# NOAA Exascale Computing Project

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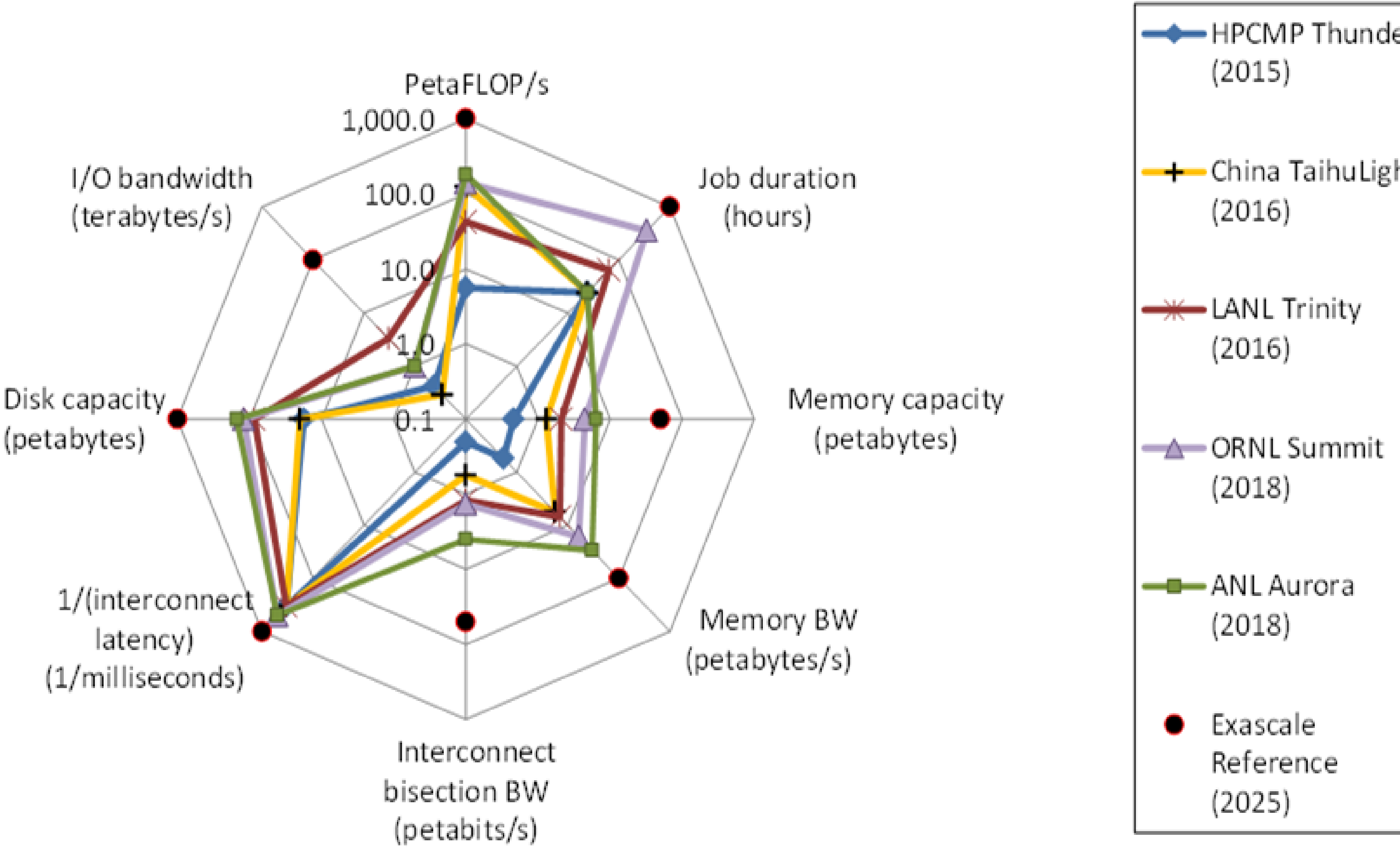
# Background

- Project began in November 2017
- To address challenges in future computing
  - Increasing diversity
  - More cores
  - I/O and inter-process communications concerns
- Key questions
  - How to expose sufficient parallelism for systems with millions of cores?
  - What is the best path to good performance and scalability?
  - Is performance – portability achievable?
  - Do we need to rewrite our applications?
    - Optimize ---> Refactor ---> Rewrite?
  - Can model and data assimilation be more tightly linked?

# Hardware & Appli

- Diverse processor, systems
  - x86, ARM, GPU, Power+GPU
  - Powerful processors / nodes
  - Slow I/O, inter-process communications
  - Massive parallelism
- Applications
  - Complex, diverse
  - Low compute intensity
  - Limited parallelism



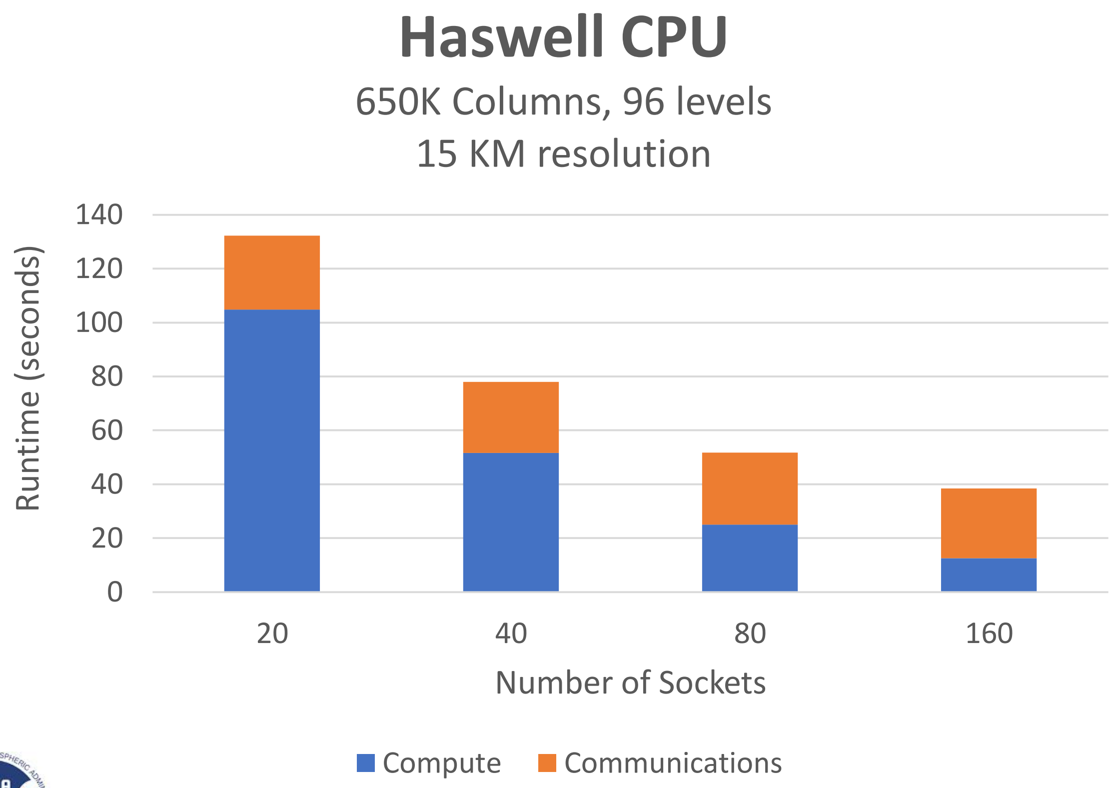

Credit: HPCMP Architectural Trends - Global to Corporate View, DOD HPC Modernization, February 2017

