- Microphysics : WSM6
- Radiation : RRTMG
- Ocean Mixed Layer (modified from WRFV3.6)

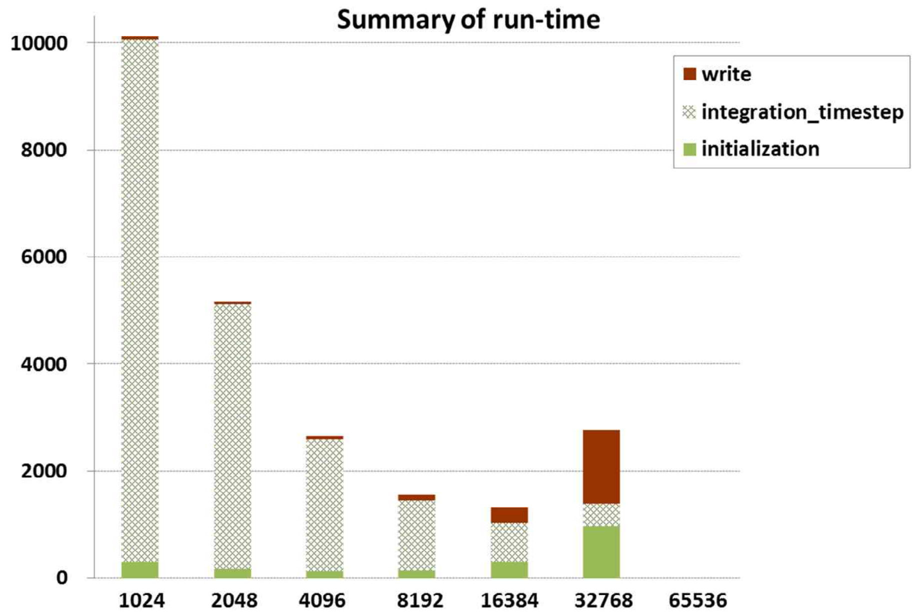
<table>
<tr><th># of cores</th><th>exp1</th><th>exp2</th><th>exp3</th></tr>
<tr><td>1024</td><td rowspan="6">CDF5</td><td rowspan="4">NetCDF4</td><td rowspan="5">CDF5</td></tr>
<tr><td>2048</td></tr>
<tr><td>4096</td></tr>
<tr><td>8192</td></tr>
<tr><td>16384</td><td rowspan="2">No PIO</td></tr>
<tr><td>32768</td><td>X</td></tr>
</table>

- We integrated the model for **6-hr forecast** with **dt=15sec → 1440 timesteps**
- 17 runs have been conducted.
  - 32768-core run for exp3 could not be completed due to the short time limit.

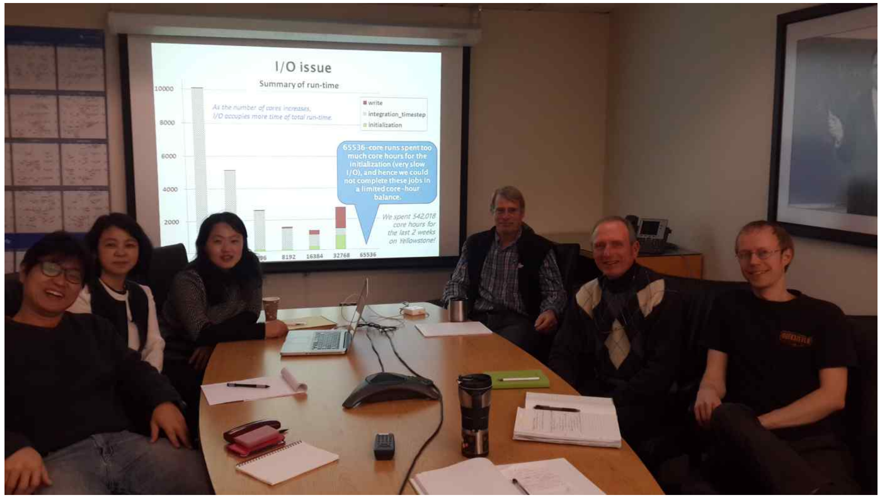
- The runs with CDF5 format show much faster I/O than those with NetCDF4 format. Therefore, we planed to run the exp3 with CDF5 format
- The runs with 16384 & 32768 cores have serious issue related to the I/O bottleneck using NetCDF4 format. Thus, we also tried not using PIO lib.

Scalability test – Total time





As the number of cores increases,
I/O occupies more time of total run-time.



Summary

NCAR
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

KISTI Korea Institute of Science and Technology Information www.kisti.re.kr

MPAS
Model for Prediction Across Scales

Optimization for
TC forecast over W.P.

K-MPAS

- ❖ CPU-GPU heterogeneous code
- ❖ MPAS-LETKF system

- ❖ What's next?
  - Coupling with Ocean model (i.e., MOM)
  - Modifying or developing physics schemes for the severe weather forecast over the East Asia

Thank you