Advanced Supercomputing Technology for Big Data Science

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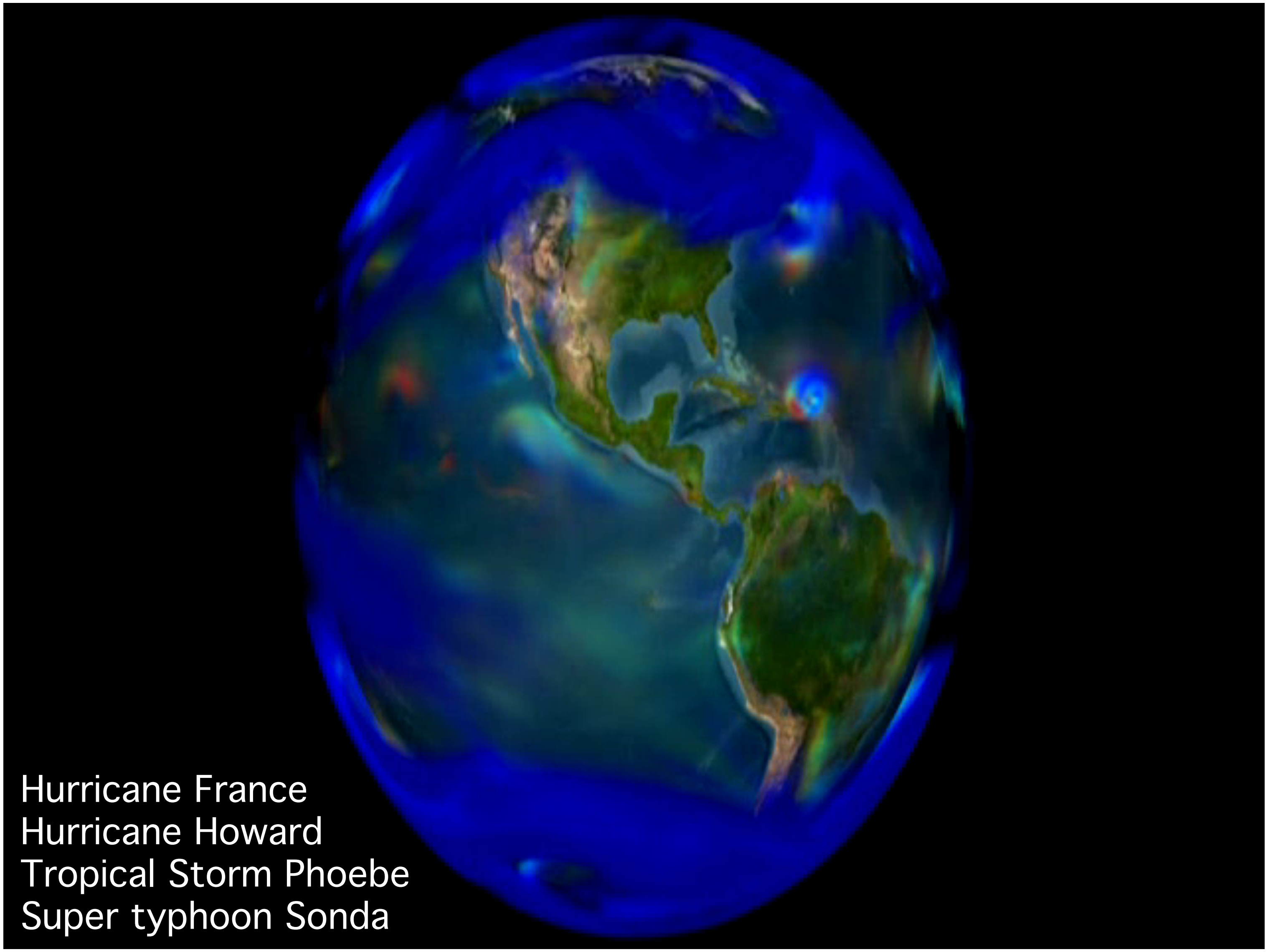
Outline

1. Introduction
2. Concurrent Visualization (and Supercomputing Technology) for Effective Data Presentation
3. Parallel Ensemble Empirical Mode Decomposition (PEEMD) for Multiscale Data Analysis and Scientific Insights
4. High-order Lorenz Models to Reveal Negative Nonlinear Feedback
5. Summary and Future Tasks

Simulations of Global Tropical Cyclones



Volume, Variety, and Velocity

- Global
- Multi-dimensional (3D)
- multivariate,
- High temporal-spatial resolution

2D Grid Cells vs. Grid Spacing

Resolution	x	y	Grid cells
2.5° (~280km)	144	91	13K
1° (~110km)	288	181	52 K
0.5° (~55km)	576	361	208 K
0.25° (~28km)	1000	721	721 K
0.125° (~14km)	2880	1441	4.15 M
0.08° (~9km)	4500	2251	10.13 M
MMF (2D CRM)	144x64	90	829 K