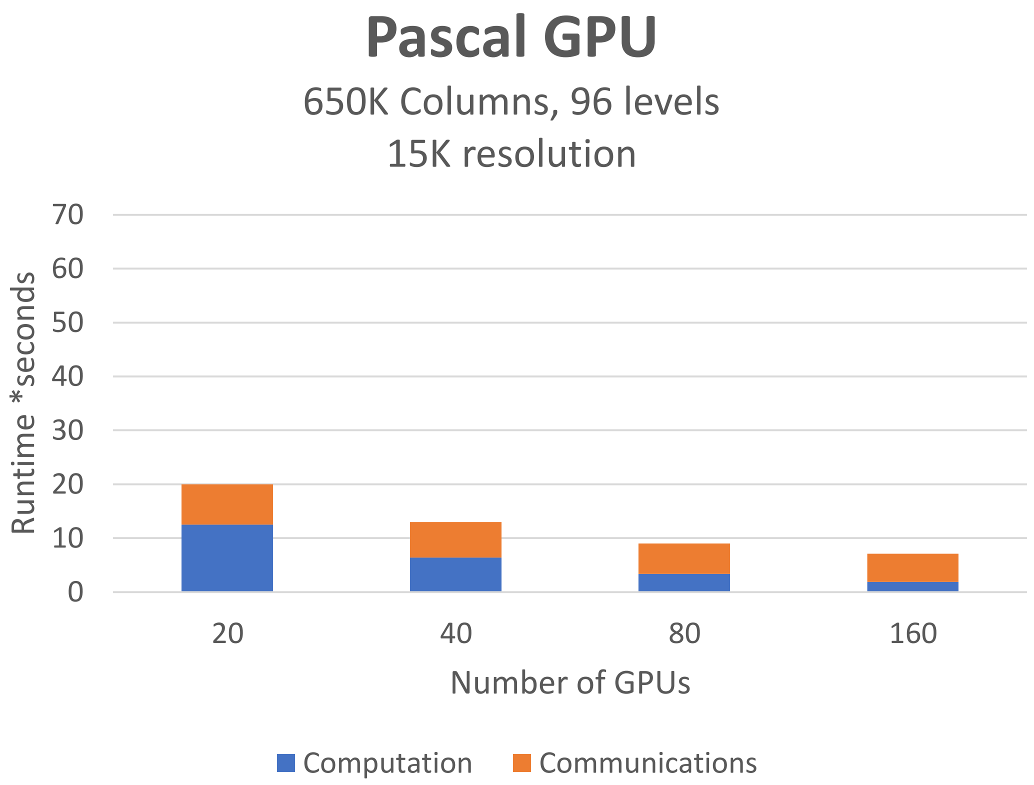
# Application Performance Measures

- Percentage-of-peak
- Speedup
- Scalability
- Time-to-solution
  - Weather Forecast
    - 1 hour to produce a 10 day forecast === > 6 minutes / day ==== > 0.65 YPD
    - 1 hour to produce an 8 day forecast === > 7.5 minutes / day ==== > 0.52 YPD
  - Climate Prediction
    - 5 years per wall clock day is reasonable today
  - How much time should we spend on assimilation versus forecast?
    - NCEP requires DA run in 20 minutes, ECMWF allows 40 minutes

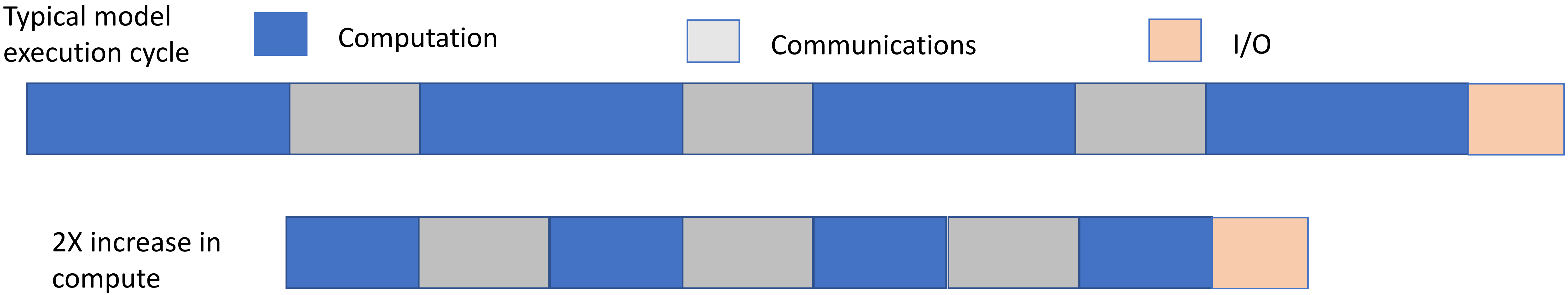
# Strong Scaling:  CPU, GPU

- CPU socket (2 per node) versus Pascal GPU (2 per node)
  - Identical system, interconnect, data movement per MPI task
  - Different communications CPU: impi, GPU: mvapich), affinity (CPU: range, GPU: pinned)



