

Scalable Computing Challenges in Ensemble Data Assimilation

CAS2K13

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NCAR - IMAGE/DAReS

12 Sept 2013

Overview

- What is Data Assimilation?
- What is DART?
- Current Work on Highly Scalable Systems

Overview of Data Assimilation

Prediction Model



Overview of Data Assimilation

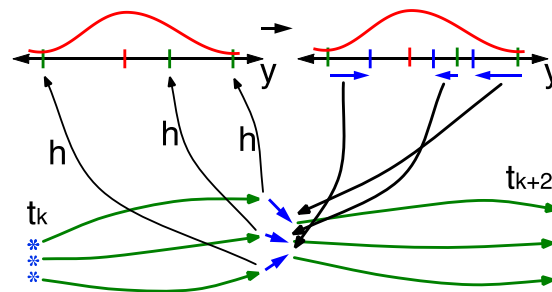
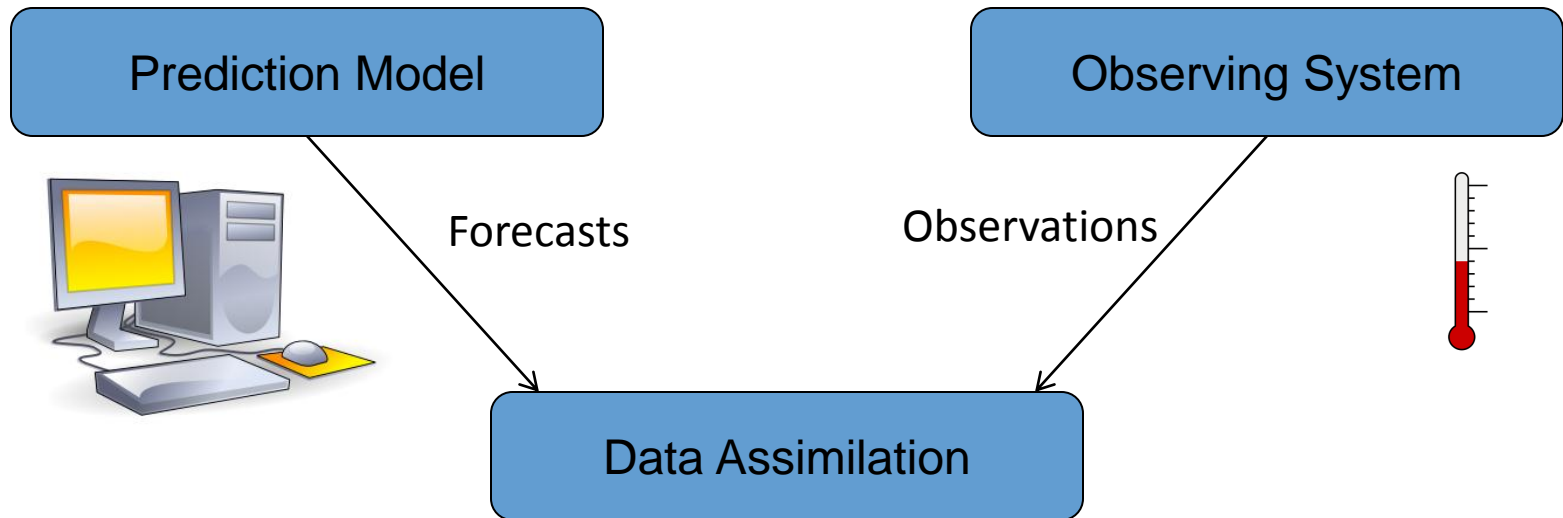
Prediction Model