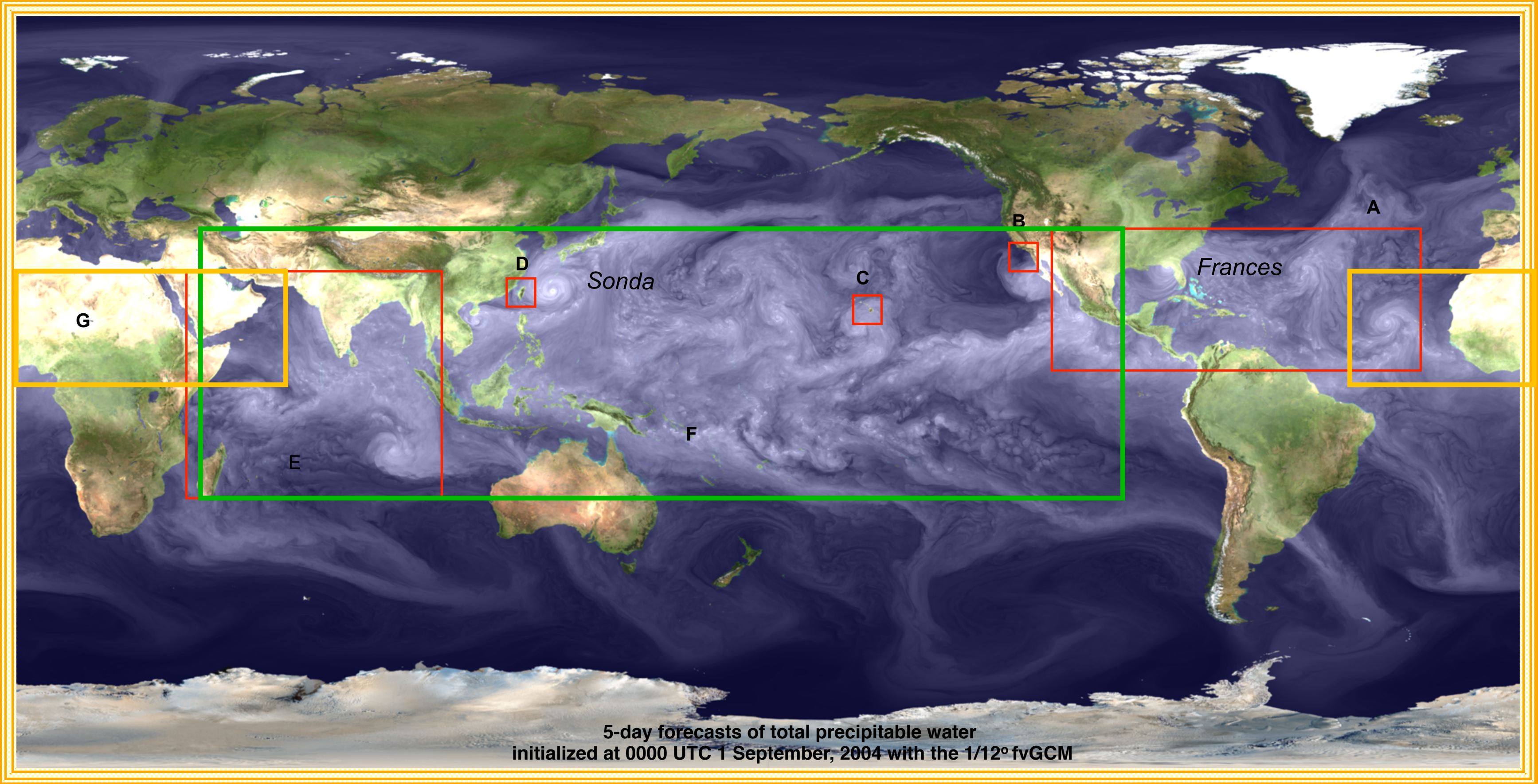
NASA Supercomputing and Visualization Systems

Pleiades Supercomputer (as Nov. 2014)

- one of a few petascale supercomputers
- R_{max} of 3,375 teraflops (LINPACK); R_{peak} of 3,988 teraflops
- 160,768 cores in total;
- 532 TB memory; 3.1 PB disk space

- Large-scale visualization system
  - 8x16 LCD tiled panel display
  - 245 million pixels
- 128 nodes with 1024 cores and 128 GPUs
- InfiniBand (IB) interconnect

Global Mesoscale Modeling on NASA Supercomputers



F: Madden-Julian Oscillation (MJO)

G: African Easterly Wave (AEW)

D: Asian Mei-Yu Front

E: Twin Tropical Cyclones

A: Atlantic Hurricanes

B: Catalina Eddy

C: Hawaiian Lee Wakes

Concurrent Visualization for Effective Data Presentation

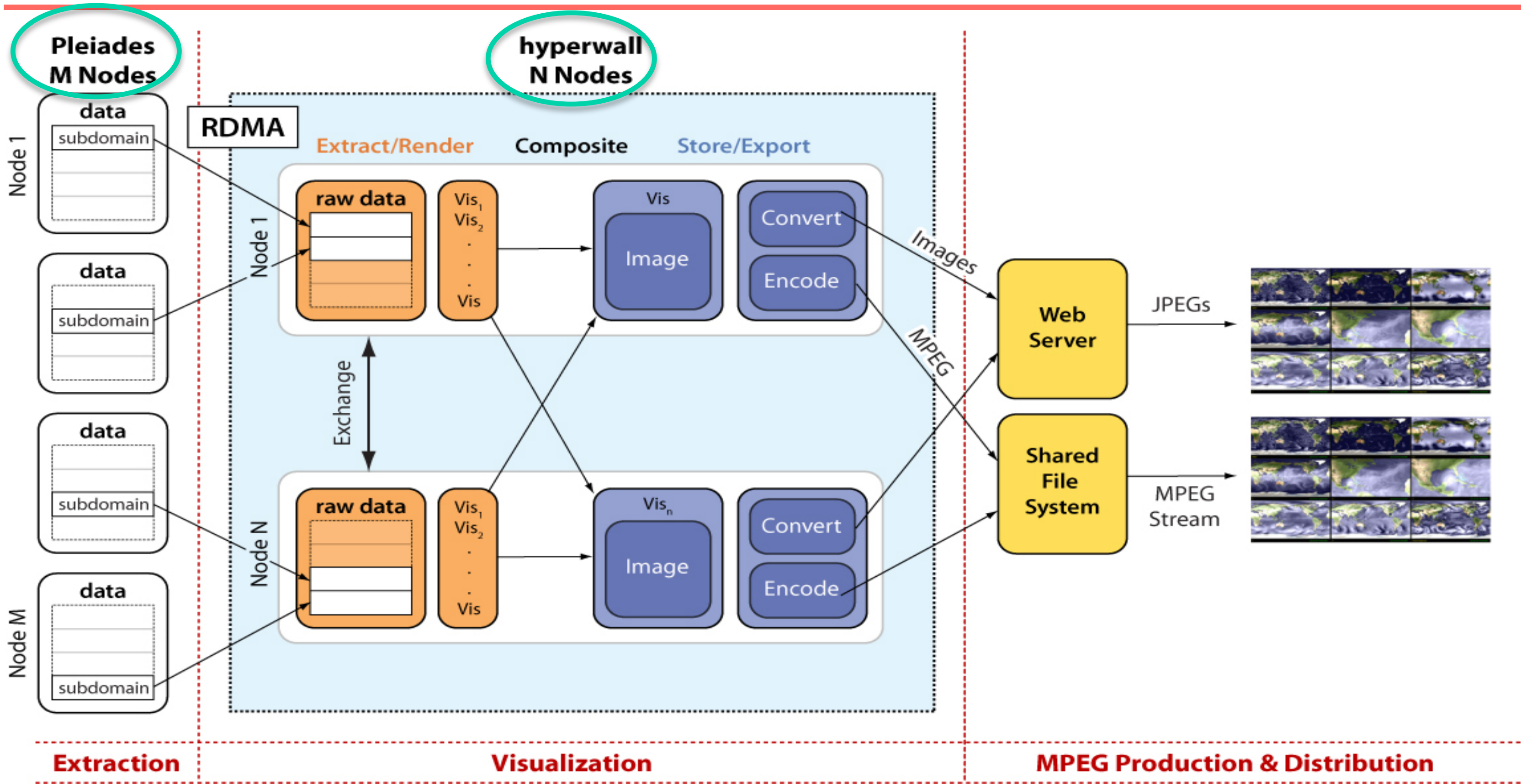
1. Large time-varying simulations generate more data than can be saved
   - Problem gets worse as processing power increases
   - Models increase spatial and temporal-resolution
2. Saving data to mass storage consumes a significant portion of runtime
3. Only a small fraction of timesteps are typically saved and important dynamics may be missed