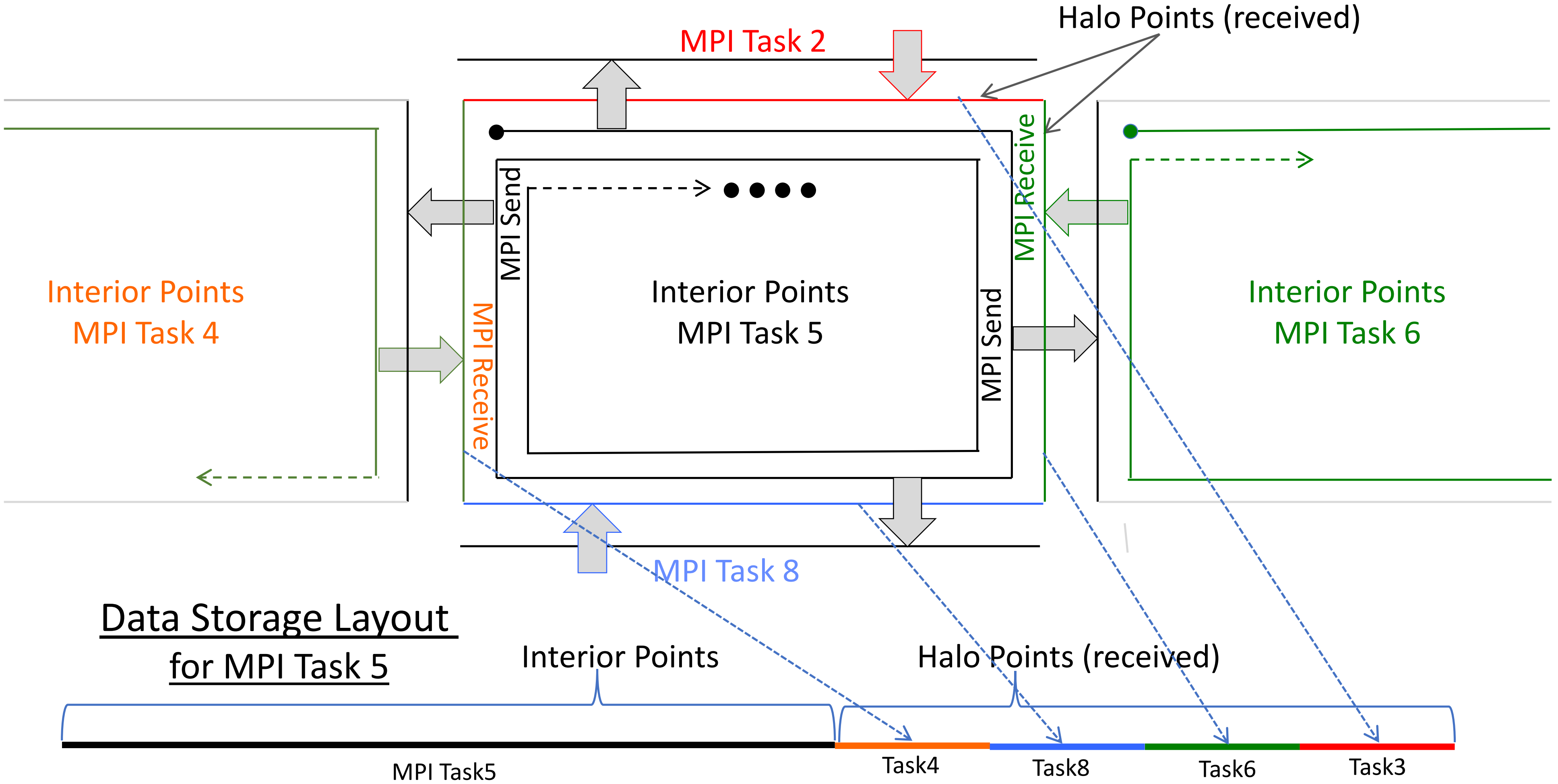



# Communications Performance & Scalability




- Inter-process communications biggest factor affecting scalability
- Common techniques to reduce impact of MPI communications
  - Overlap communications with computation
  - Aggregation
  - Reduce frequency & volume of data
  - Reorder points to avoid MPI pack / unpack (Middlecoff, 2015)

# Spiral Grid Ordering

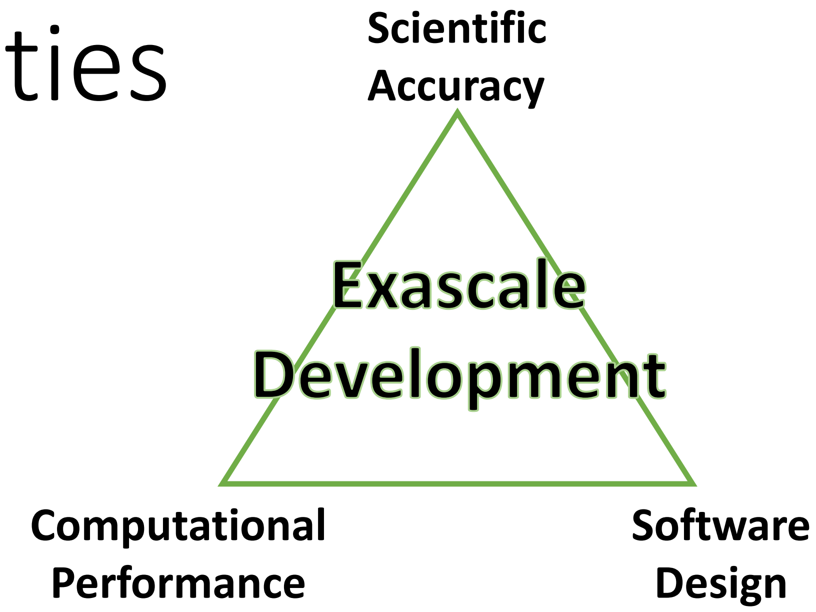



Parallelization and Performance of the NIM on CPU, GPU and MIC Processors, Bulletin of the AMS, Govett, et al, 2017

# Performance - Portability

- Goal to have same code for x86, ARM, GPU, etc
- Languages
  - Fortran, C, C++, CUDA
  - Domain-Specific Languages (DSLs)
    - Source to source, high level to machine abstractions
  - Libraries:  MPI, SMS, RSL
- Directives
  - OpenMP, OpenACC, SMS

# Exascale Development Activities




- Model Dwarfs
  - Advection
  - Grid staggering
- Data Assimilation
  - Prototypes
  - TL & ADJ generation
  - Optimization
- Machine Learning
- I/O
- Software Design

- Evaluate scientific accuracy and computational efficiency
- Improve software process
- Incorporate science & computational aspects into design

# Advection Dwarf Development & Beyond

Duane Rosenberg, Bryan Flynt

AGU, December 10-14, 2018

**Characterizing and Improving Scientific Algorithms and I/O for Exascale: Nimble Dwarfs,**

*Bryan T. Flynt, Duane Rosenberg, Yonggang Yu and Mark Govett*

# Scientific Motivation & Scope

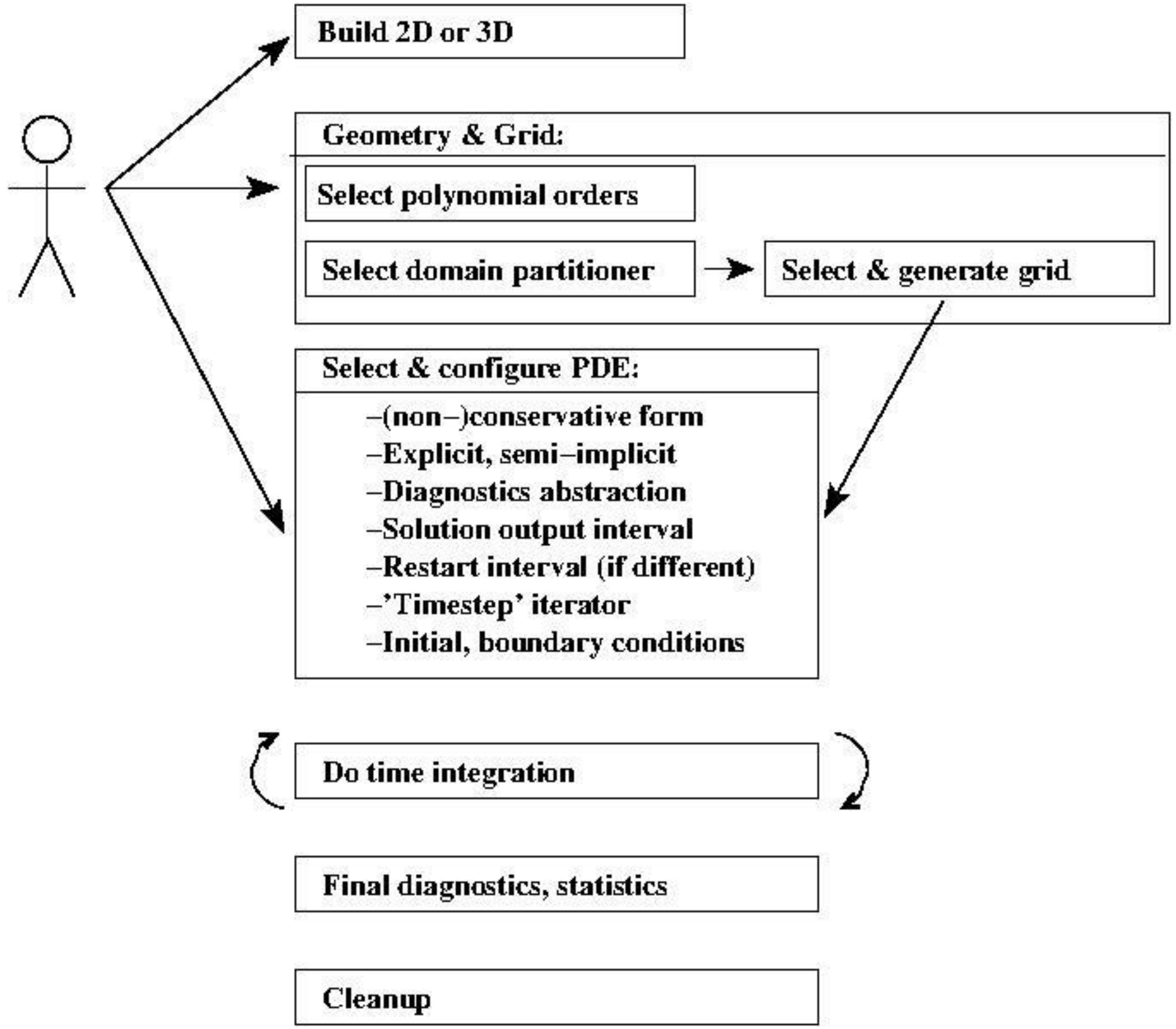
To develop highly accurate, high performance models for atmosphere (and ocean)