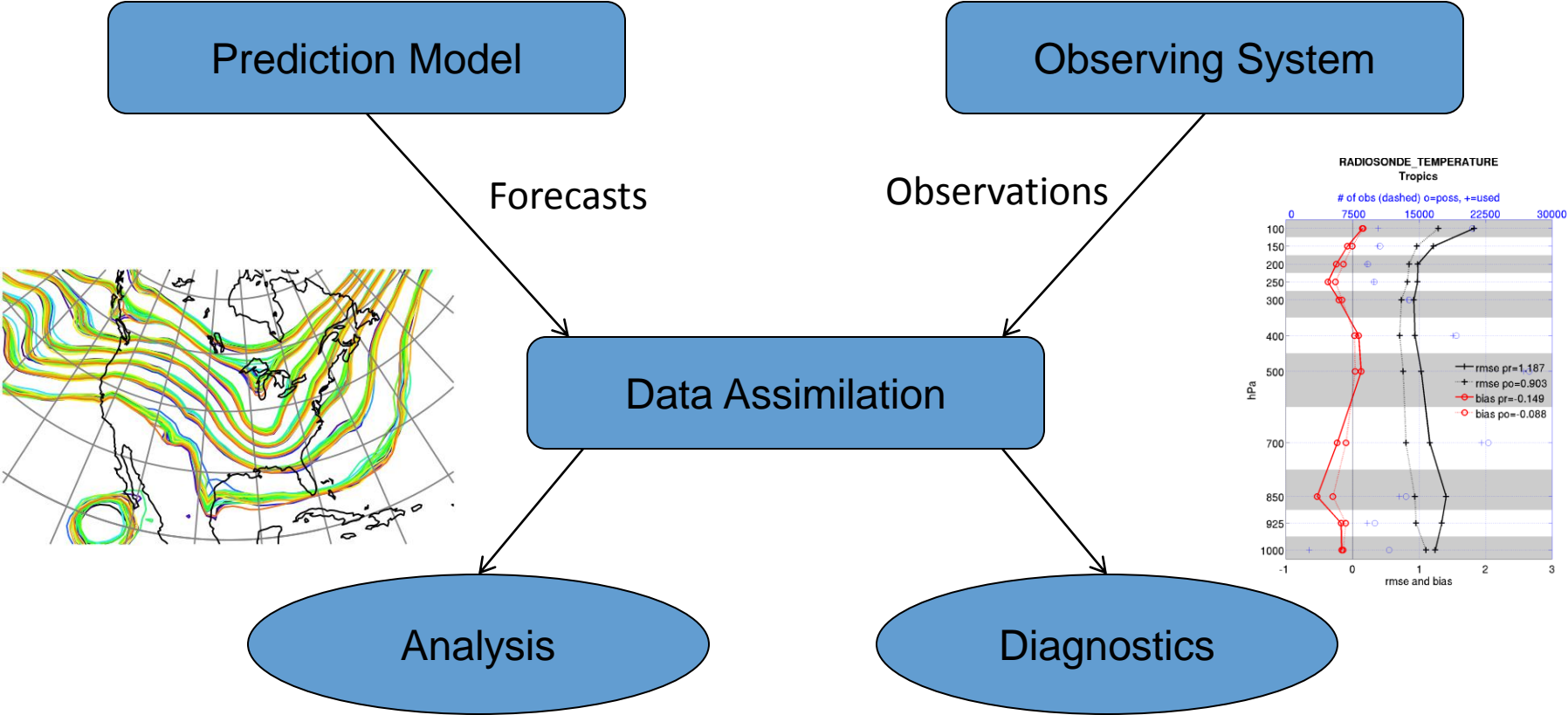
Observing System



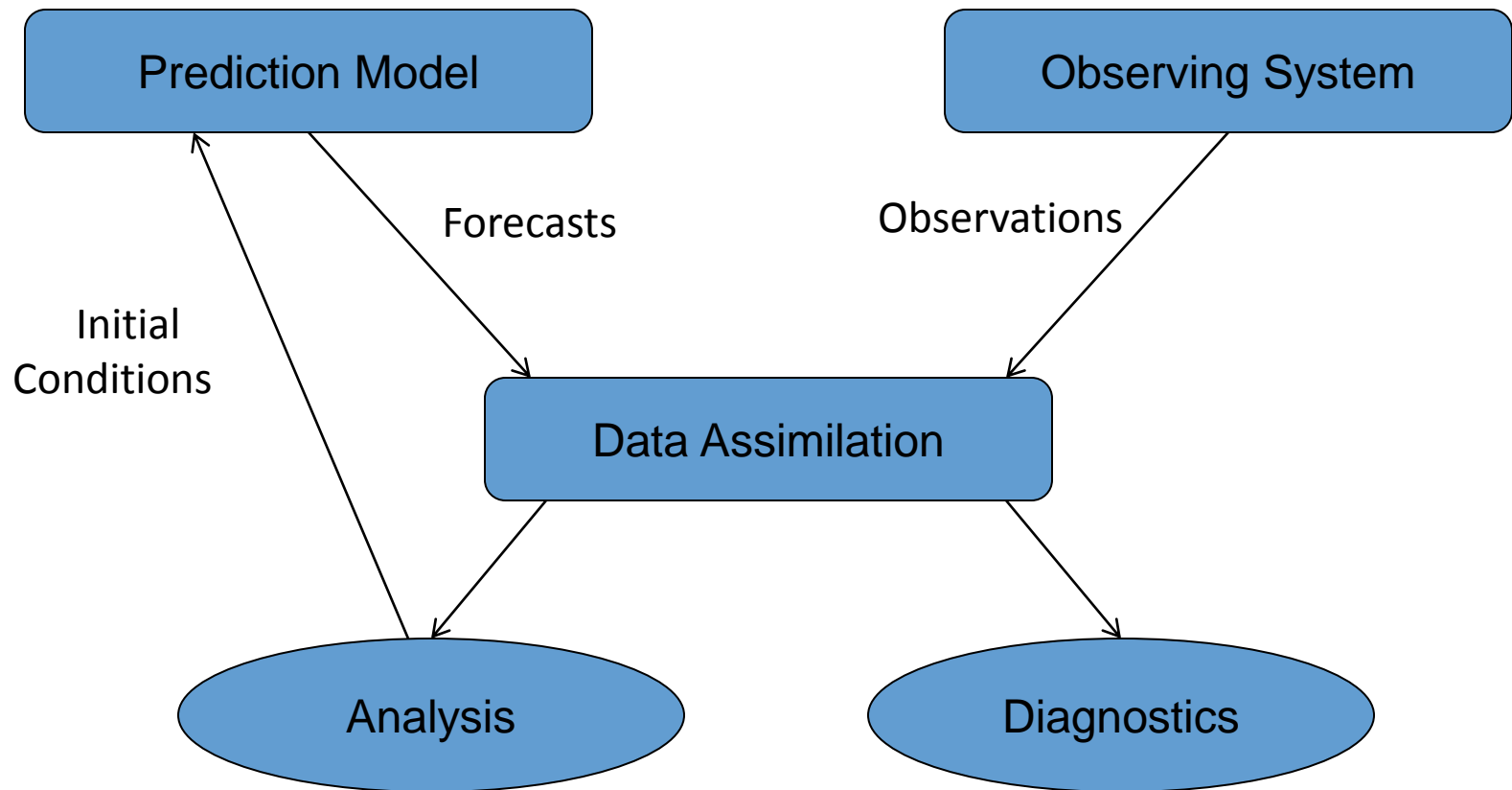
Overview of Data Assimilation



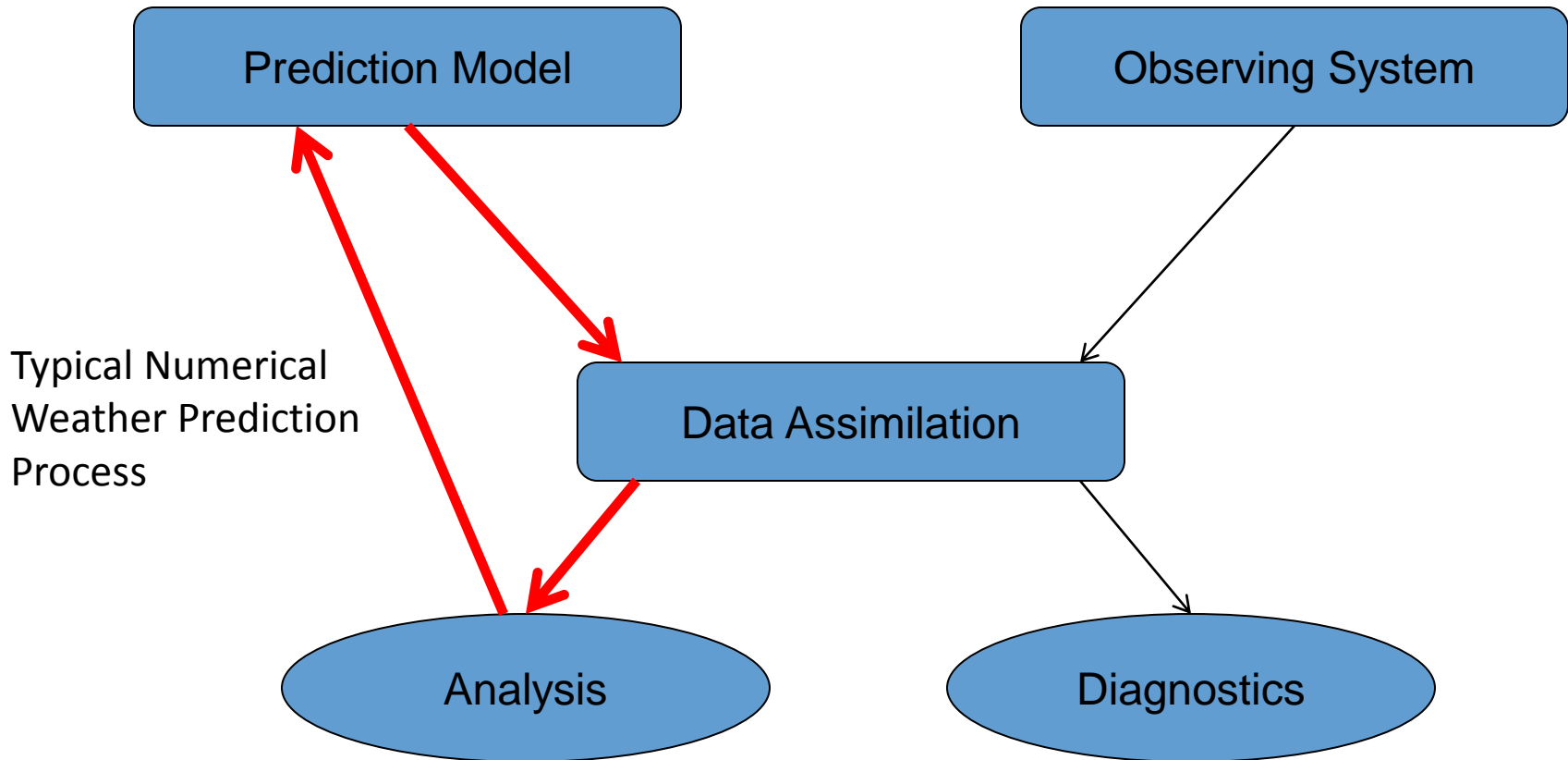
Overview of Data Assimilation



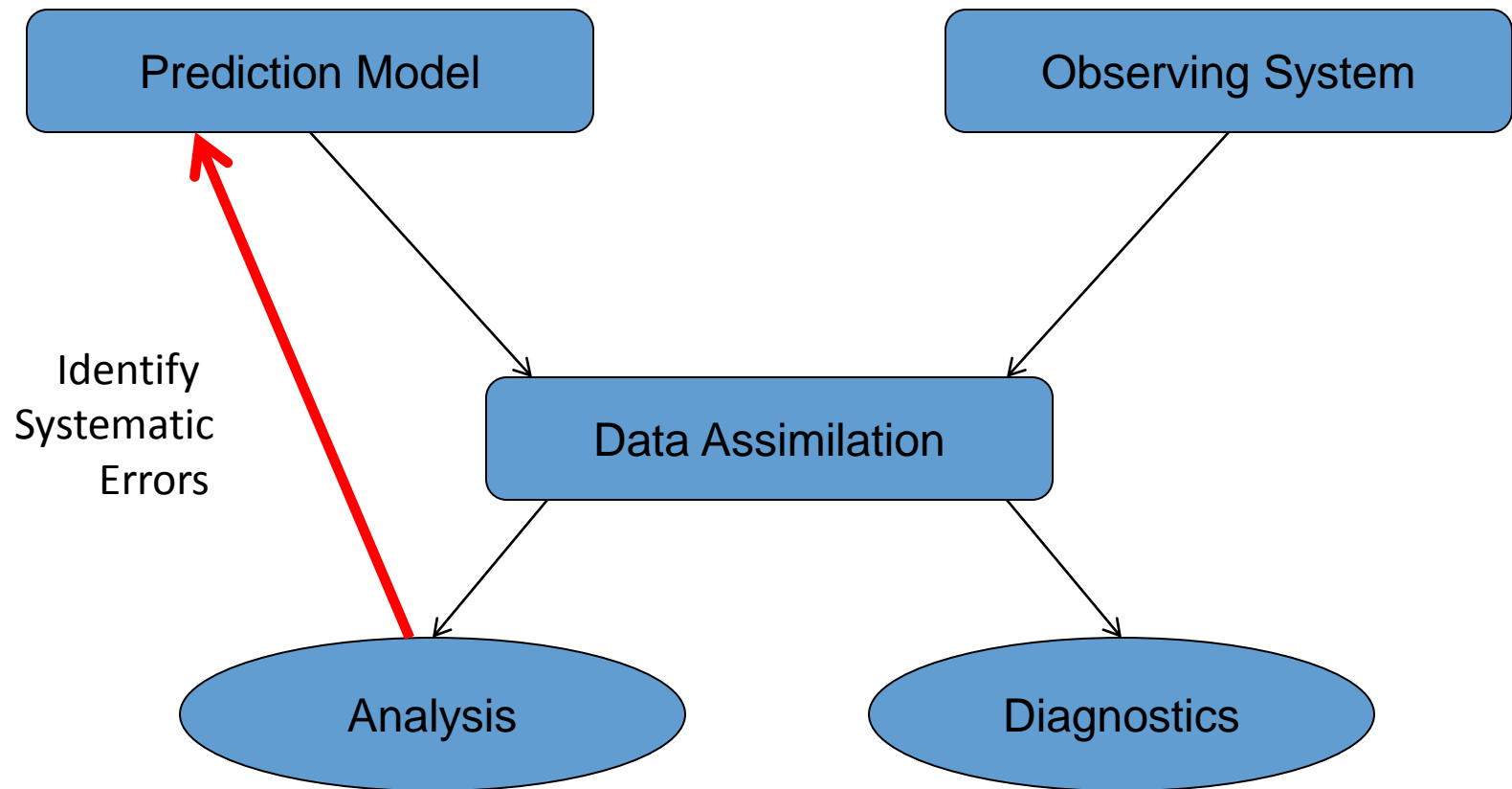
Overview of Data Assimilation



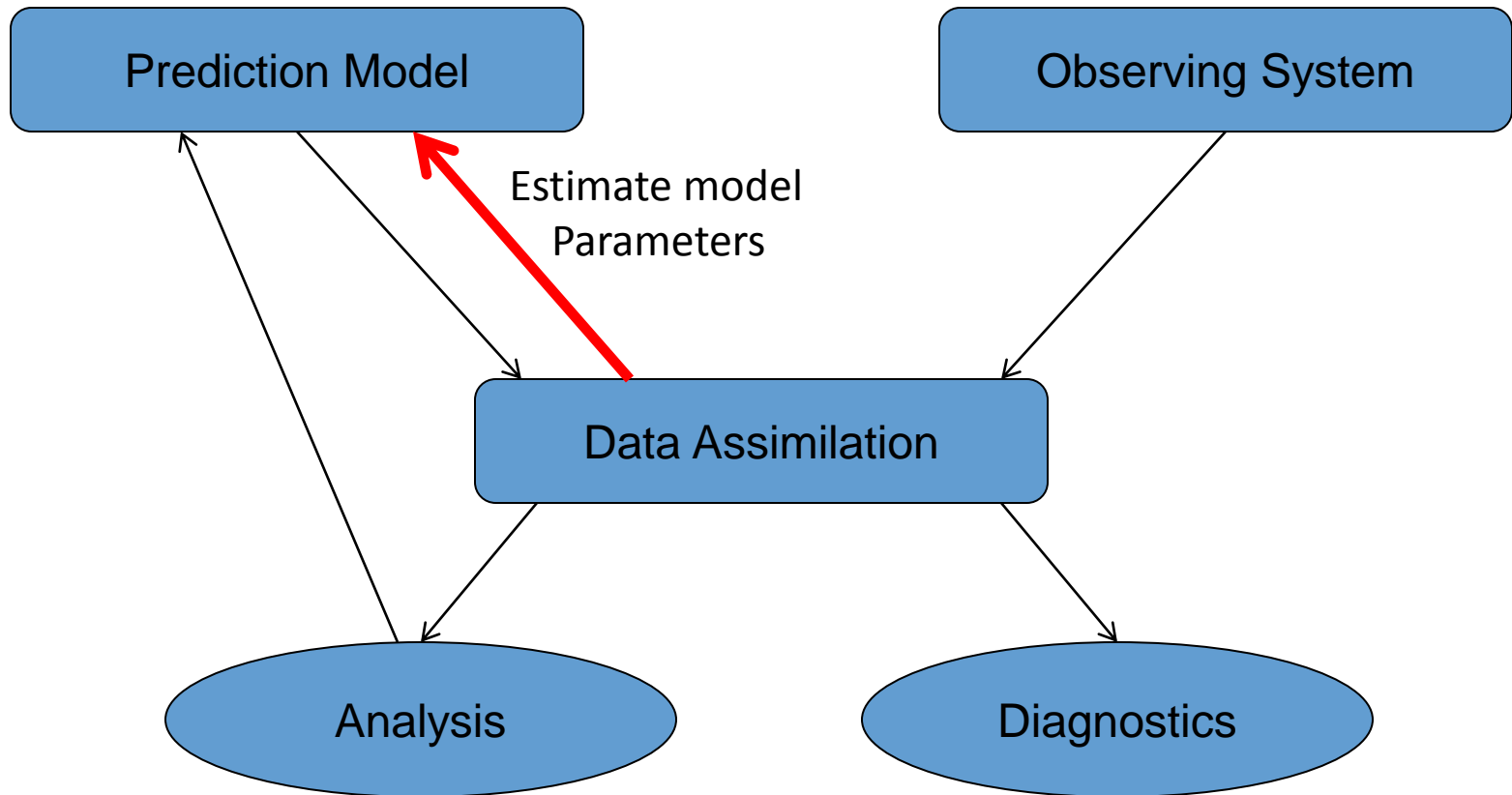
Overview of Data Assimilation



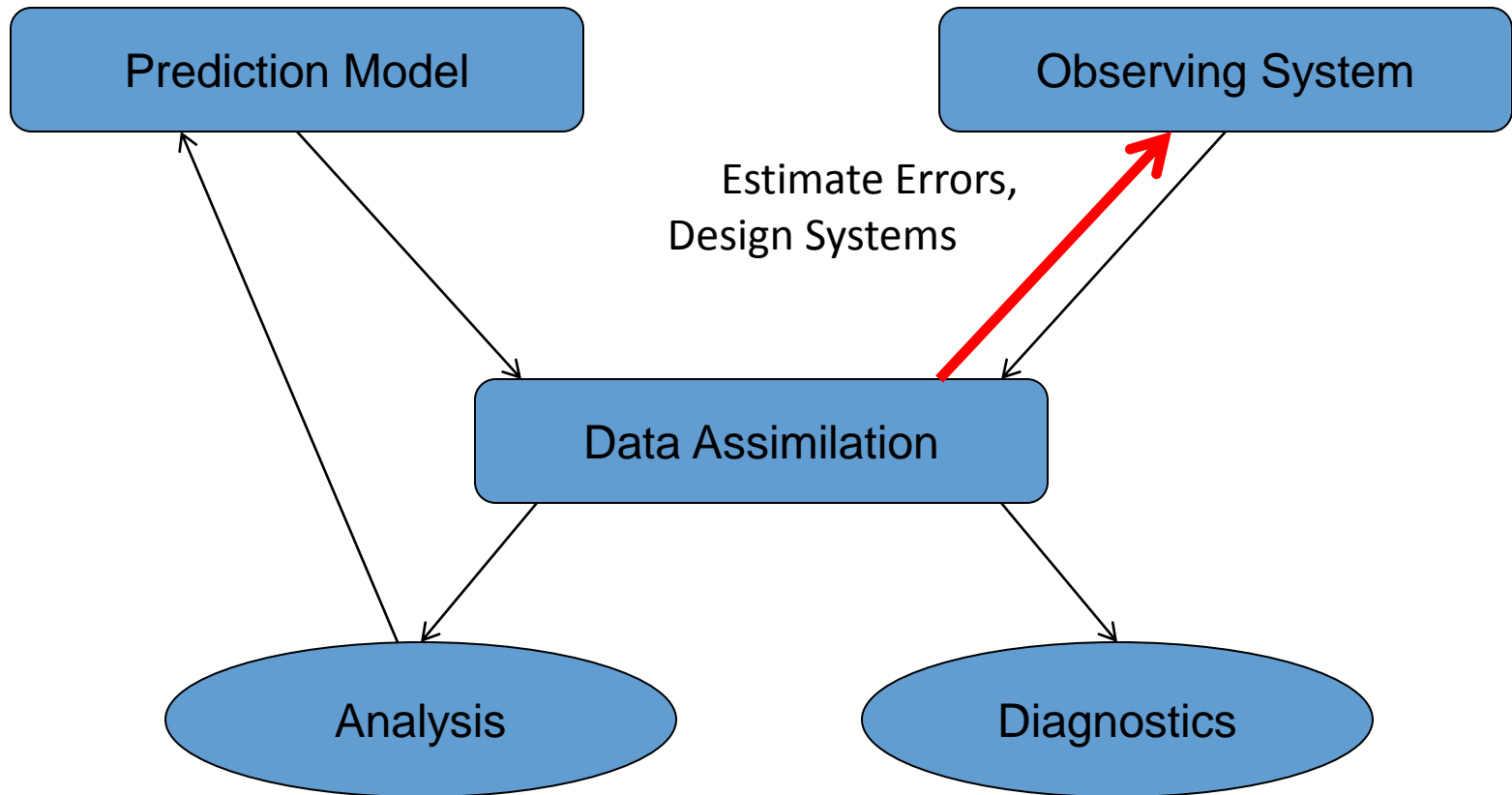
Overview of Data Assimilation



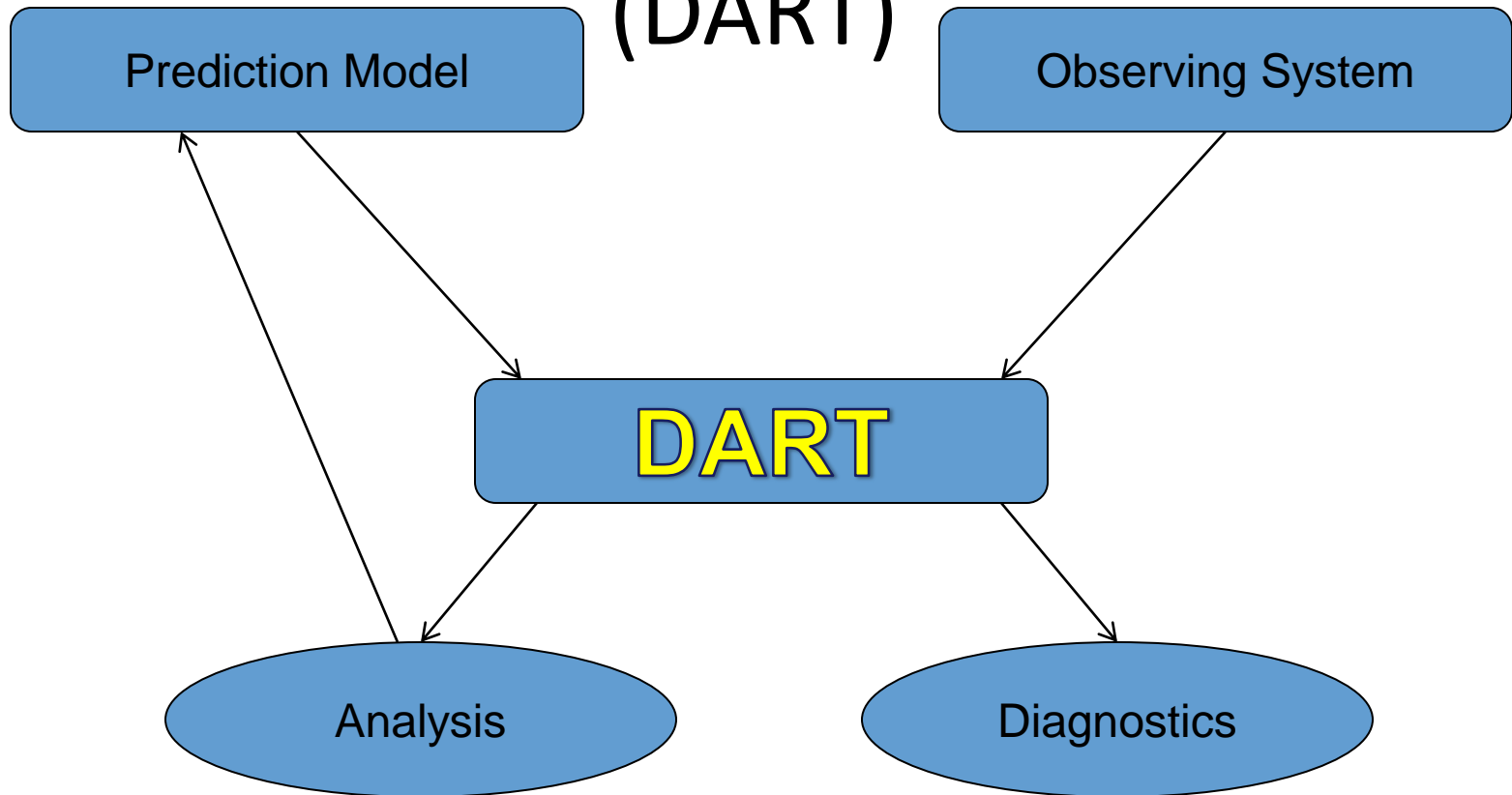
Overview of Data Assimilation



Overview of Data Assimilation



Data Assimilation Research Testbed (DART)



DART is a *community* ensemble assimilation facility.