process huge data efficiently

1. Extract data directly from running simulation for asynchronous processing
   - Add instrumentation to the simulation code, usually quite minimal
2. Simultaneously produce a series of visualizations
   - Many fields;
   - Multiple views
3. Generate and store images, movies, and "extracts"
4. Send visualizations of current simulation state almost anywhere, including web
   - Images of current state kept up-to-date in web browser
   - Stream progressively growing movies to remote systems
5. Use hyperwall-2 for parallel rendering and asynchronous I/O

generate visualizations while model is still running

M-on-N Concurrent Visualization Model



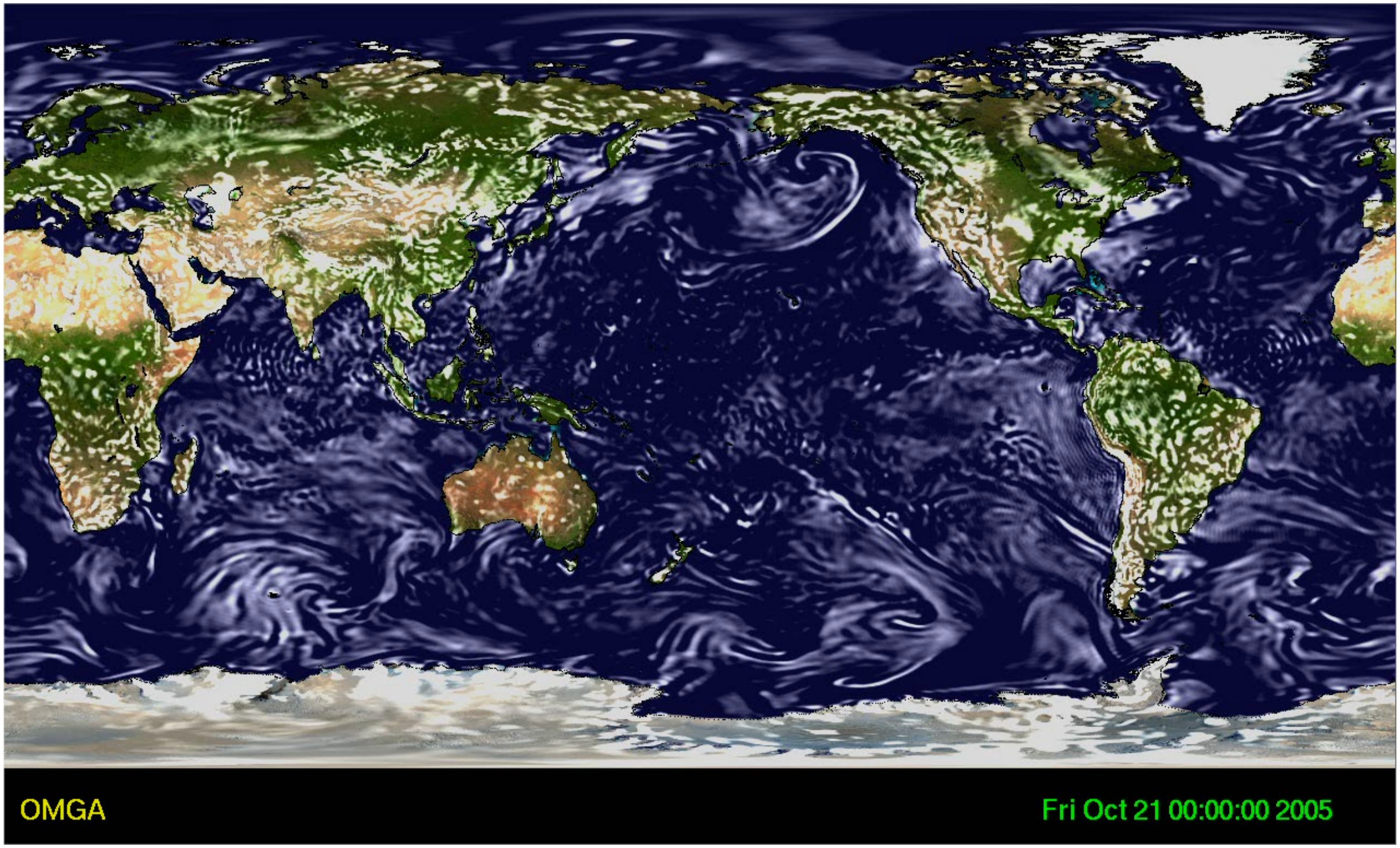
- M-on-N model takes advantage of new Pleiades-hyperwall-2 IB network topology
- Uses the simulation's parallel decomposition
- These new features enable Large-scale 3D Concurrent Visualization

Green, B., C. Henze, B.-W. Shen, 2010: Development of a scalable concurrent visualization approach for high temporal- and spatial-resolution models. AGU 2010 Western Pacific Geophysics Meeting, Taipei, Taiwan, June 22-25, 2010.

Concurrent Visualization: Benefits

- Higher temporal resolution than post-processing
  - Avoids disk space and write speed limits
  - Output typically 10-1000x greater than standard I/O
- See current state of simulation as its running
  - Application monitoring or steering
  - Detect serious job failures that might otherwise cause waste of system resources
- Minimal impact to application
  - Data is offloaded to vis cluster for concurrent processing
- Reveals features not otherwise observable
  - Has consistently revealed previously unknown dynamics

Concurrent Visualizations: Butterfly Effect?



Green, B., C. Henze, **B.-W. Shen**, 2010: Development of a scalable concurrent visualization approach for high temporal- and spatial-resolution models. Eos Trans. AGU, 91(26), West. Pac. Geophys. Meet. Suppl., Abstract A23B-142. AGU 2010 Western Pacific Geophysics Meeting, Taipei, Taiwan, June 22-25, 2010.

Shen, B.-W., B. Nelson, W.-K. Tao, and Y.-L. Lin, **2013a**, "Advanced Visualizations of Scale Interactions of Tropical Cyclone Formation and Tropical Waves," Computing in Science and Engineering, vol. 15, no. 2, pp. 47-59, March-April 2013, doi:10.1109/MCSE.2012.64

Coupled Modeling and Visualization Systems: Why?