Evaluate primary components of geofluid models with spectral element/DG and finite-volume approaches to examine parallel performance and scientific accuracy

# Dwarf Development:  Requirements and Initial Focus

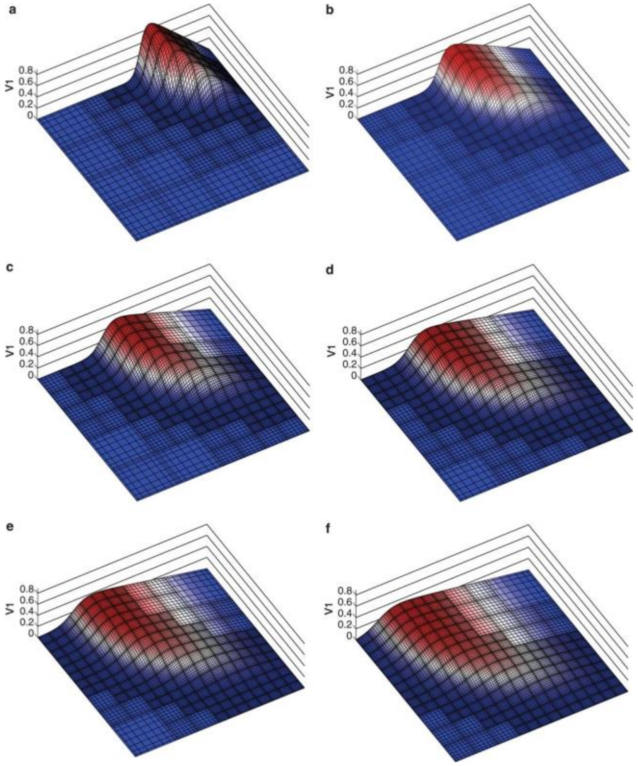
| Requirements | Initial Focus |
| --- | --- |
| Simplest framework to *test* linear, nonlinear, (non-)conservative, transport in idealized setting<br>Extensible to allow different grid types, PDEs | Advection-diffusion: Burgers equation, DG and CG forms:<br>$\partial_t \mathbf{u} + \nabla \cdot (\mathbf{u}\mathbf{u}) = \mathbf{u}\nabla \cdot \mathbf{u} + \nu \nabla^2 \mathbf{u} \quad (1)$<br>$\partial_t \mathbf{u} + \mathbf{c}(\mathbf{u}) \cdot \nabla \mathbf{u} = \mathbf{f} + \nu \nabla^2 \mathbf{u} \quad (2)$ |
| Must be discretized on the sphere, 2D and 3D | Icosahedral (2D) and spherical-polar (3D) |
| Must allow different time stepping methods, explicit & semi-implicit | Explicit: Runga-Kutta |
| Relatively small, self-contained & *manageable;* compiler,  platform portable | Object-oriented; test-driven development |
| Must accommodate ‘coarse’ and ‘fine’-grain parallelization | MPI-ready, building in OpenACC/OpenMP offloading |

# Configuration Framework



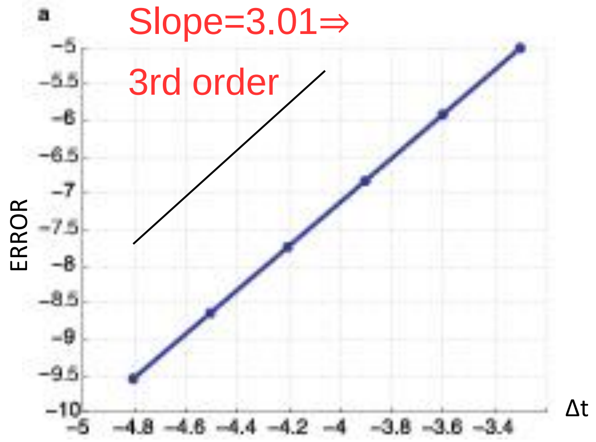
# Evaluation of Accuracy and Complexity

Select initial conditions, e.g. N-wave, and evolve:

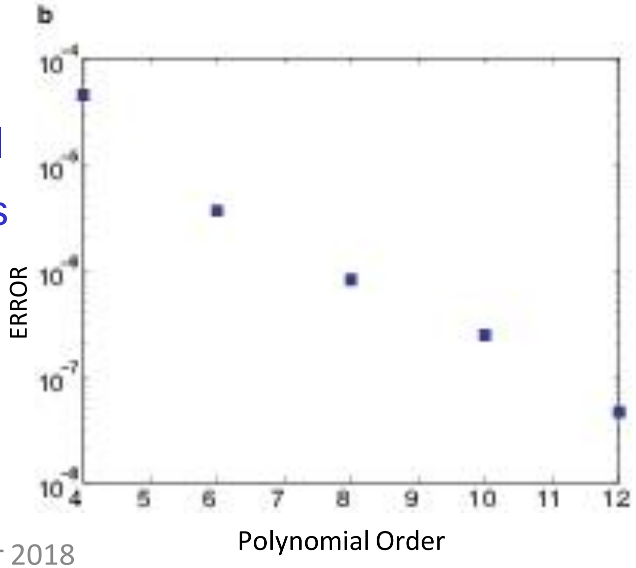


Use (semi-)analytic solution to find:

Error vs **Δ**t yields temporal truncation error

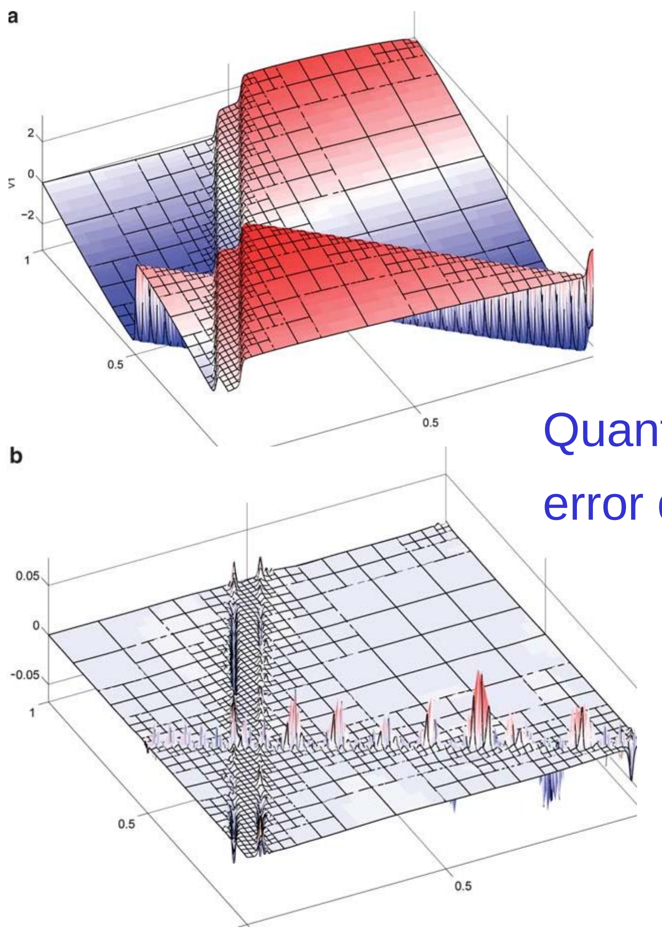



Error vs polynomial order demonstrates spatial spectral convergence



# Accuracy and Complexity

Interacting fronts:




Quantify spatial error distribution

Quantify via:

**Communication complexity:**

Comm. volume/Flops (per elem)

**'Accuracy efficiency':**

F[T log(Error) / T_0 log(Error_0)]

(T is solution time)

**Compare with low order:**

$\log N_{cells} \sim p \log(pE)$

(p ≡ poly. order; E ≡ # elements)

# Grid Staggering

## Evaluate the Scientific Accuracy and Computational Performance of the A-grid and C-grid staggering

Yonggang Yu

AMS, January 6 -10

Session: Developing and Preparing Models for Exascale Computers

**Comparison of A-grid and C-grid Shallow Water Model Solver on Icosahedral Grids**

Yonggang Yu, Ning Wang and Mark Govett

**Design and performance testing for A-grid and C-grid Shallow Water Model Solvers for Exascale,** Jacques Middlecoff, Yonggang Yu, and Mark Govett

## Scope

Small software solving shallow water model on sphere to test computational cost versus scientific accuracy using different spatial staggering schemes

### Design principles for this code:

- ❖ Algorithmic Versatility
  - Solving PDE by spatial discretization on A-grid, C-grid, etc
  - Support icosahedral grid and the associated Voronoi cell
- ❖ Support HPC enabling technologies
  - MPI, OpenMP, OpenACC
- ❖ Small and self-contained codes
  - Icosahedral grid generation (Ning Wang)
- ❖ Suitable for profiling and tests

### Advantages:

- ❖ Fair comparison among numerical schemes
  - Fixed time integration method (Runge-Kutta $4^{th}$ order)
  - Avoid bias from different icos grid generators (NCAR, CSU, ESRL)
  - Same level of MPI optimization (e.g. using SMS for message [un]packing, Spiral grid optimization (Jacques Middlecoff))
- ❖ Compilation and Run time consistency
  - Keeping the same compiler option (on same hardware)

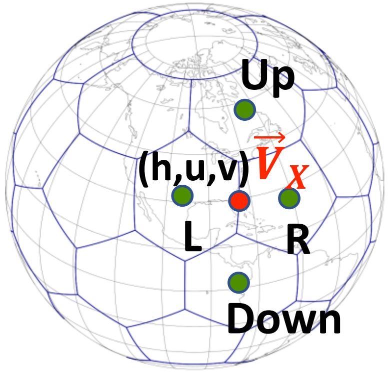
# Solving Shallow Water Model on Icosahedral Grids using A-grid and C-grid Staggering Schemes

**Dynamic equations:**

$$\frac{\partial h}{\partial t} + \nabla \cdot \left(h\vec{V}\right) = 0$$

$$\frac{\partial \vec{V}}{\partial t} + \left(2\vec{\Omega} + \nabla \times \vec{V}\right) \times \vec{V} + \nabla\left(\frac{1}{2}\vec{V}\cdot\vec{V} + gh\right) = 0$$

## A-grid (NICAM method)




$$\vec{V}_X = \frac{1}{2}\cdot\begin{bmatrix}\left(\alpha_1\vec{V}_L + \beta_1\vec{V}_R + \gamma_1\vec{V}_U\right) + \\ \left(\alpha_2\vec{V}_L + \beta_2\vec{V}_R + \gamma_2\vec{V}_D\right)\end{bmatrix}$$

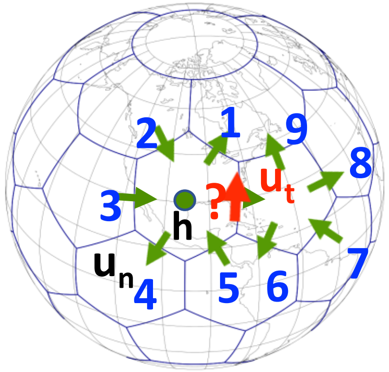
$\alpha_1 + \beta_1 + \gamma_1 = 1$

$\alpha_2 + \beta_2 + \gamma_2 = 1$

⋮

Finite volume approach

## C-grid (MPAS method)




$$U_t^e = \frac{1}{d_e}\sum_{e'=1}^{9\text{ or }10} W_{ee'}\, l_{e'}\, U_n^{e'}$$

$$t_{ev}\left(\hat{U}_n^{e'} \times \hat{U}_n^{e}\right)\cdot\hat{k}\, W_{ee'}$$

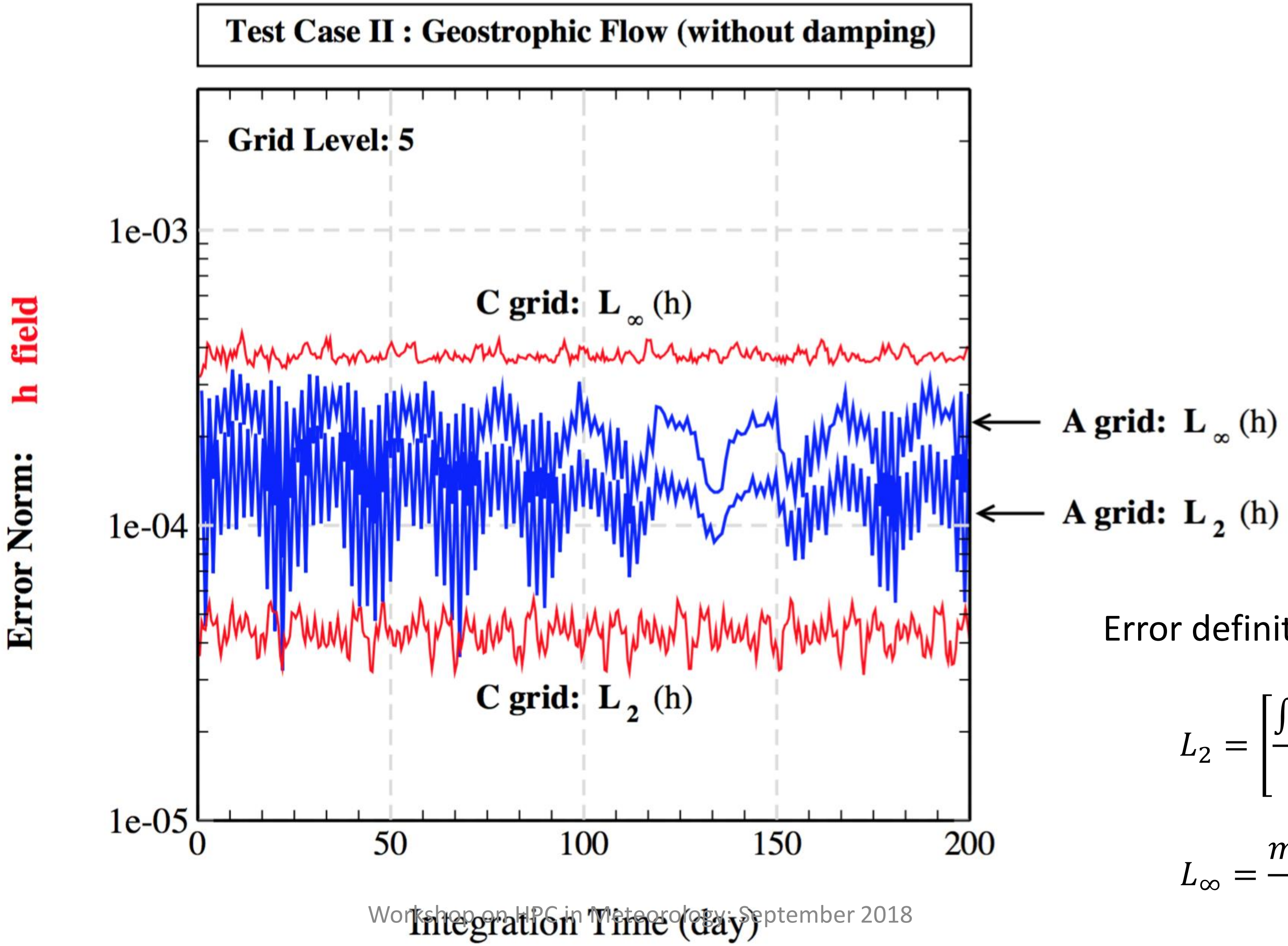
$$= \sum_{ip} R_{ip}^{(v)}\,\hat{U}_n^{e'}\cdot\hat{U}_{e'}^{out}$$

$$\frac{\partial U_n}{\partial t} + (\mathrm{f} + \xi)U_t + \hat{U}_n^e\cdot\hat{n}^{out}\,\frac{\partial(K+\Phi)}{\partial n} = 0$$