Data Assimilation Types

- Variational Systems
 - Used by operational NWP forecasting centers
- Ensemble Systems
 - Make many forecasts
 - Easier to develop a DA system, especially for large models
 - Feasible for individual researchers, small groups
 - Produces uncertainty information

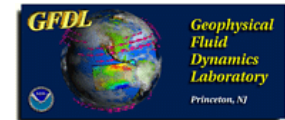
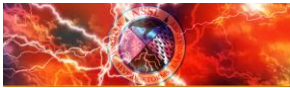
Data Assimilation Research Testbed

- DART software is used for:
 - Building Ensemble Data Assimilation systems
 - A Teaching tool
 - A DA Research tool
- Users can run it:
 - Out of the box
 - Add their own new models
 - Add their own new observation types
 - Change the assimilation algorithms



DART is used at:

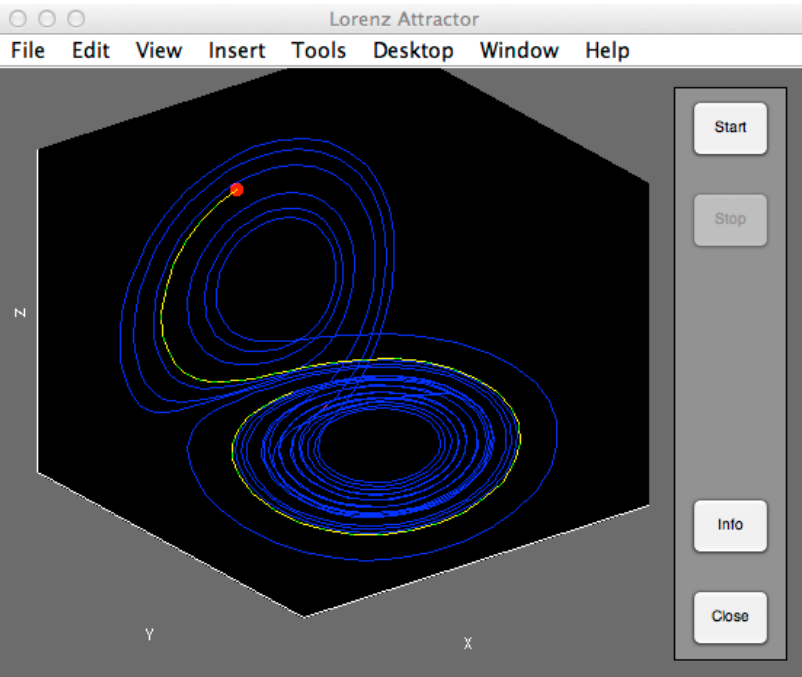
48 UCAR member universities
More than 100 other sites



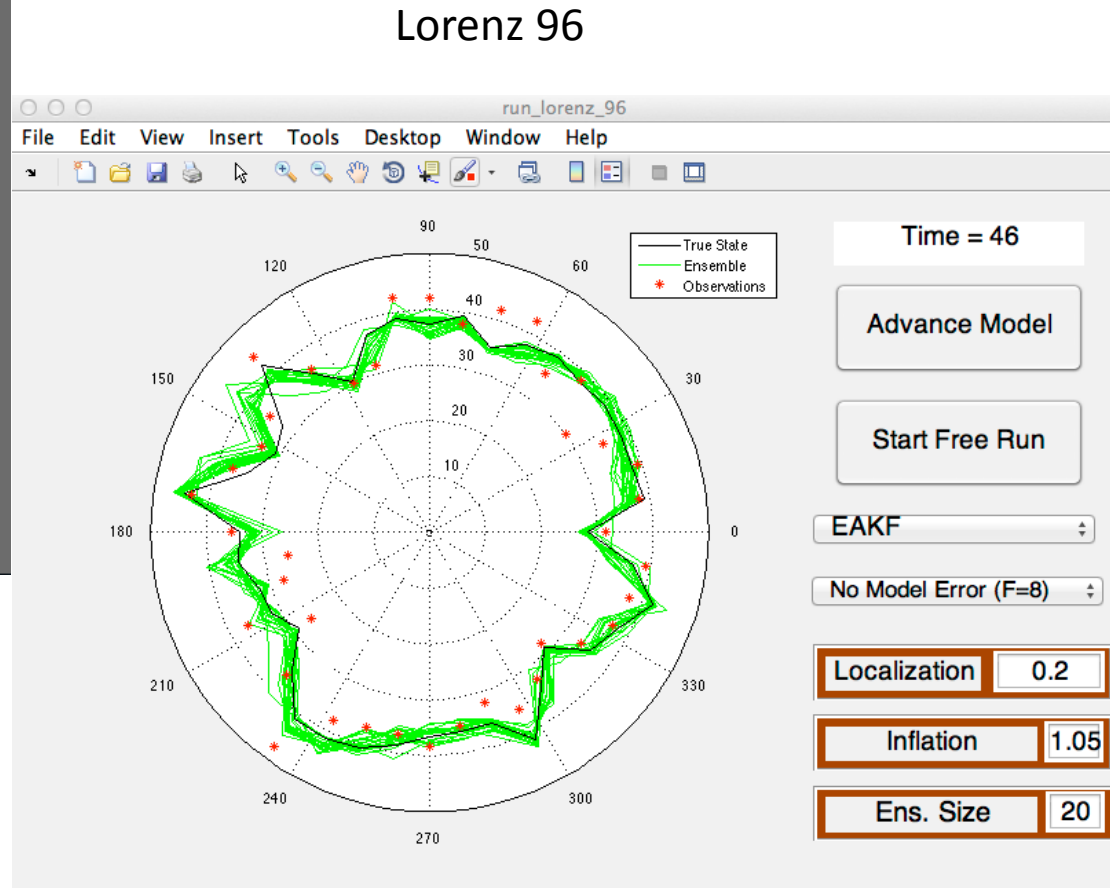
DART Models

- 1D, 2D+
 - 6 Lorenz models, simple chaotic models (e.g. Ikeda, Null, 9var, SQG, PE2LYR, Bgrid_solo)
- Full Geophysical Models
 - Coupled Climate, Weather, Ocean, Land, ...
(e.g. CESM, WRF, POP, MITgcm, COAMPS, GITM, MPAS, TIEgcm, Rose, NOAH, NOGAPS)
- Economic, Epidemiological, Ecosystem, etc

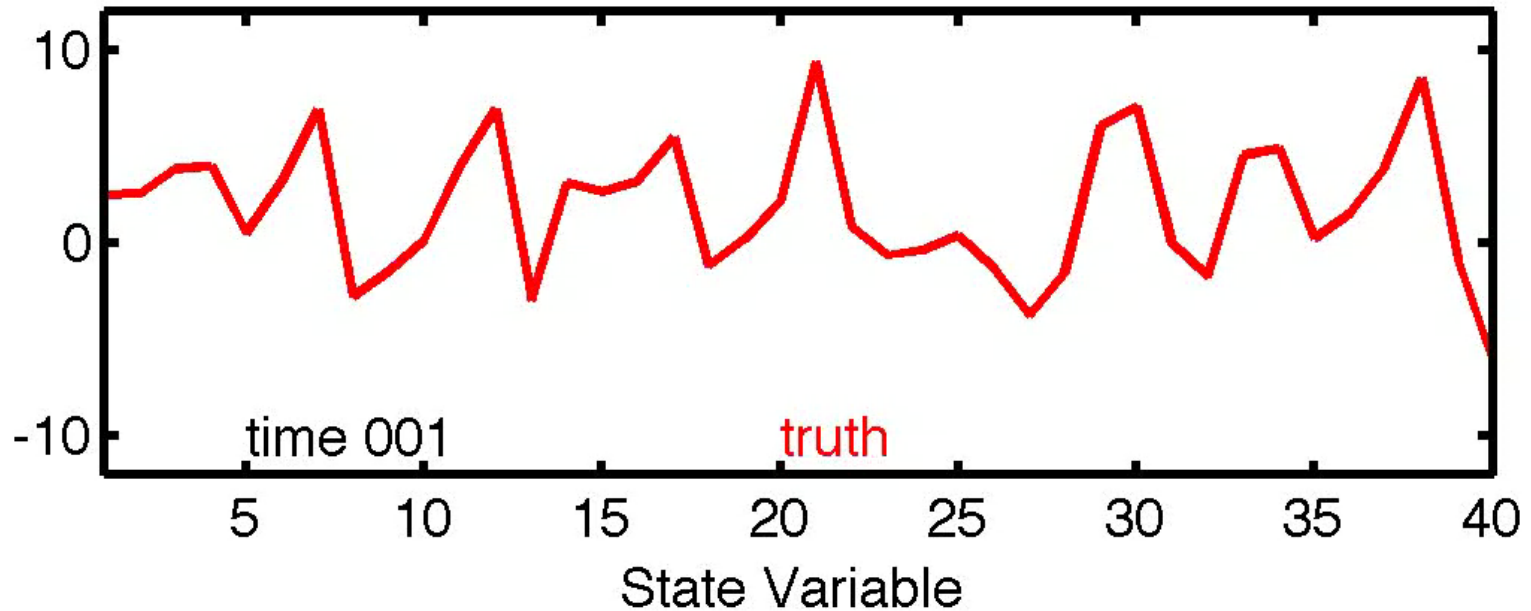
Lorenz Models



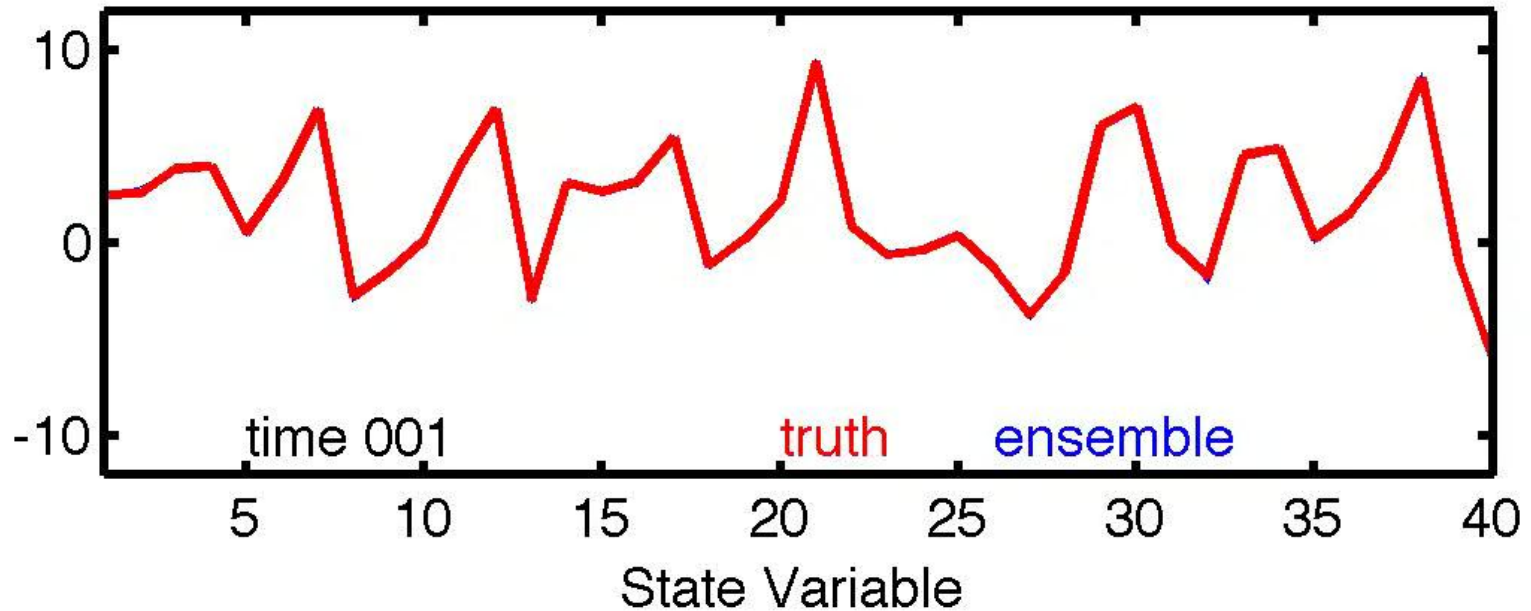
Lorenz 63 (butterfly)



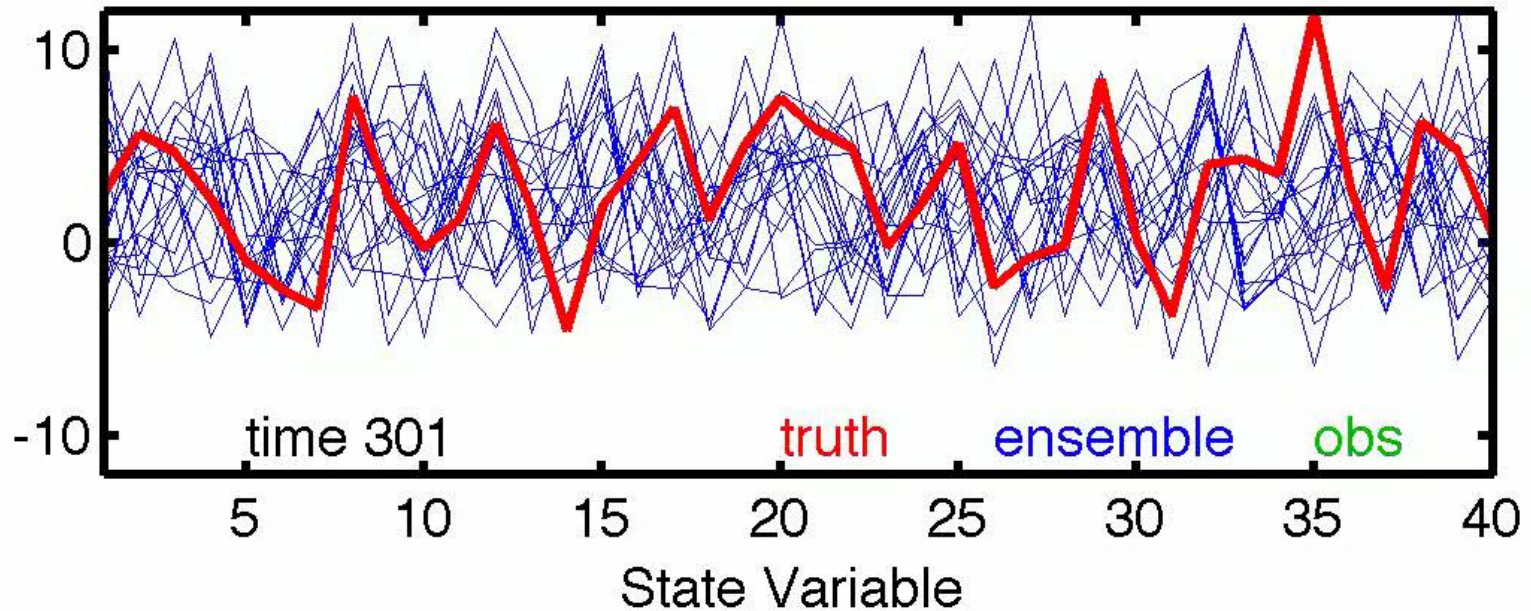
Lorenz 96 Free Run



Lorenz 96 Ensembles



Lorenz 96 with DA



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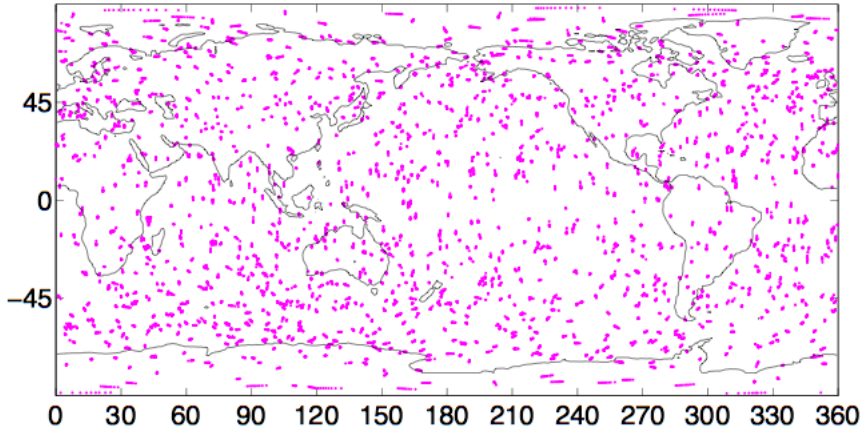
Example Dart Observation Types