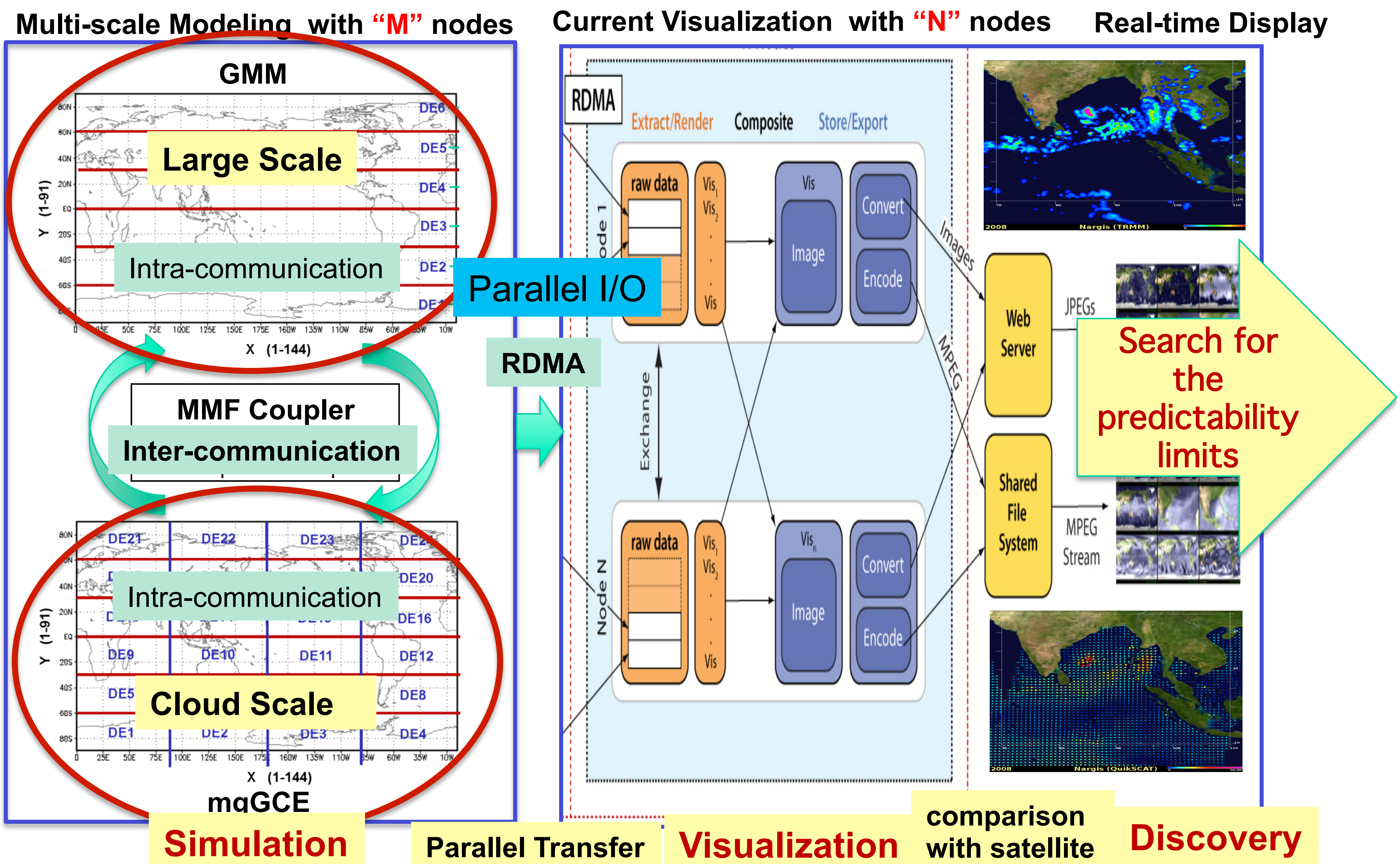
Model form	Representation of solutions	Remarks
Mathematical equations (linear)	Analytical solutions	math symbols or functions
Mathematical equations (nonlinear)	numerical solutions (contour lines)	complicated functions; graphics
Numerical models (one component)	data; Complicated graphics; 2D visualizations	graphics
Coupled models (multiple components)	huge data; (local) 3D visualizations	visualizations with a zoomed-in view
(loosely or tightly) coupled numerical model with visualization systems	massive data; (global) "Live" 3D visualizations; (a "live" visualization refers to as the one at high spatial and temporal resolutions)	Visualizations with both zoomed-in and zoomed-out views, the latter of which focus the relationships between local and remote events

Live 3D Visualizations: Benefits

- Inspire and motivate young students and researchers, who live in the world full of fancy visualizations, to investigate hurricanes dynamics;
- Improve the public understanding of hurricane dynamics and predictions, namely the understanding of hurricane dynamics by non-experts;
- Help numerical modelers quickly understand the dependence of TC simulations on the changes of model's grid spacing, physics parameterizations, and land surface processes etc;
- Promote the "integrative" (global; non-local) view on the scale interactions of hurricane dynamics and scale dependence of predictability among hurricane experts in Earth Science community, including the horizontal interactions (termed as "horizontal phasing") between two approaching systems; and processes that lead to vertical coherence (termed as "vortex phasing" for TCs).

Architecture of the CAMVis v1.0

(the Coupled Advanced Multiscale modeling and concurrent Visualization systems; Shen e al. 2011)



Empirical Mode Decomposition (EMD) for Multiscale Data Analysis and Scientific Insights

1. HHT (Hilbert Huang Transform, Huang et al., 1998; Huang and Shen, 2005,2014) consists of Empirical mode decomposition (EMD) and Hilbert Transform.
2. The data-driven EMD method is Complete, Orthogonal, Local, and Adaptive (COLA), which is ideal for the local and nonlinear analysis.
3. EMD generates a set of intrinsic mode functions (IMFs), each of which has features with comparable scales (Wu and Huang 2009, and references therein).
4. EMD performs like a filter bank (e.g., a dyadic filter); the unique feature suggests a potential for hierarchical multiscale analysis.