Reference:

- Tomita, H., M. Tsugawa, M. Satoh, and K. Goto, 2001: Shallow Water Model on a Modified Icosahedral Geodesic Grid by Using Spring Dynamics. J. Comput. Phys., 174, 579–613, doi: 10.1006/jcph.2001.6897.
- Thuburn, J., T. Ringler, J. Klemp and W. Skamarock, 2009: Numerical representation of geostrophic modes on arbitrarily structured C-grids, J. Comp. Phys., 2009: 228 (22), 8321
- Ringler, T. D., J. Thuburn, J. B. Klemp, and W. C. Skamarock, 2010: A unified approach to energy conservation and potential vorticity dynamics for arbitrarily-structured C-grids. J. Comput. Phys., 229, 3065–3090, doi:10.1016/j.jcp.2009.12.007.
- Arakawa and Lamb: Computational Design of the Basic Dynamical Processes of the UCLA General Circulation Model, in Methods in Computational Physics: Advances in Research and Applications, Vol. 17, p 173 (1977)

# Computational Accuracy Study for A-grid v.s. C-grid Staggering




Error definition:

$$L_2 = \left[ \frac{\int (h - h_0)^2 d\Omega}{\int {h_0}^2 d\Omega} \right]^{\frac{1}{2}}$$

$$L_\infty = \frac{max|h - h_0|}{max|h_0|}$$

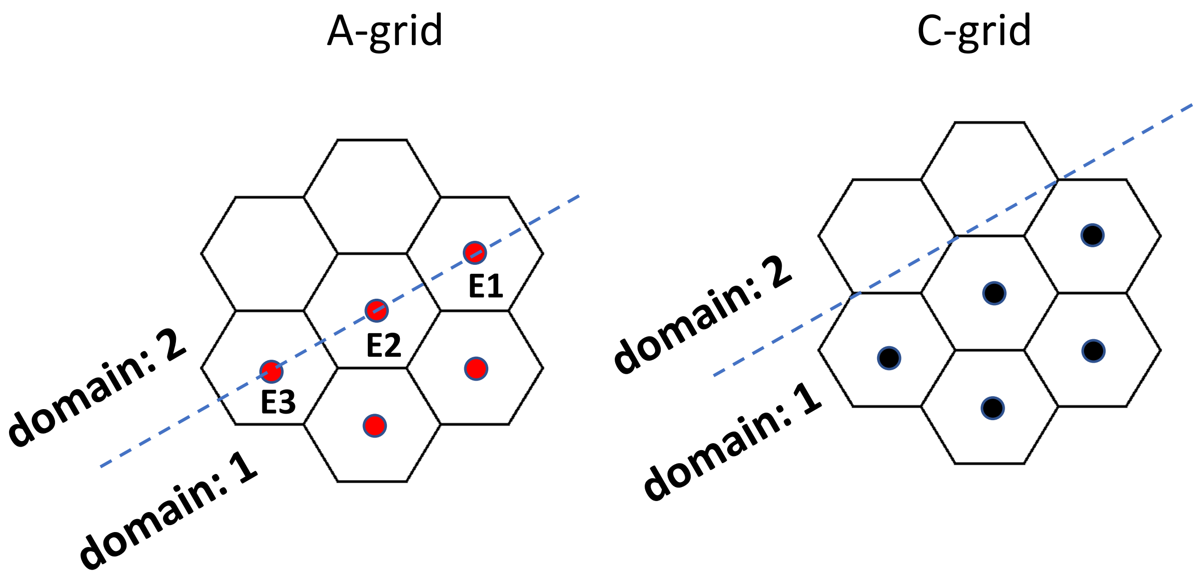
# Parallellization and Performance Measurement for A-grid v.s. C-grid Staggering

## MPI parallelization schemes:

- Loop over basin centers
- domain decomposition and halos

## GPU parallelization schemes:

- Loop over basin centers and edges



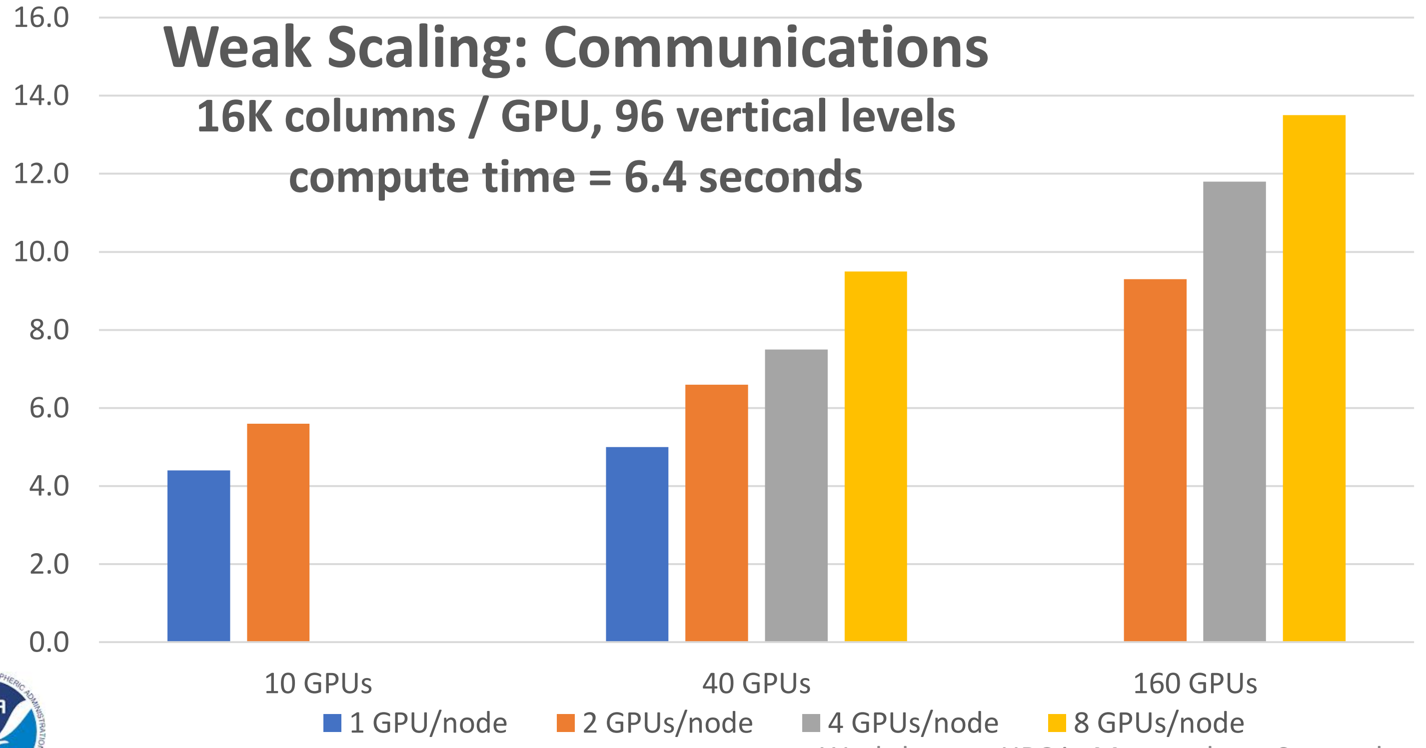

### Impose metrics for fair comparison:

- Fair comparison among numerical schemes
  - Fixed time integration method (Runge-Kutta 4th order)
  - Disable numerical damping
  - Avoid bias from different icos grid generators (NCAR, CSU, ESRL)
  - Same level of MPI optimization