- Atmospheric Obs
 - Radiosondes (balloons) Temperature, Winds
 - Aircraft, Satellite Winds, Surface Obs, GPS (T, Q)
- Ocean Obs
 - Temperature, Salinity, Sea Surface Temp/Height
- Land Obs
 - Snow cover, CO Fluxes from Towers
- Novel Obs Types
 - Gravity/Length of Day, Leaf Area Index, COSMOS
Neutron Soil Moisture

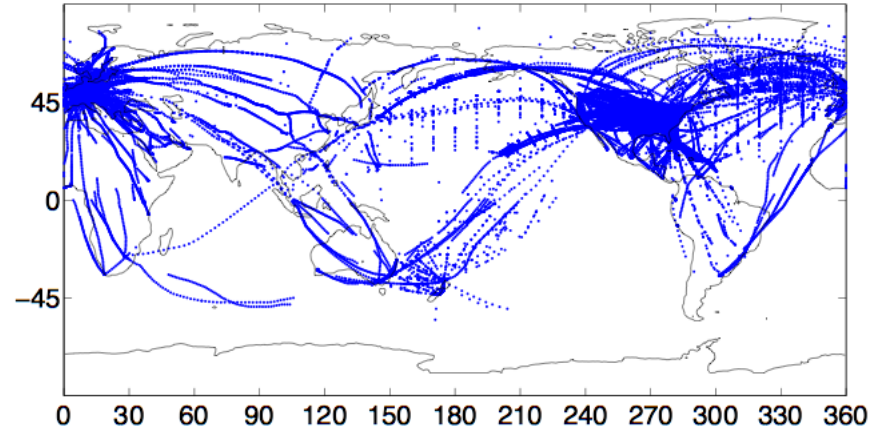
Examples of Observation Density by Obs Type

Observations 1 December 2006

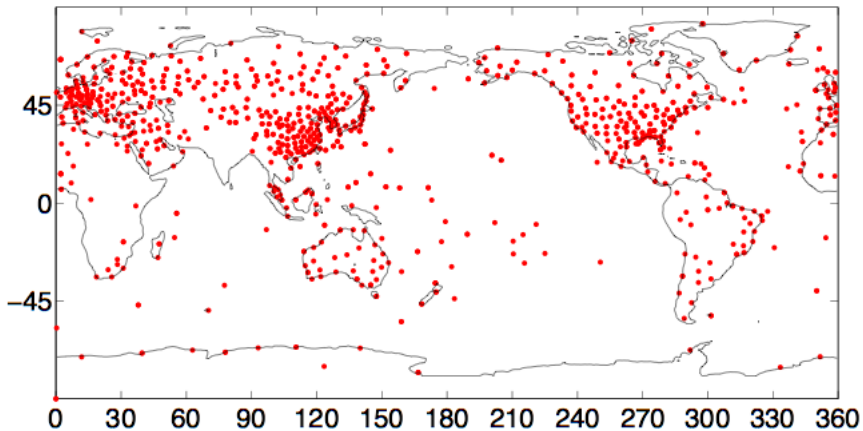
GPS



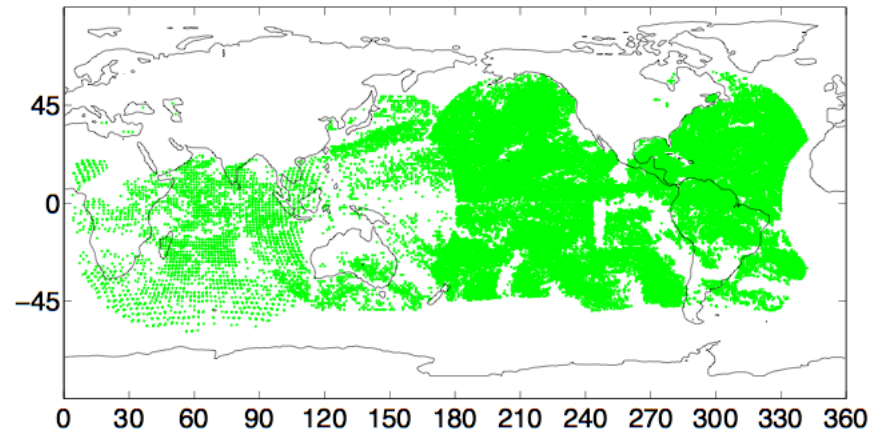
ACARS and Aircraft



Radiosondes



Sat Winds

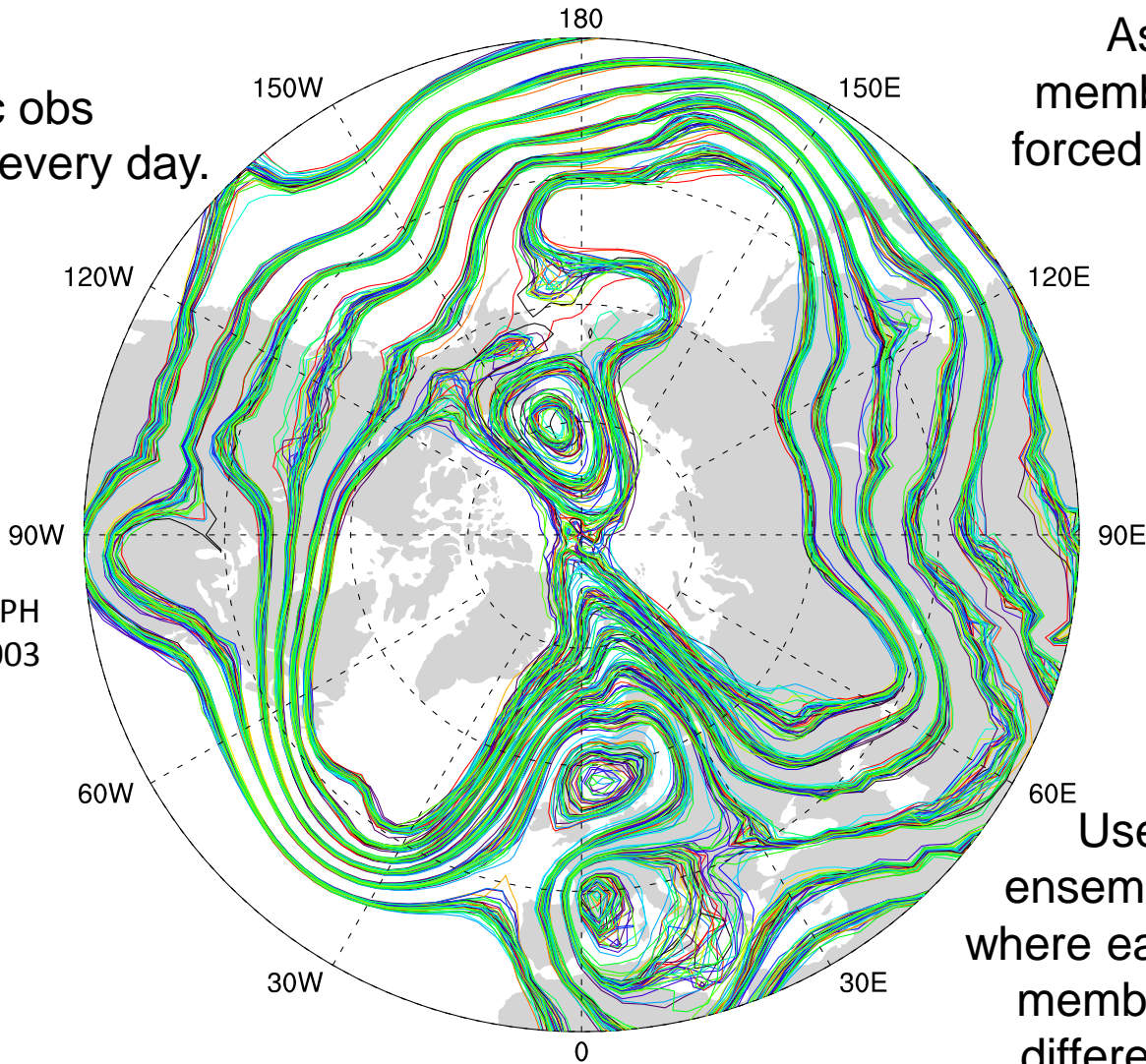


Atmospheric Reanalysis

O(1 million)
atmospheric obs
assimilated every day.

Assimilation uses 80
members of 2° FV CAM
forced by a single ocean.

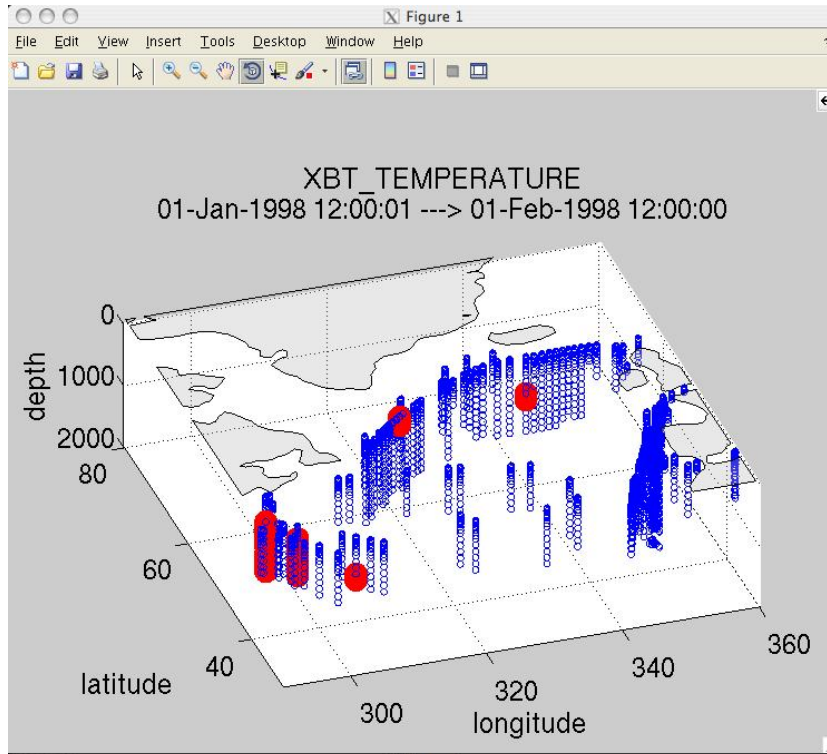
500 hPa GPH
Feb 17 2003



CONTOUR FROM 5200 TO 5700 BY 100

Used in turn to force an
ensemble of ocean models
where each ocean ensemble
member is matched with a
different atmosphere state

Observation Visualization Tools



MATLAB 7.9.0 (R2009b)

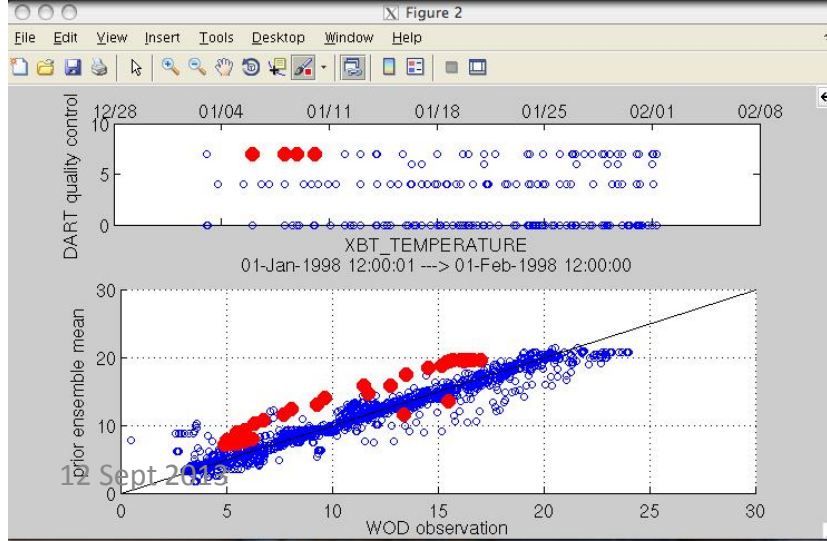
Current Folder: /fs/image/home/thoar/DART/models/POP/work

Shortcuts How to Add What's New

Variable Editor - obsmat

obsmat <2739x9 double>

	1	2	3	4	5	6	7	8	9
236	340.0700	61.0000	200	8.8950	8.8613	0	613	7.2976e+05	
237	340.0700	61.0000	250	8.9310	8.8631	0	614	7.2976e+05	
238	340.0700	61.0000	300	8.6230	8.8421	0	615	7.2976e+05	
239	340.0700	61.0000	400	7.0700	8.6502	0	616	7.2976e+05	
240	340.0700	61.0000	500	6.6250	8.3299	0	617	7.2976e+05	
241	340.0700	61.0000	600	6.2390	8.0034	7	618	7.2976e+05	
242	340.0700	61.0000	700	5.8530	7.6989	7	619	7.2976e+05	
243	340.0700	61.0000	800	5.4670	7.2985	0	620	7.2976e+05	
244	340.0700	61.0000	900	5.0810	6.7805	0	621	7.2976e+05	
245	340.0700	61.0000	1000	4.6940	6.2161	0	622	7.2976e+05	
246	340.0700	61.0000	1100	4.3740	5.6387	0	623	7.2976e+05	
247	340.0700	61.0000	1200	4.1000	5.1041	0	624	7.2976e+05	
248	350.5500	42.1500	0	15.6000	NaN	4	1	7.2976e+05	
249	350.5500	42.1500	10	15.5900	NaN	4	2	7.2976e+05	
250	350.5500	42.1500	20	15.5600	NaN	4	3	7.2976e+05	
251	350.5500	42.1500	30	15.5400	NaN	4	4	7.2976e+05	
252	350.5500	42.1500	50	15.5000	NaN	4	5	7.2976e+05	



Command Window

```
>> link_obs(fname, ObsTypeString, ObsCopyString, CopyString, QCString, region);
N = 1520 FLOAT_SALINITY (type 15) tween levels 0.00 and 1400.00
N = 7019 FLOAT_TEMPERATURE (type 16) tween levels 0.00 and 1500.00
N = 670 MOORING_SALINITY (type 27) tween levels 0.00 and 20.00
N = 16228 MOORING_TEMPERATURE (type 28) tween levels 0.00 and 500.00
N = 1419 BOTTLE_SALINITY (type 30) tween levels 0.00 and 5000.00
N = 1568 BOTTLE_TEMPERATURE (type 31) tween levels 0.00 and 5000.00
N = 4328 CTD_SALINITY (type 32) tween levels 0.00 and 5000.00
N = 4916 CTD_TEMPERATURE (type 33) tween levels 0.00 and 5000.00
N = 38 XCTD_TEMPERATURE (type 39) tween levels 0.00 and 1000.00
N = 1440 MBT_TEMPERATURE (type 41) tween levels 0.00 and 500.00
N = 23881 XBT_TEMPERATURE (type 43) tween levels 0.00 and 1750.00
DART quality control is QC copy 2
DART quality control is QC copy 2
replacing copies with [1 < QC flag < 5] with NaN
QC summary follows:
(DART quality control == 0) 1904 obs [assimilated]
(DART quality control == 4) 594 obs [prior forward operator failed]
(DART quality control == 6) 7 obs [prior QC rejected]
(DART quality control == 7) 234 obs [outlier rejected]
```