Fourier, Wavelet and EMD/HHT Analysis

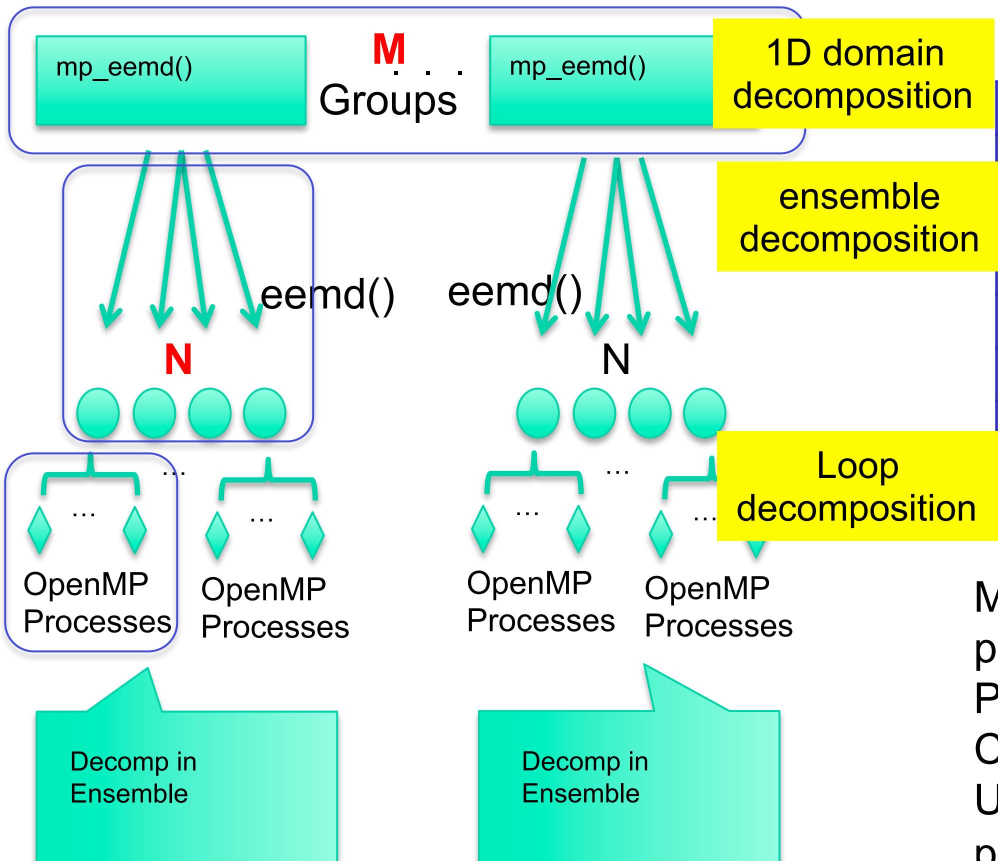
	Fourier	Wavelet	Hilbert/EMD
Basis	a priori	a priori	adaptive
Frequency	convolution: global, uncertainty	convolution: **regional,** uncertainty	differentiation: local, certainty
Presentation	energy-frequency	energy-time-frequency	energy-time-frequency
Nonlinearity	no	no	yes
Nonstationarity	no	yes	yes
Feature extraction	no	discrete: no, continuous: yes	yes
Theoretical base	theory complete	theory complete	empirical

Huang (2005); Huang et al., (1998);

Note: The above table with the major change (highlighted in blue) is updated based on the more recent table of Huang (2005). In addition, the uniqueness of the EMD method is indicated by the recent study of Daubechies et al (2011) who developed the synchrosqueezed wavelet transform, a special kind of wavelet method, to capture the flavor and philosophy of the EMD approach.

Benchmark with the Three Level Parallelism

The 3-Level parallelism is achieved with the fine-grain OpenMP inside all the N members in each M process.



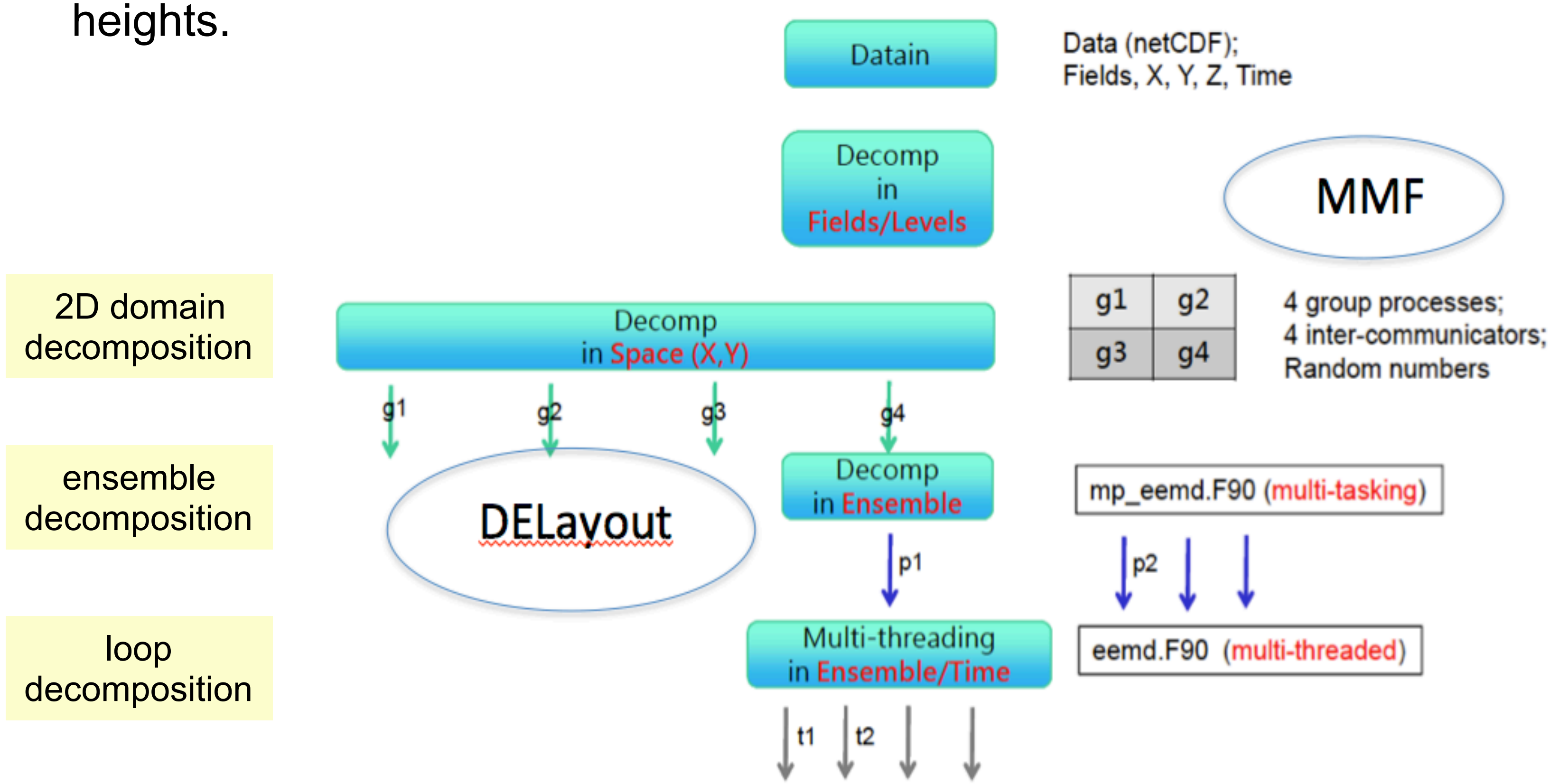
Speedup

M	N	OMP1	OMP2	OMP4
2	1	1.99	3.66	6.28
2	2	3.79	6.33	10.92
4	2	7.46	12.52	21.57
4	4	13.72	21.65	33.99
25	4	80.40	127.79	200.50
100	4	286.35	459.04	721.30
100	16	449.16	100 nodes	

Multiple runs for the MRG case with 1001x1001 points and en=1000 were performed on Pleiades. Sandy processors were used; each CPU has 8 cores, and each node has 16 cores. Using 100 nodes, the MPI-OMP hybrid parallelism produces the best performance.