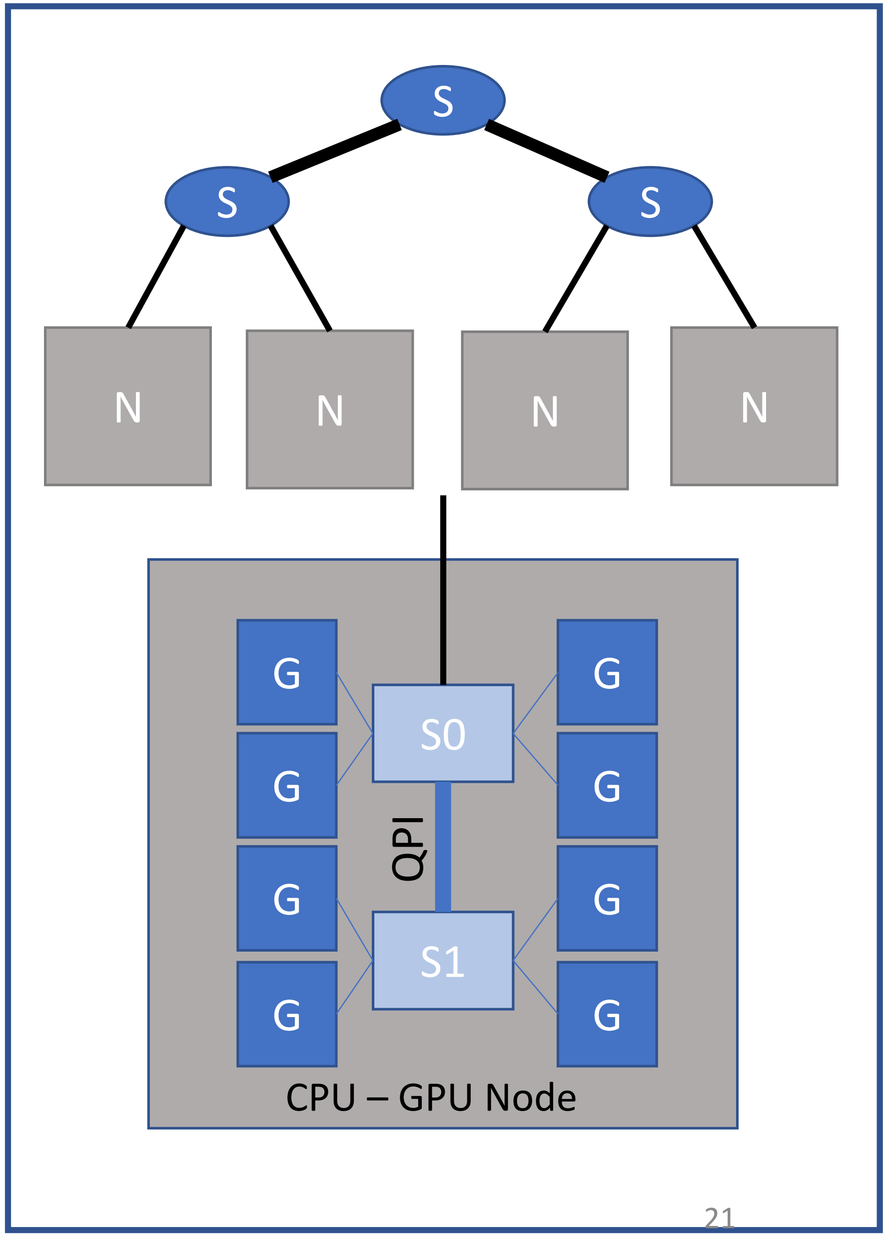
- Compilation and Run time consistency
  - Keeping the same compiler option (on same hardware)

# Scalability & Performance

- NOAA GPU System with 800 P100 GPUs
  - 20 core Haswell CPU and 8 P100 GPUs,
  - 100 nodes, mellanox QDR (upgrade?)
- DoE Summit




NOAA GPU System



# Data Assimilation

Isidora Jankov, Lidia Trailovic, Chris Harrop

# Shallow Water Model for Application in 4DVar

Shallow Water Equations: non-conservative form, simplified

$$\frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} + \frac{\partial (hv)}{\partial y} = 0$$

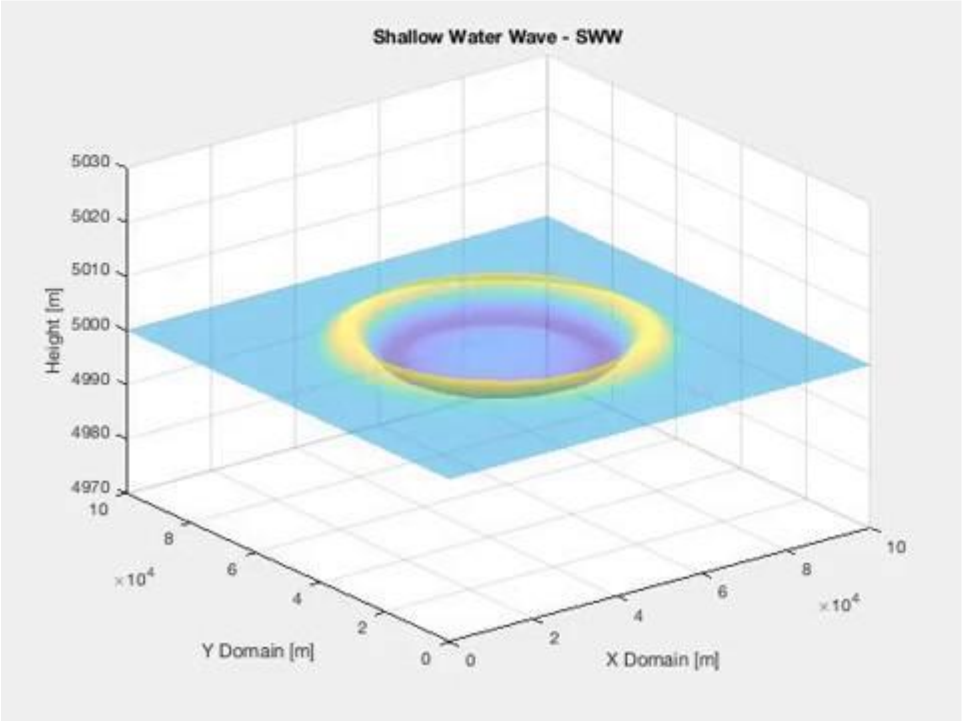
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial h}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + g\frac{\partial h}{\partial y} = 0$$

- Square grid, no viscosity, no bottom profile
- Initial condition h0: Gaussian pulse in the middle
- Boundary condition: reflective
- Proof of concept:
- Discretization & Linearization

Space (x,x+dx),(y,y+dy) grid (i,i+1),(j,j+1)

Time (t, t+dt) is (k, k+1)