Parallel Computation Issues

- Model algorithms are usually grid based
 - Subregions of the model grid are distributed to different processors for parallel computation
 - Best distribution puts nearest neighbors on same processors and communicates across boundaries
- DART parallelizes differently than most apps
 - 3 distinct data decompositions for parallelism

Ensemble Filter For Large Geophysical Models

1. Use model to advance **ensemble** (3 members here) to time at which next observation becomes available.

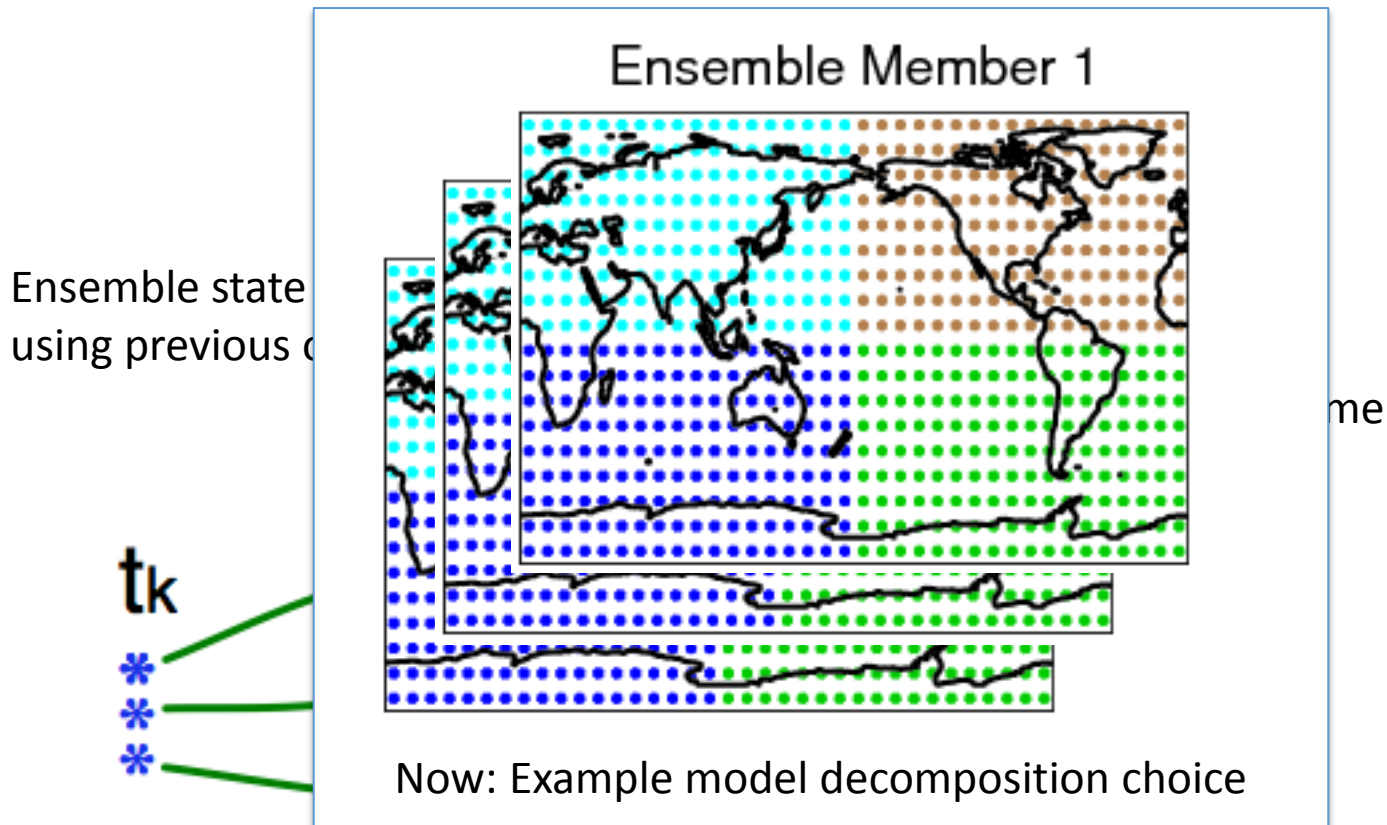
Ensemble state estimate, $x(t_k)$, after using previous observation (**analysis**)

Ensemble state at time of next observation (**prior**)



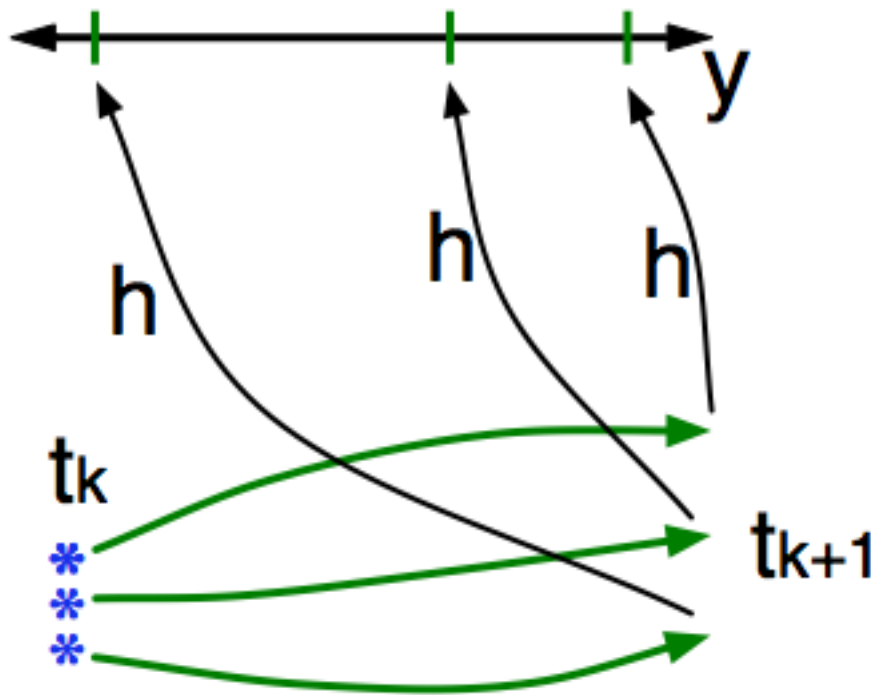
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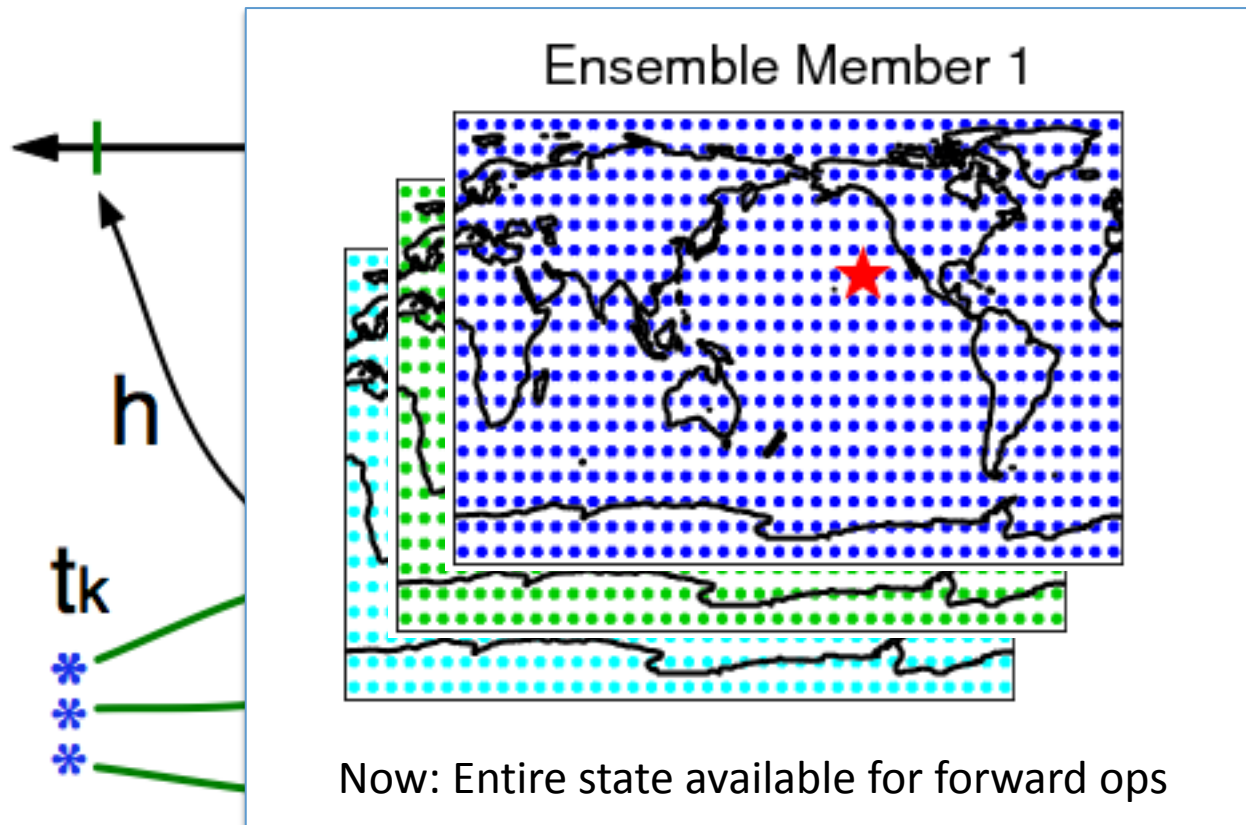
2. Get prior ensemble sample of observation, $y = h(x)$, by applying forward operator h to each ensemble member.



Theory: observations from instruments with uncorrelated errors can be done sequentially.

Ensemble Filter For Large Geophysical Models

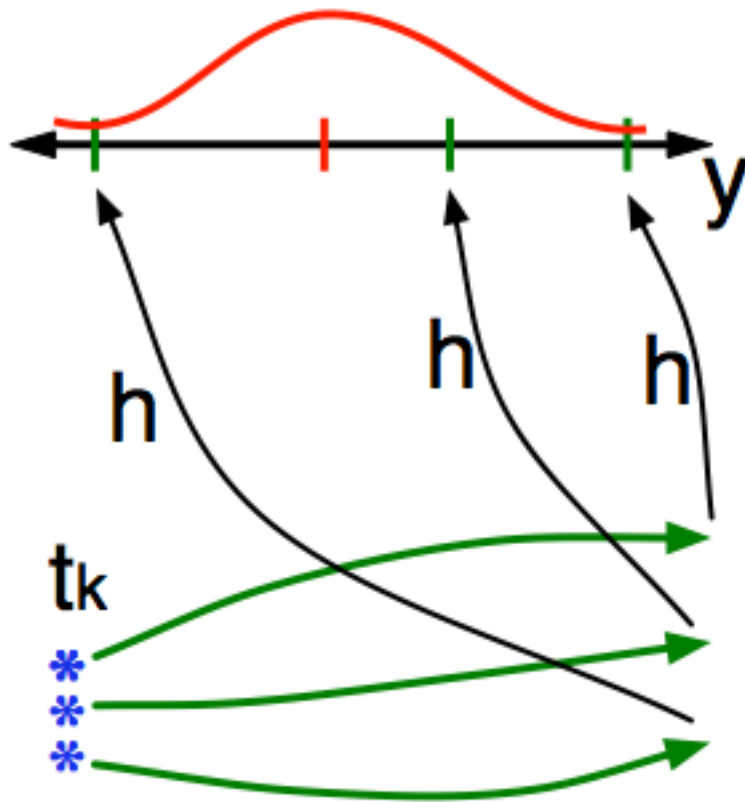
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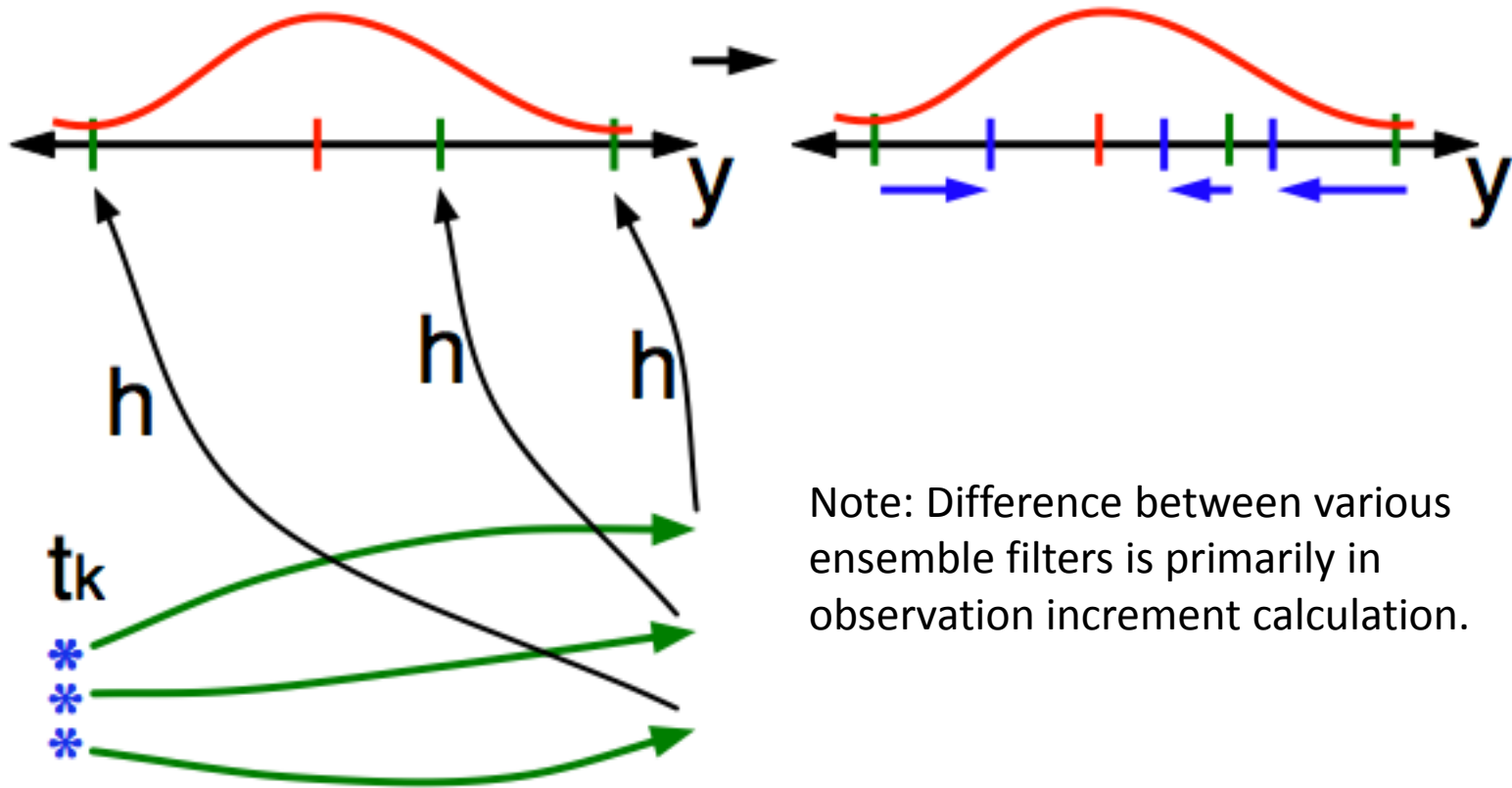
Ensemble Filter For Large Geophysical Models