Four-level Parallelism in EEMD

The EEMD method requires large computational resources that are linearly proportional to the number of ensemble trials. A parallel version is proposed to extend the 1D EEMD to multi-dimensional EEMD for multiple fields at different heights.

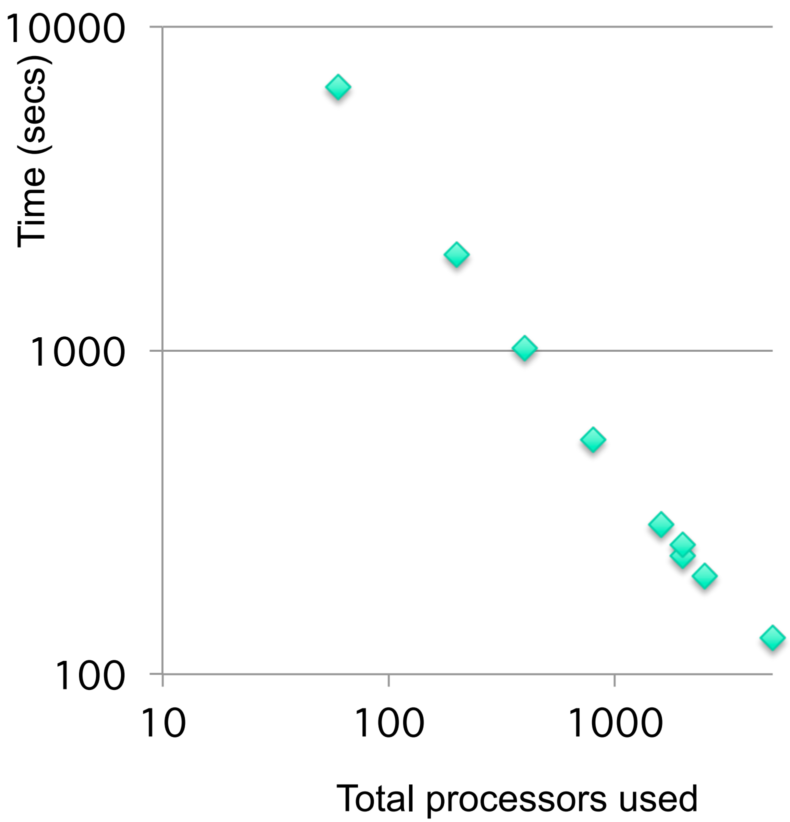


“Grid-Ensemble-OpenMP” 4 levels Parallelism.

PEEMD: Scaling of 5000 Cores

MRG Case, Grid:1000x1000 (400MB), Ivy Bridge Processors

4-Level Parallelization
SGI MPT library is used

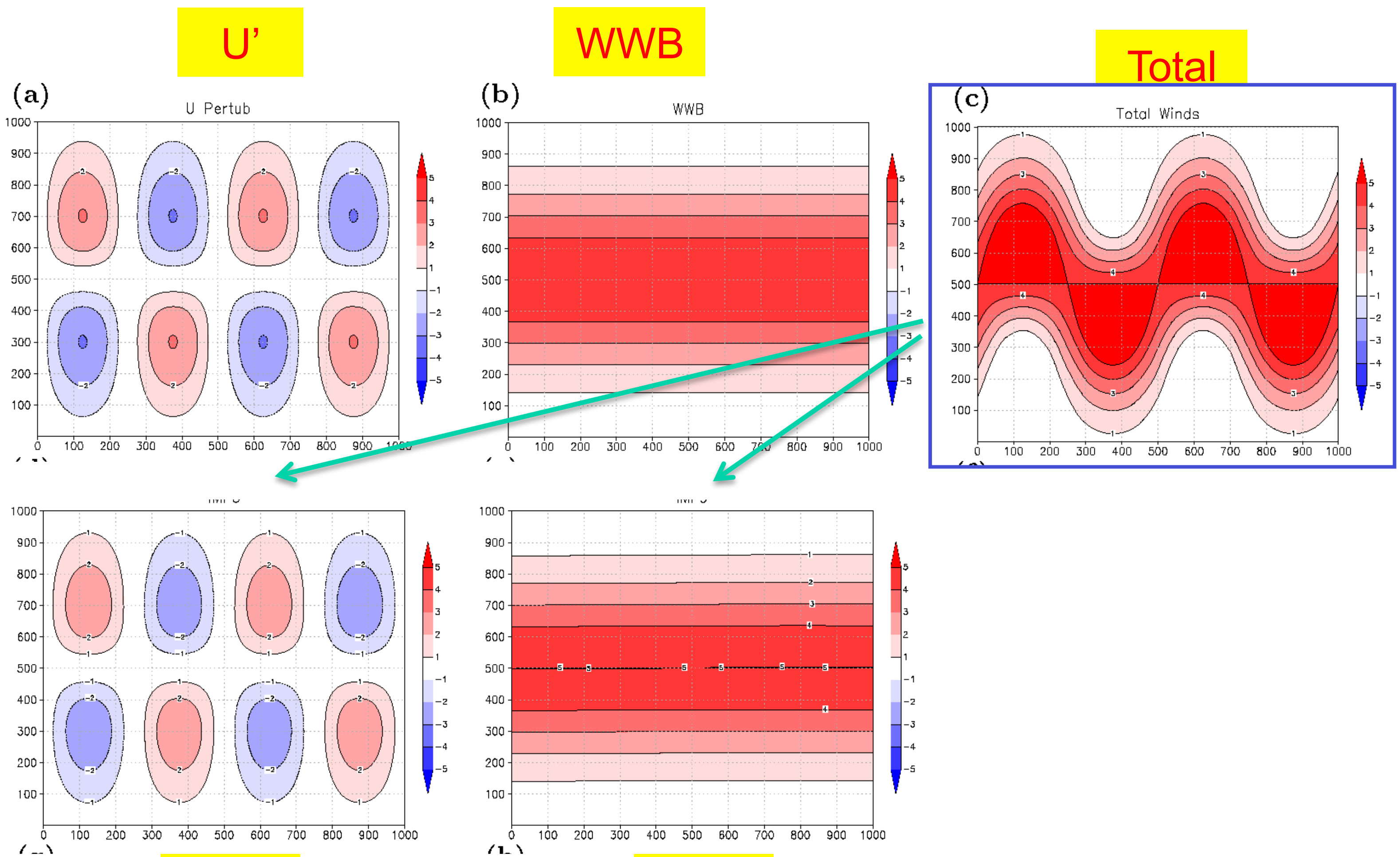


Grid DELayout I	J	Ens	OMP	Total	Time (secs.)	Speed Up
5	6	2		60	6543.56	1.0
10	10	2		200	1983.25	3.3
10	10	4		400	1021.10	6.4
20	20	2		800	531.36	12.3
20	20	4		1600	289.42	22.6
25	40	2		2000	231.69	28.2
25	20	2	2	2000	251.21	26.0
25	25	4		2500	200.60	32.6
25	25	4	2	5000	129.68	50.4
50	50	2		5000	123.85	52.8