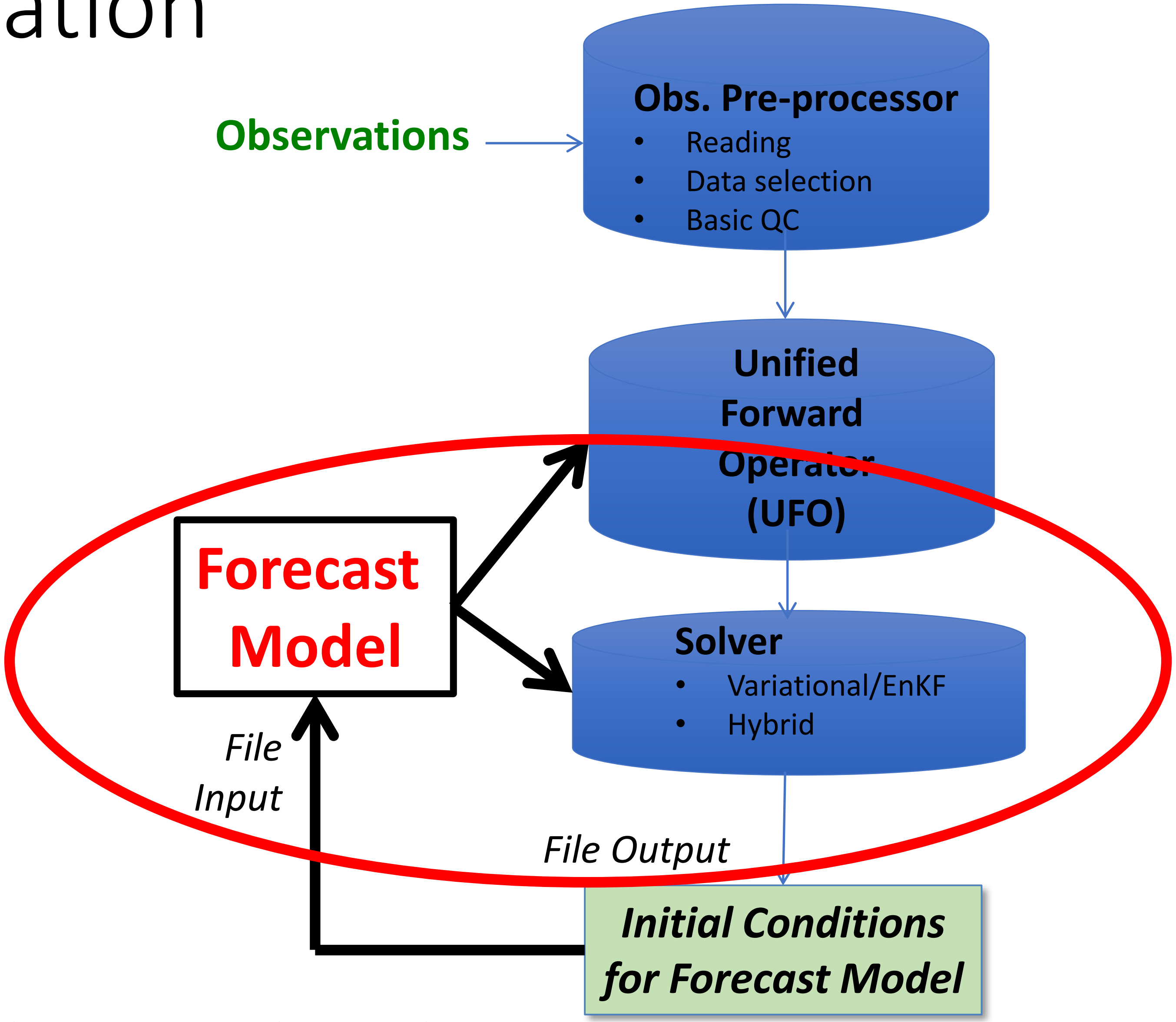

VIdeo: the first 1500 time steps

**Next Steps:**

- SW model with its TL and Adj will be made available in JEDI as an additional "toy" model (SW will include MPI, which will make it a unique "toy" model)
- Compare performance of code generators for Adj and TL (e.g. Tapanade) and manually produced & optimized models
- Add MPI option for B matrix preconditioning in JEDI and test different flavors of B
- Evaluate impact of various flavors of B and R matrices for application in existing operational systems (e.g. RAP, HRRR and UFS)

# JEDI Data Assimilation

- Development
  - CRTM Optimization
  - MPI into JEDI
- Link Model and DA development and evaluation
  - Shallow water
  - More complex models



# I/O Developments

Bryan Flynt, Ed Hartnett

AMS, January 6 -10

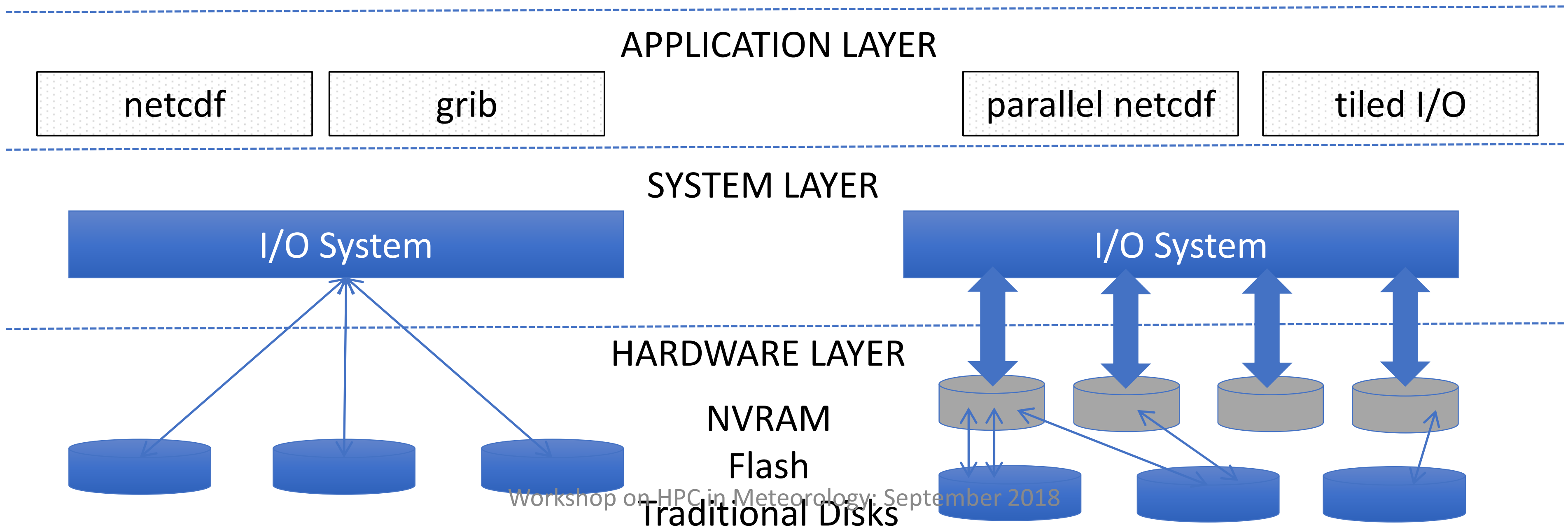
**NetCDF-4 Performance Improvements Opening Complex Data Files**, Ed Hartnett

**Characterizing and Improving Scientific Algorithms and I/O for Exascale: Nimble Dwarfs,**

*Bryan T. Flynt, Duane Rosenberg, Yonggang Yu and Mark Govett*

# Scope

- To develop realistic I/O projections for exascale
  - 1 - 3KM global deterministic, 3 – 5 KM ensembles
  - hourly output?
- Test & tune on HPC systems
- Share with vendors, support procurements



# Summary

- Exploring ways to more effectively design, develop and run modeling systems on exascale systems
- Models and HPC systems are tremendously complex which limits the ability to develop, run and maintain modeling systems (DA, Model)
- We are exploring a development strategy that strongly links scientific, computational and software development from inception
  - Development team is composed of scientists, software engineers, computer scientists who work **together** to design, build, test, optimize, evaluate, etc.

Scientific Algorithms

Model Code

Optimization

Refactoring

Integration