3. Get **observed value** and **observational error distribution** from observing system.



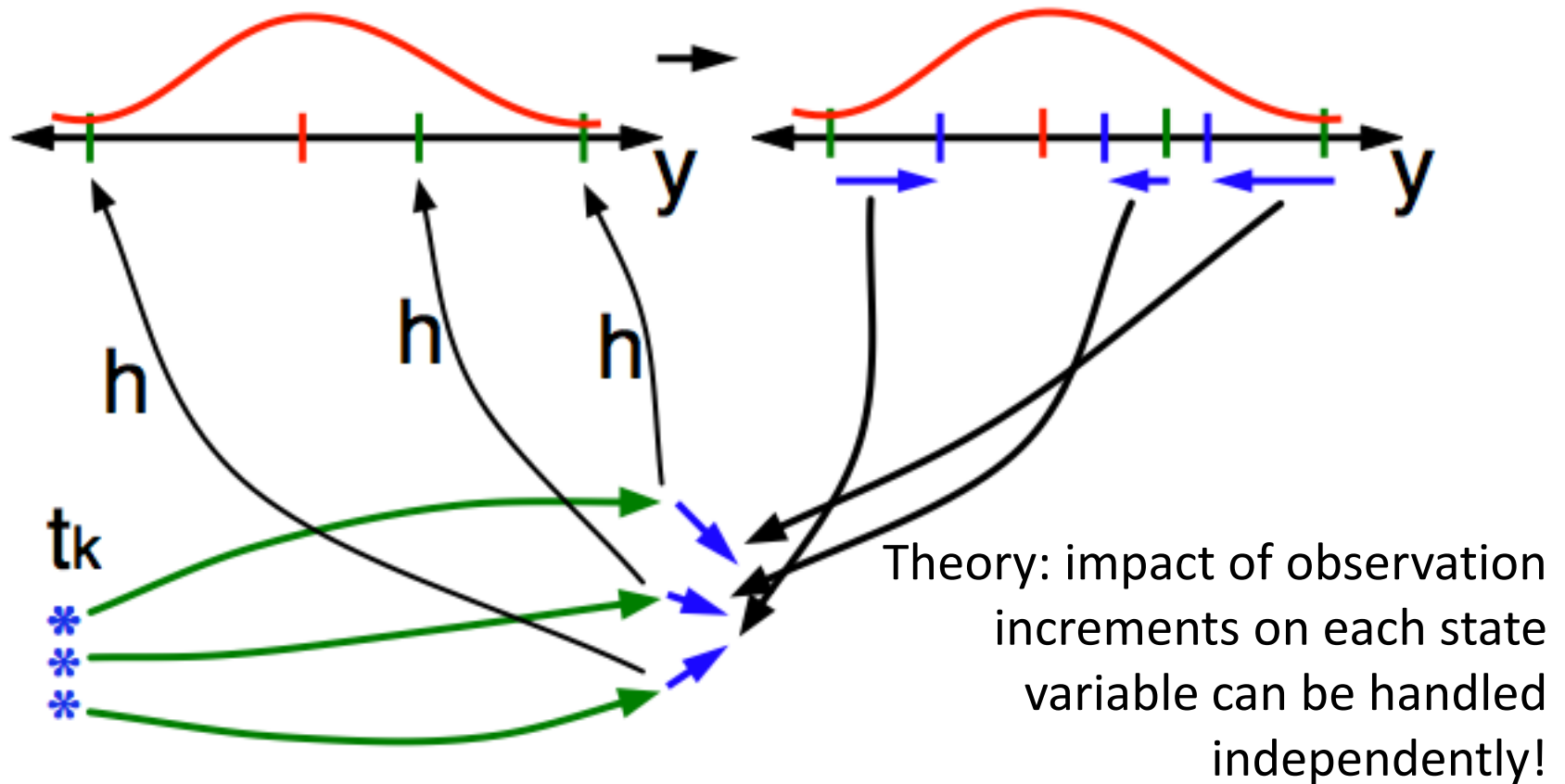
Ensemble Filter For Large Geophysical Models

4. Compute the **increments** for the prior observation ensemble (this is a scalar problem for uncorrelated observation errors).



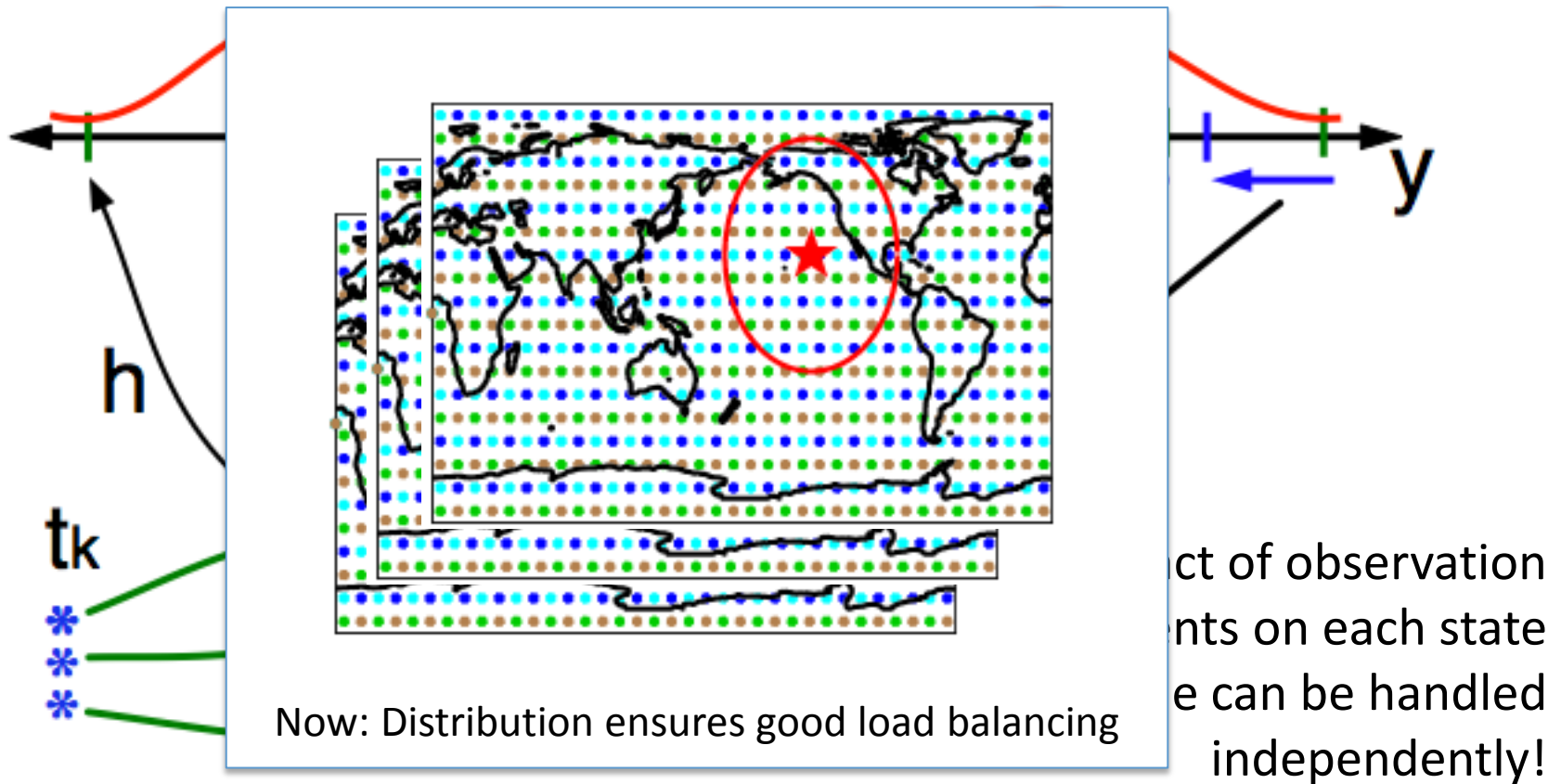
Ensemble Filter For Large Geophysical Models

5. Use ensemble samples of y and each state variable to linearly regress **observation increments** onto state variable increments.



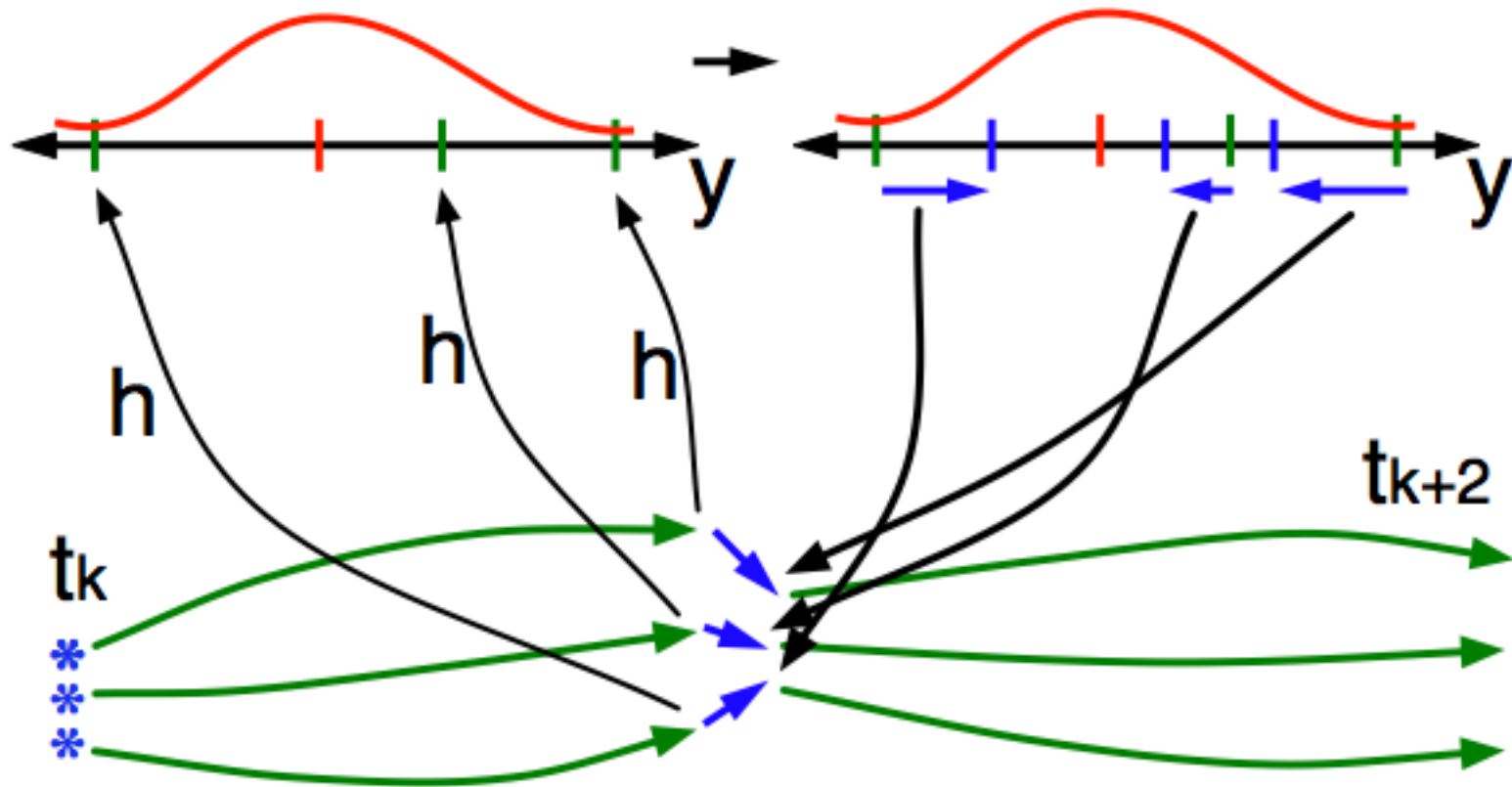
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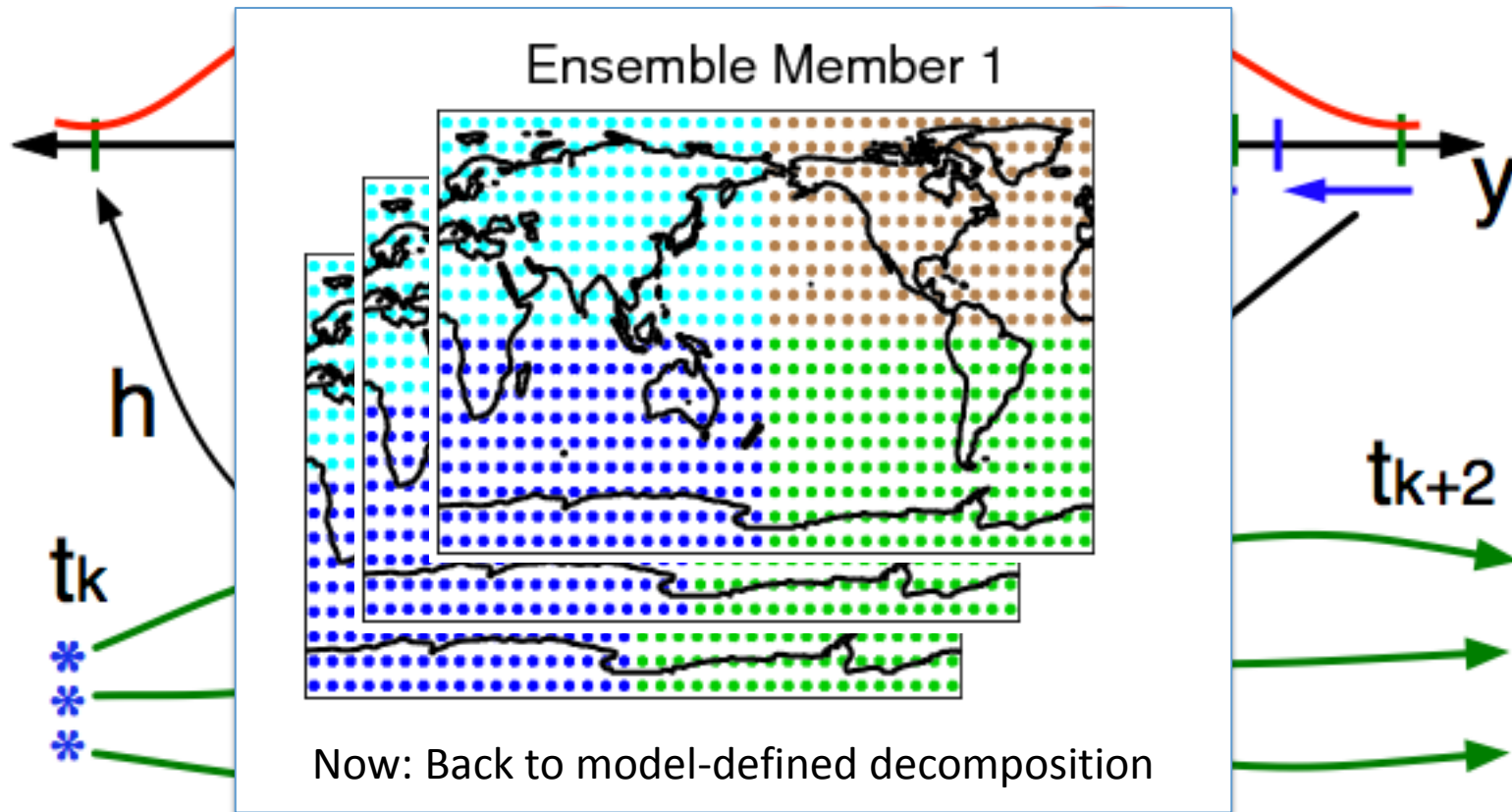
Ensemble Filter For Large Geophysical Models

6. When all ensemble members for each state variable are updated, there is a new analysis. Integrate to time of next observation ...