Parallel efficiency:
2000 cores, 28.2/(2000/60)=84.6%
5000 cores, 52.8/(5000/60)=63.4%

Decompositions of an MRG wave with the PEEMD

Analytical Solutions



IMFs

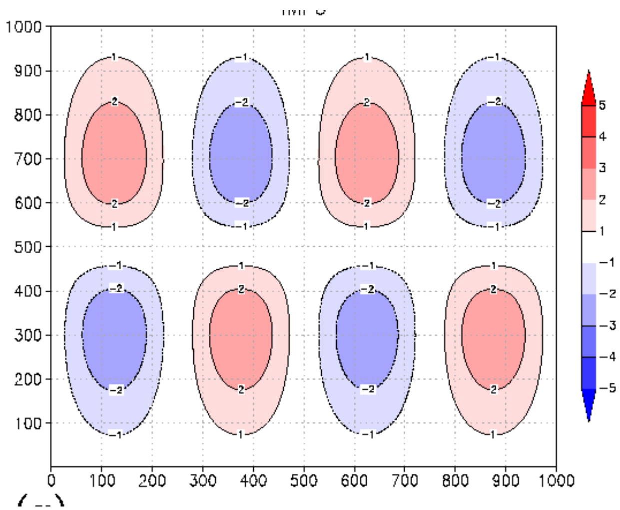
IMF6

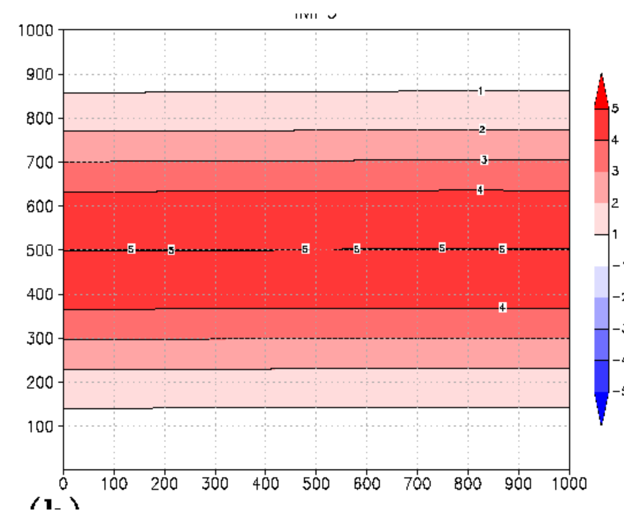
(an oscillatory mode)

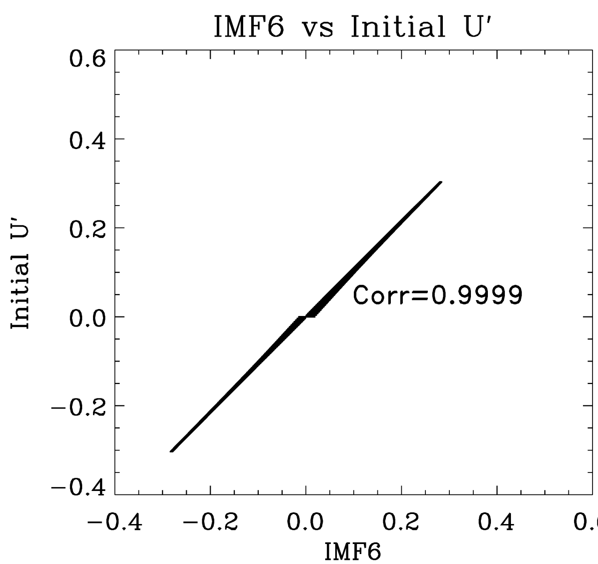
IMF9

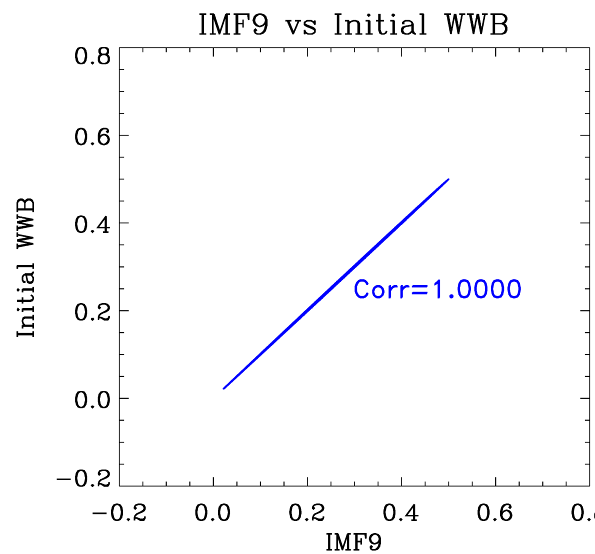
(a trend mode)

Correlation Plots







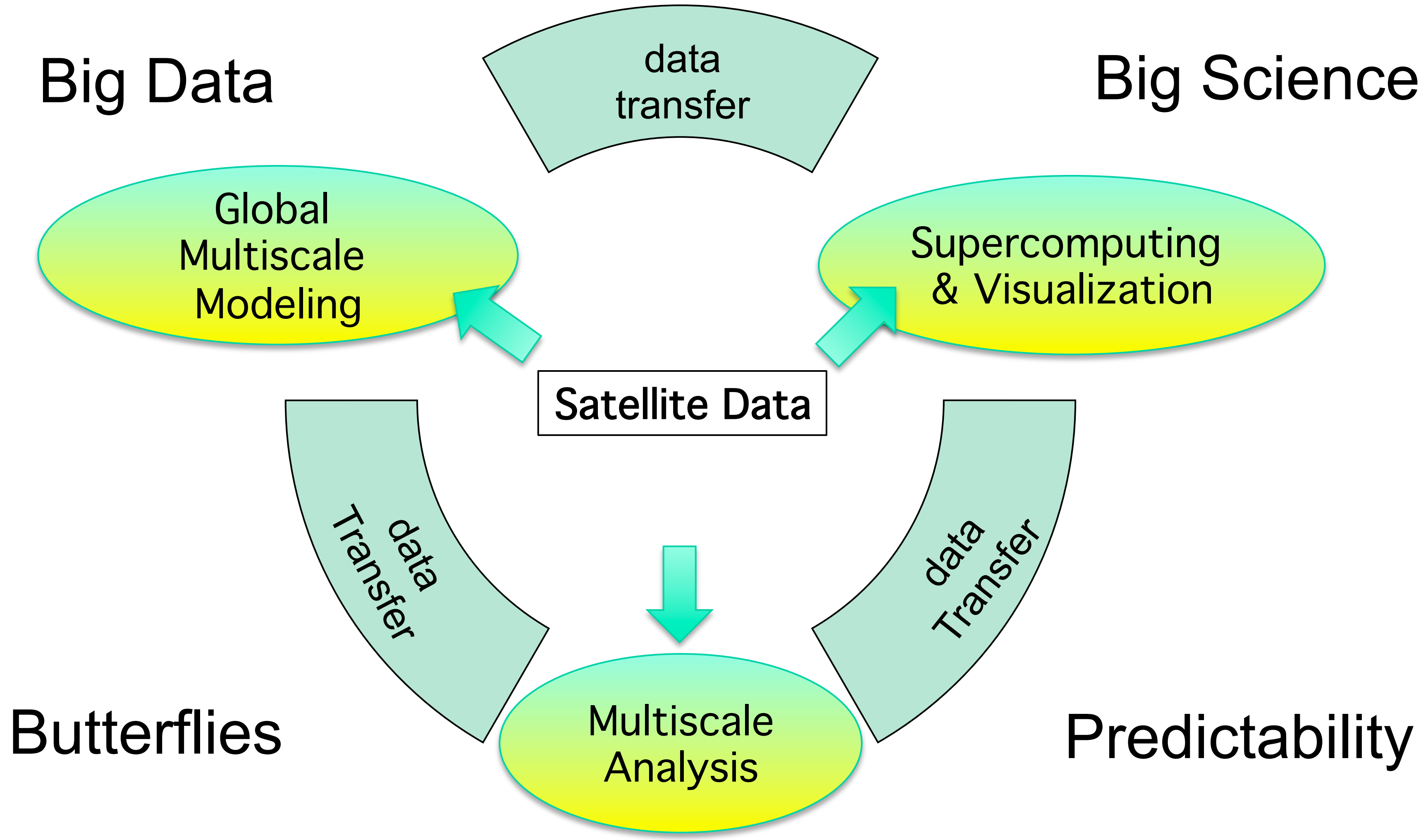


Ensemble Empirical Mode Decomposition (EEMD) Implementations

- R Implementation
  - Designed for education & experimentation purposes (prototyping release)
  - Easier to use
  - Easier to setup
  - More Portable
  - 10 files with 1155 lines (with four test cases)

- FORTRAN Implementation
  - Designed for research purposes (production release)
  - Fast, Scalable
  - 250x faster than R implementation (using the MRG case with 101x101 grid points)
  - Used in PEEMD
  - 52 files with 5497 lines (including four standard tests)

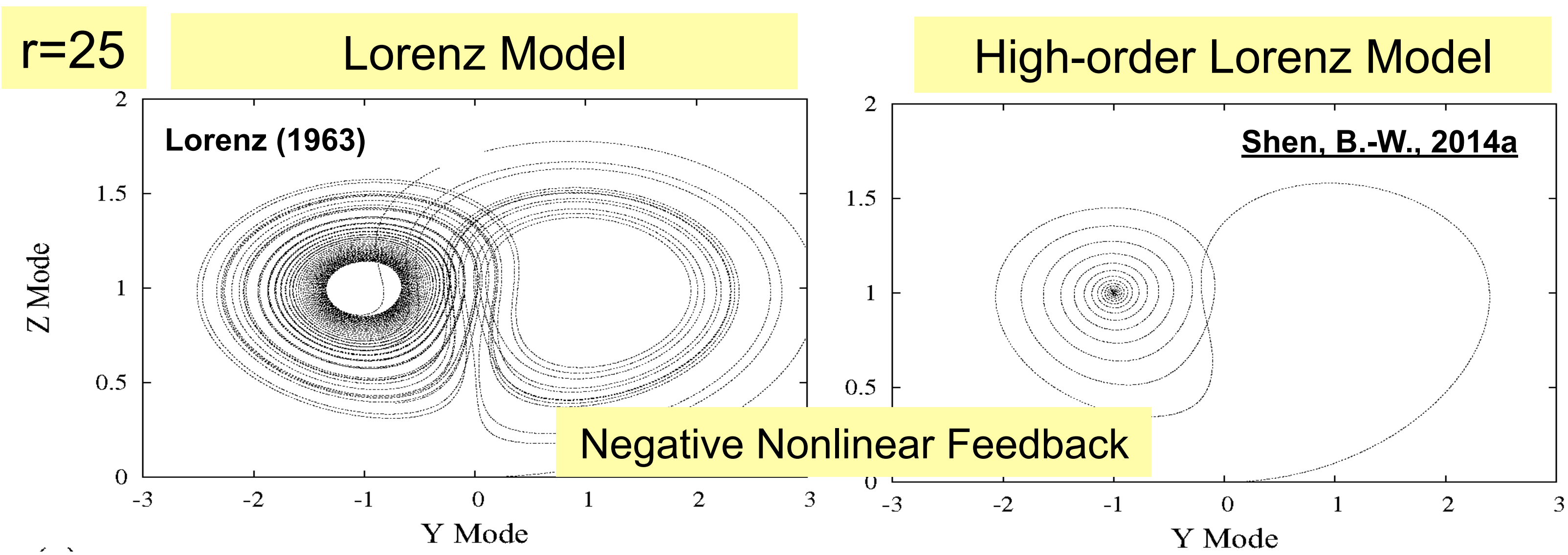
Summary



Parallel Ensemble Empirical Mode Decomposition (PEEMD)

Butterfly Effect vs. Multiscale Processes

- Lorenz's studies suggested finite predictability and nonlinearity as the source of chaos.
- Increased degree of nonlinearity (e.g., multiscale interactions) can stabilize solutions and thus improve simulations (Shen, 2014a,b; 2015).



Shen, B.-W., 2014a: Nonlinear Feedback in a Five-dimensional Lorenz Model. *J. of Atmos. Sci.* **71**, 1701–1723. doi: http://dx.doi.org/10.1175/JAS-D-13-0223.1

Shen, B.-W., 2014b: On the Nonlinear Feedback Loop and Energy Cycle of the Non-dissipative Lorenz Model. *Nonlin. Processes Geophys. Discuss.,* 1, 519-541, 2014. www.nonlin-processes-geophys-discuss.net/1/519/2014/

Shen, B.-W., 2015: Nonlinear Feedback in a Six-dimensional Lorenz Model. Impact of an Additional Heating Term. (submitted to *Nonlin. Processes Geophys; accepted as a discussion paper, March 2, 2015*)