Ensemble Filter For Large Geophysical Models

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DART Evolution Challenges

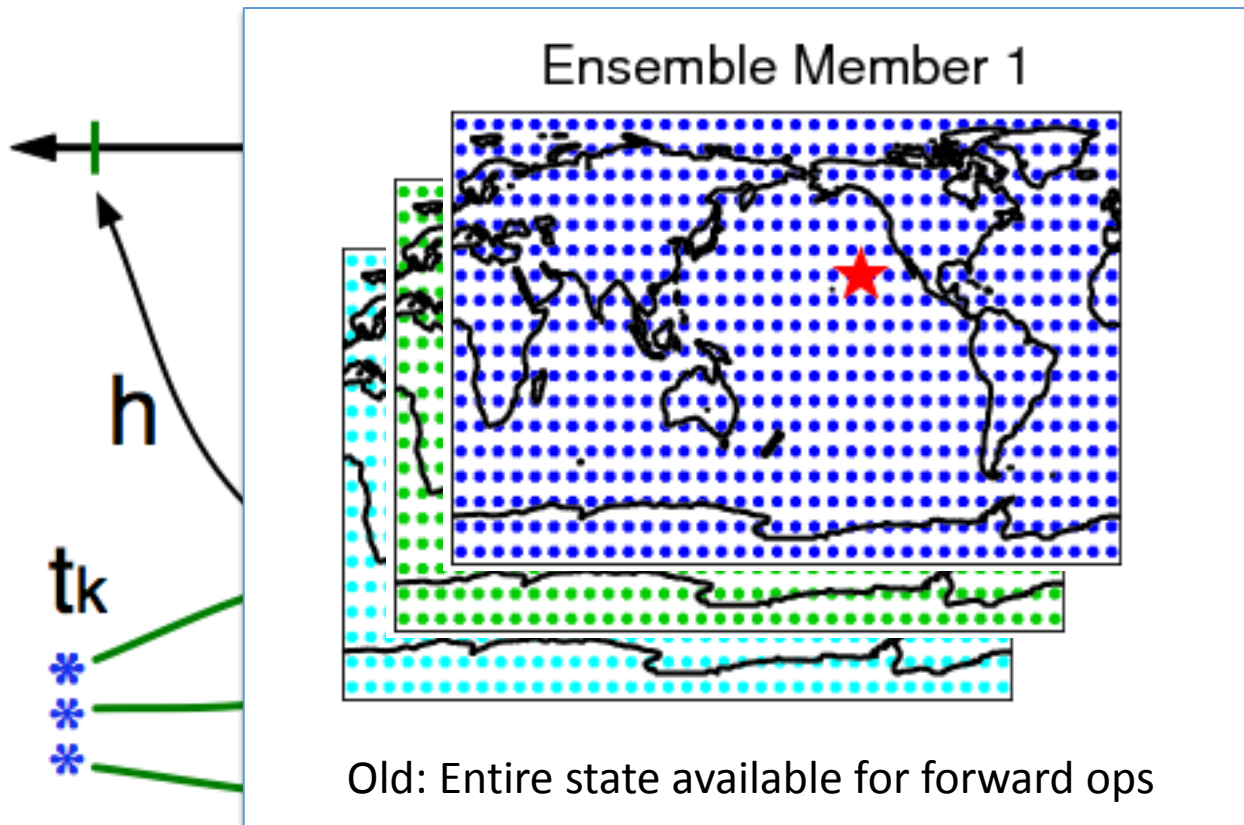
- DART runs well on $O(10 - 1000)$ processors
- New architectures $O(100,000)$ processors
- Highly scalable systems require less global communication, more asynchronicity
 - Less memory per node, more nodes, lower power
 - Harder to program Geophysical applications

Addressing Shrinking Memory Sizes

- Redesigning forward operator algorithms to avoid the need for entire state of one ensemble member in single task memory
- Requires additional communication for some types of forward operators
- Keeping spatial locality lowers communication overhead but presents load balancing issues

Ensemble Filter For Large Geophysical Models

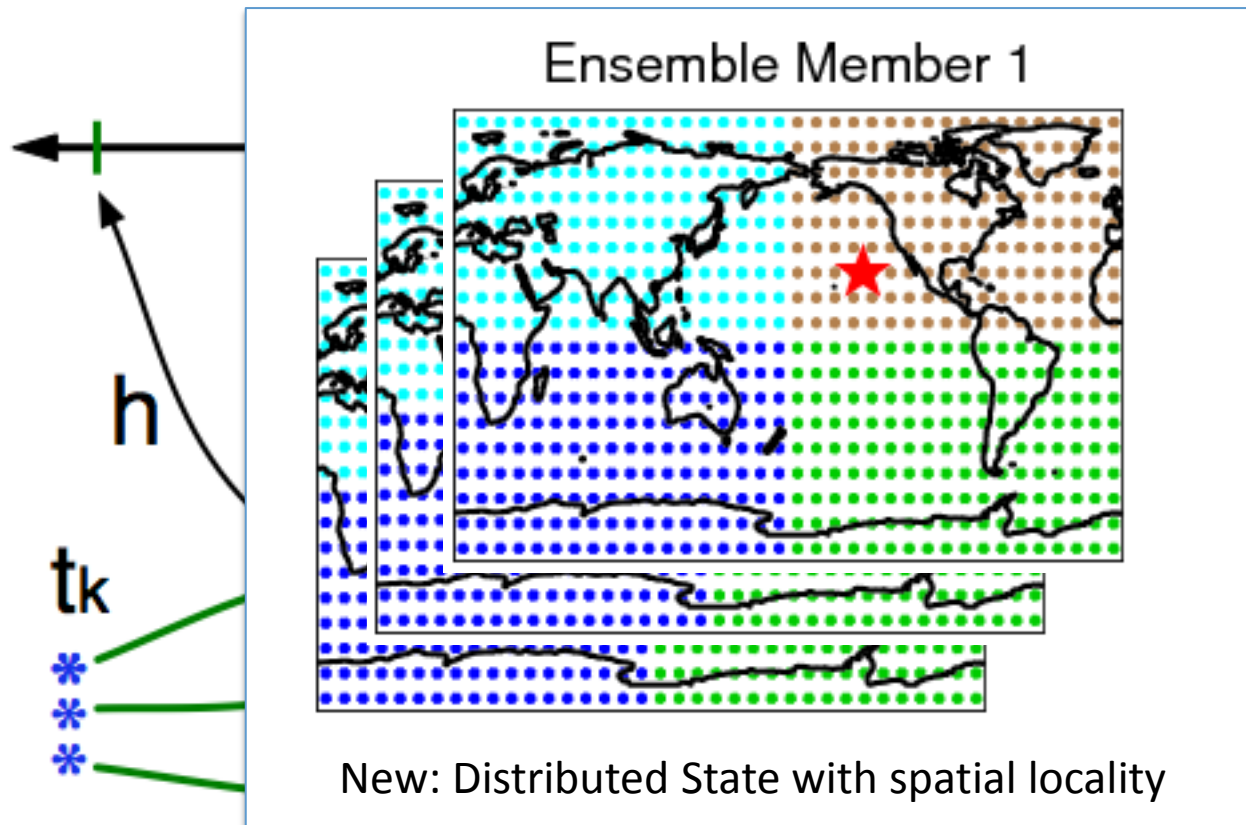
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ions from
uncorrelated
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Ensemble Filter For Large Geophysical Models

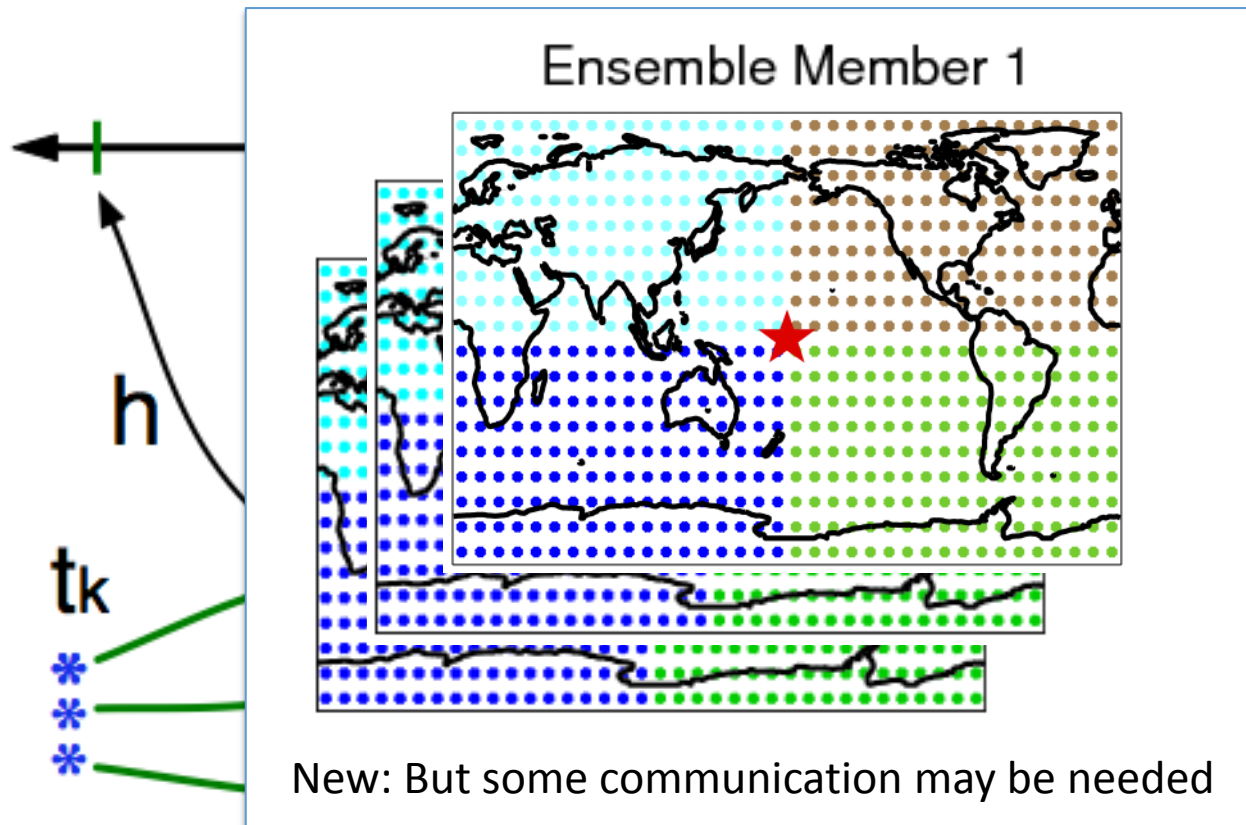
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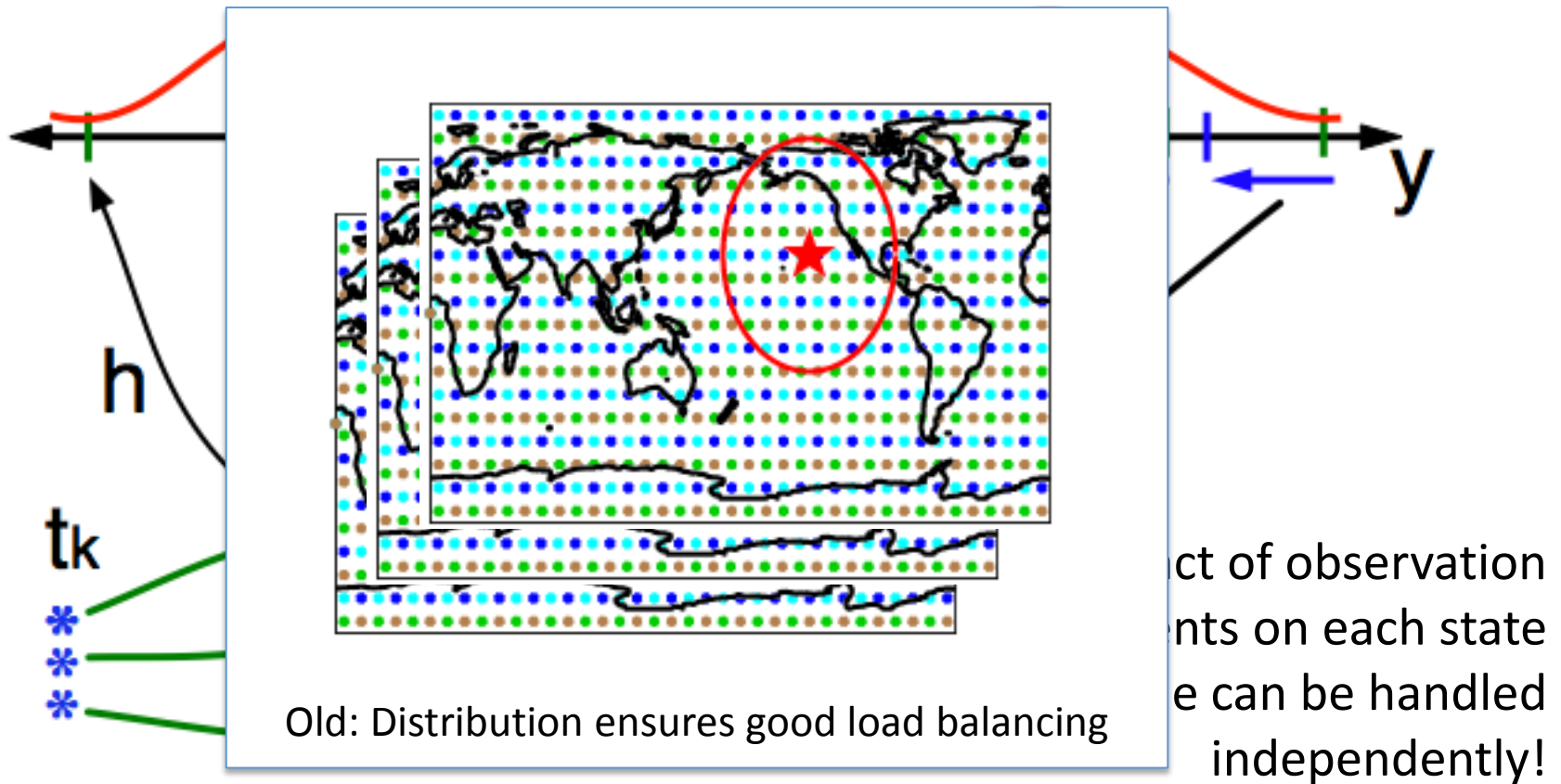


Avoiding Global Communication

- Current implementation transposes data for load balancing during state adjustment phase
- Global operations prohibitively expensive on $O(100,000)$ processor counts
- Avoiding transposes avoids global operation but again raises more load balancing issues

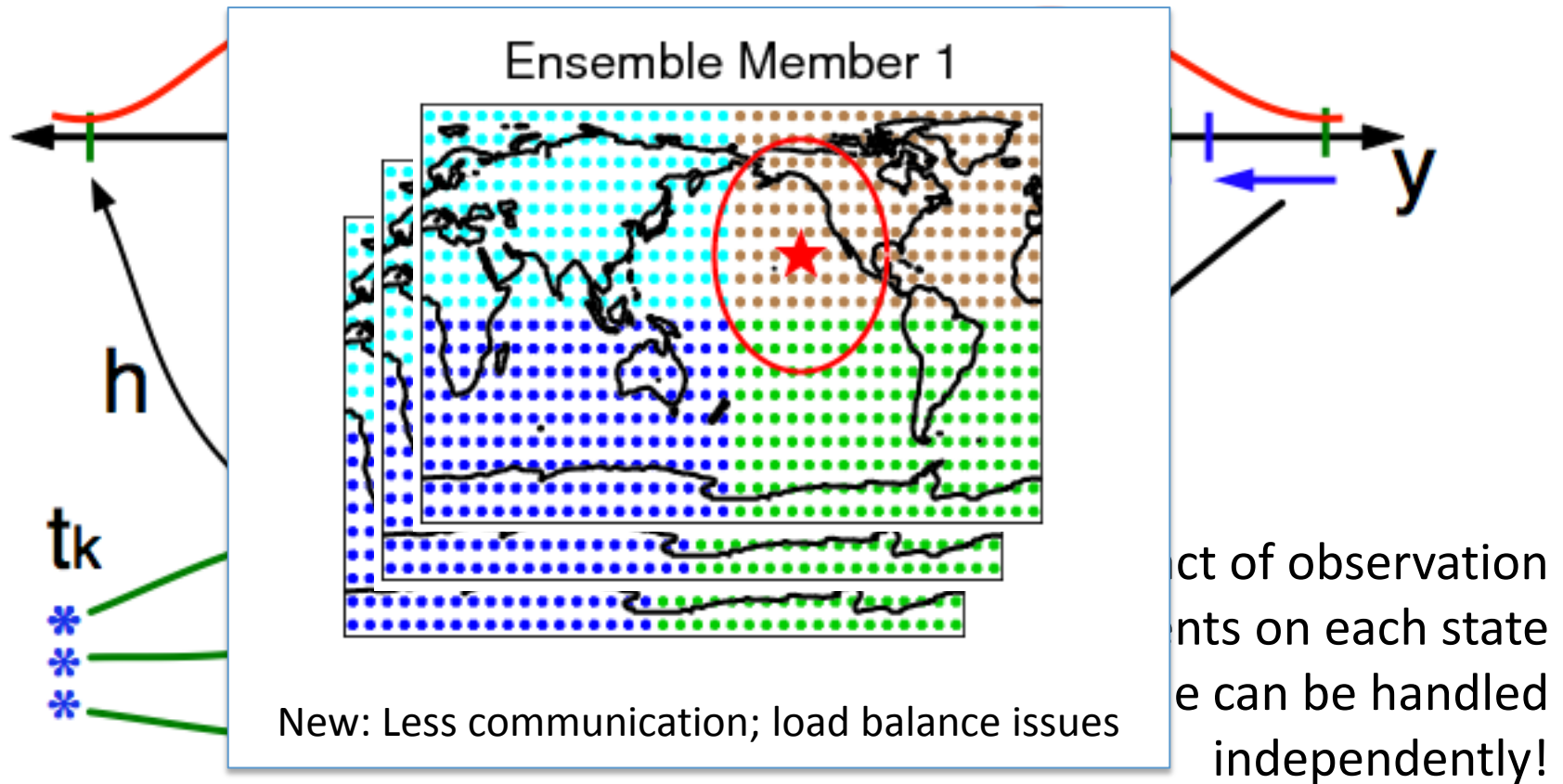
Ensemble Filter For Large Geophysical Models

5. Use ensemble samples of y and each state variable to linearly regress **observation increments** onto state variable increments.



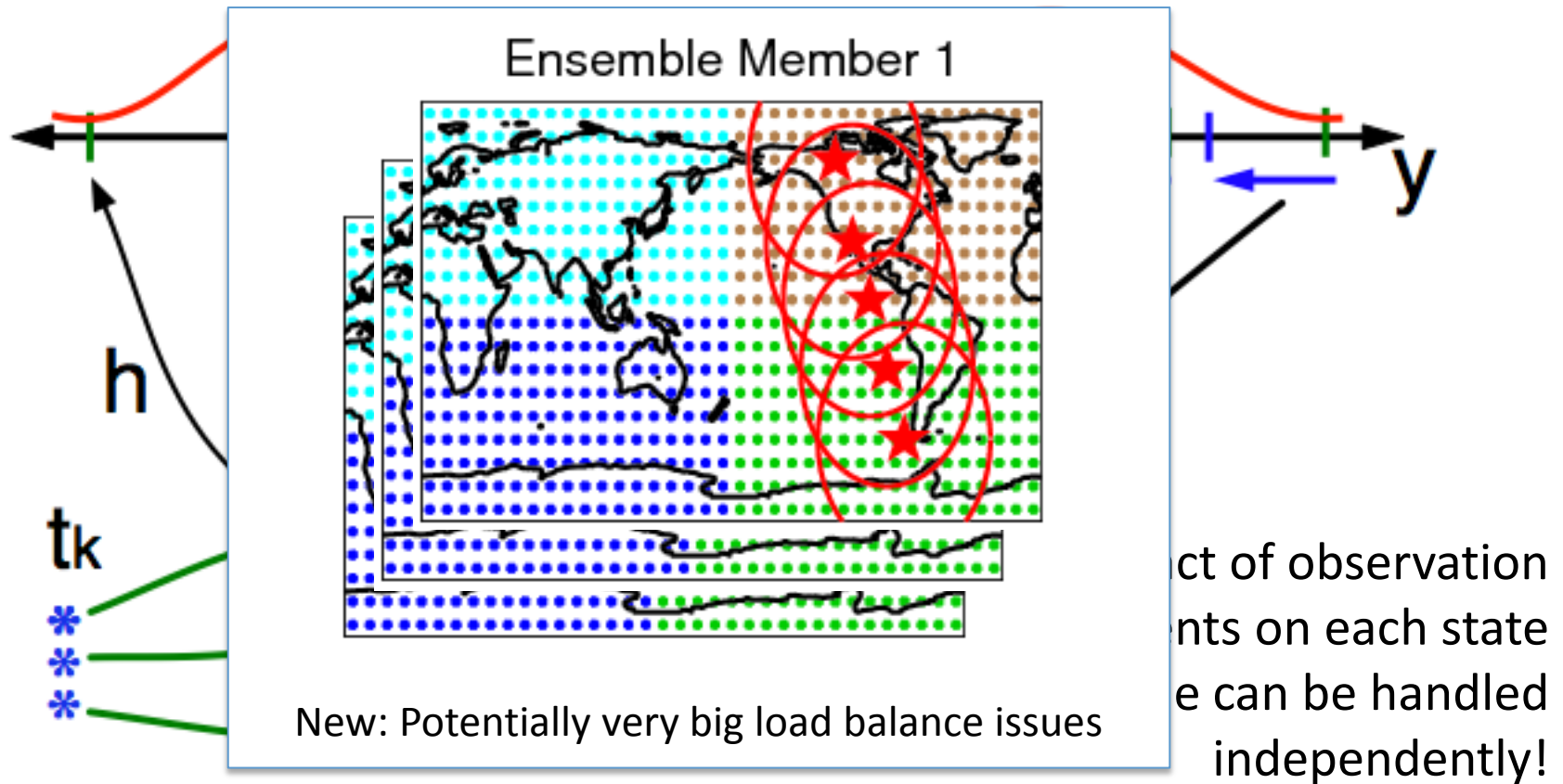
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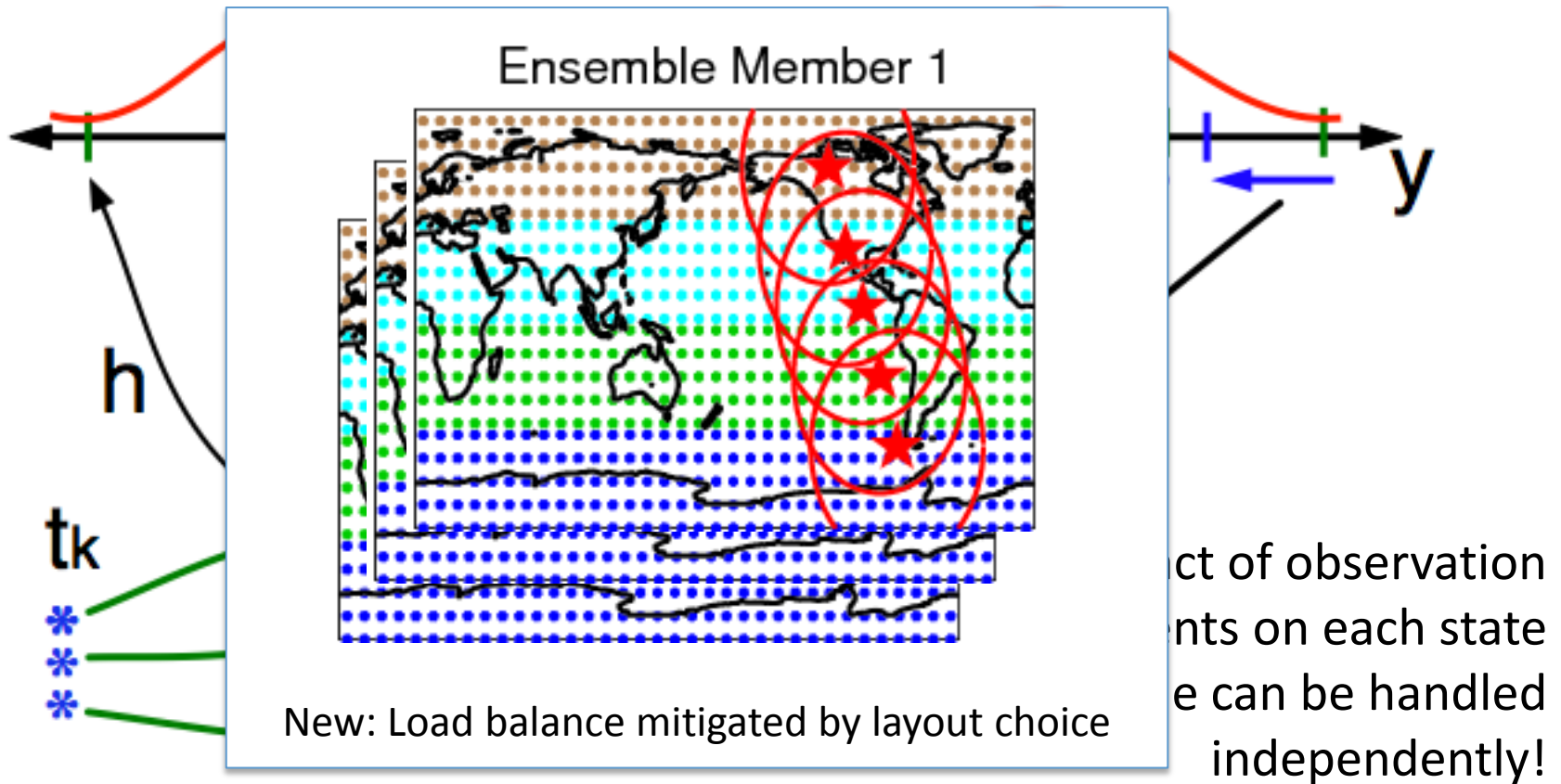
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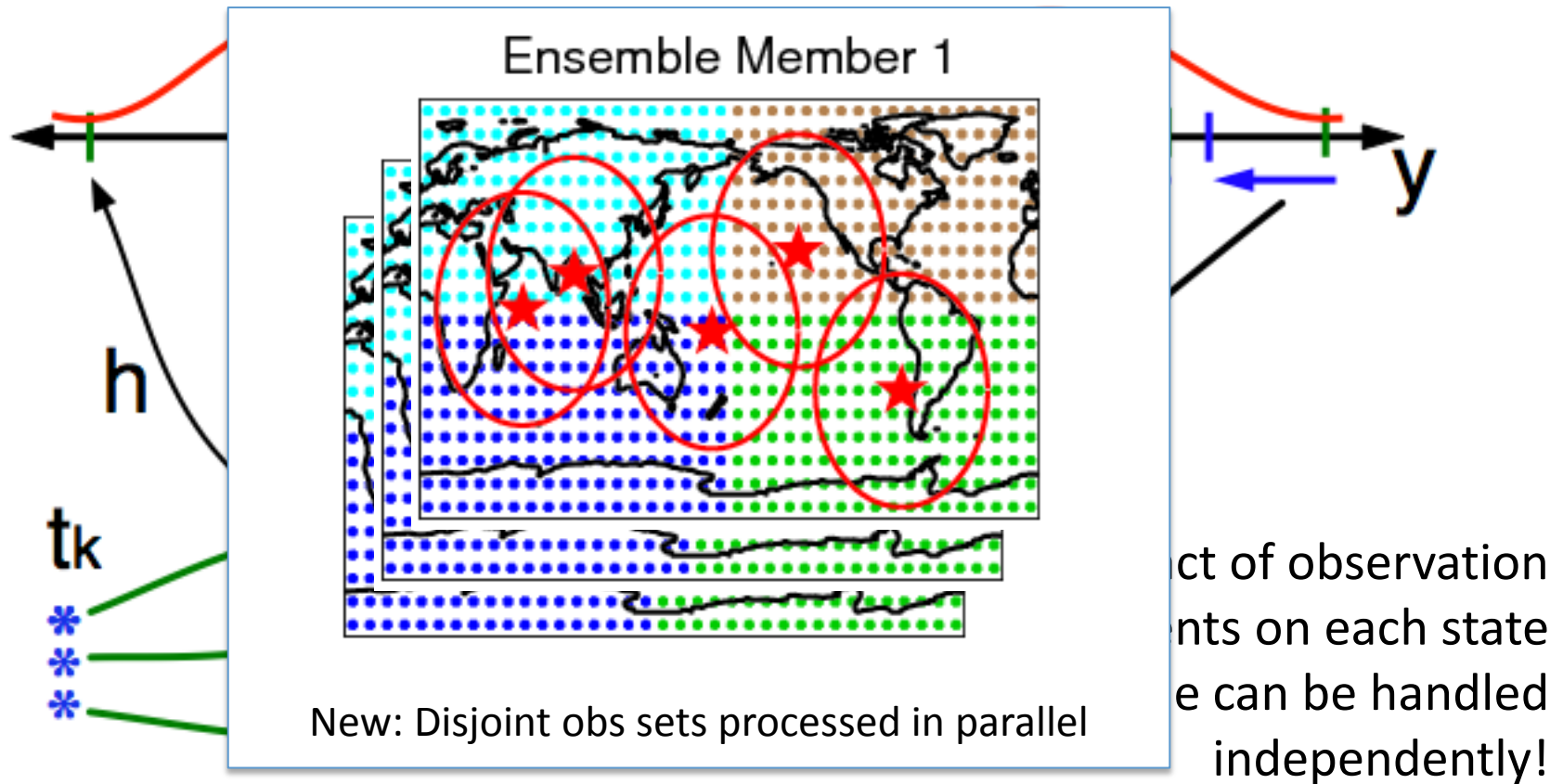
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DART Evolution for MPP Systems

- Allow single ensemble state to span multiple tasks
 - Decompose across a small number of nodes
 - Data movement confined to subsets of nodes
- Support distributed forward operator computations
 - Spatially local decomposition minimizes communication
 - One-sided MPI-2 communication avoids barriers
- Avoid global communication at state adjustment phase
 - Smarter decomposition for load balancing
 - Parallel adjustments of disjoint observation sets

DART Evolution (cont)

- Maintain reasonable interfaces that enable user-extensible sections of the code
 - Support for modification by domain scientists
 - Clear and understandable process for adding new models and new observation operators
 - Encapsulate MPI code at a level where user does not have to understand the details
- Transformational hardware architecture changes may require transformational algorithmic choices

Thank you!

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www.image.ucar.edu/DARes

