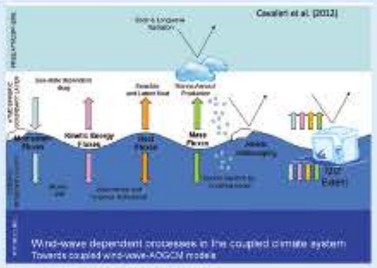
WW3 Performance in E3SM for Global Climate Simulations

Erin Thomas[1], Stephen Brus[2], Olawale Ikuyajolu[3,4], Luke van Roekel[1]
ethomas@lanl.gov

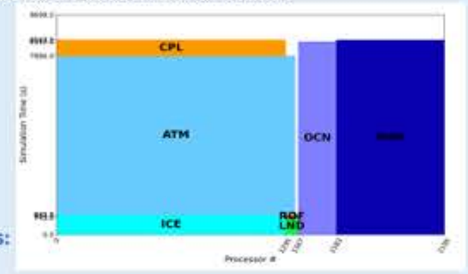
Introduction



- Wind-generated waves are an important interfacial process in the climate system
- Important interactions include:
  - Ocean vertical mixing
  - Sea-state dependent drag
  - White-capping albedo
  - Sea-ice floe size

WAVEWATCHIII (WW3) spectral wave model is being fully coupled into Energy Exascale Earth System Model (E3SM), **however, it is necessary to improve the computational efficiency of WW3 in order to run the fully coupled system with waves on climate time scales.**

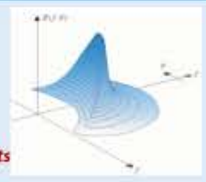
We are testing the impact of several configuration options on the performance of WW3 for use in global climate-scale simulations such as:



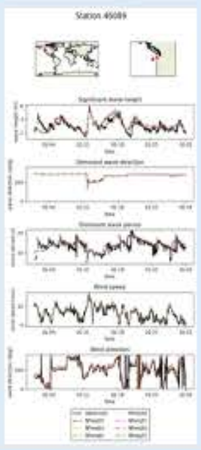
i) **Unstructured, regionally refined mesh grids**
ii) **Appropriate spectral resolution**
iii) **Porting the wave action source terms to GPUs**
iv) **Domain Decomposition Parallelization methods**
v) **Implicit numerical scheme**

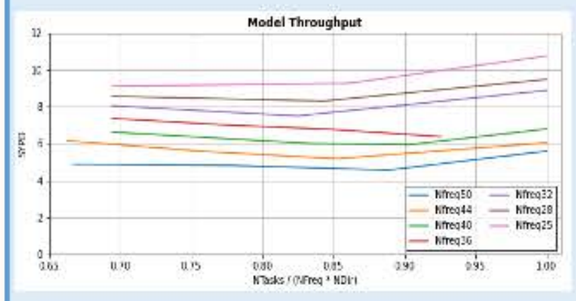
Spectral Resolution

- Waves are modeled in a phase-averaged sense in spectral space
- Source term calculations of Wave Watch code are the most time consuming due to spectral loops in code
- Reducing the spectral resolution directly increases speed/throughput of ww3 model
- ***Reducing from 50 to 25 frequencies increases WW3 throughput by ~1.8x and has negligible impact on accuracy of results***



Note: the spectral resolution is tied spatial resolution of the mesh grid, therefore, sensitivity testing is required to determine appropriate spectral resolution for any given grid.



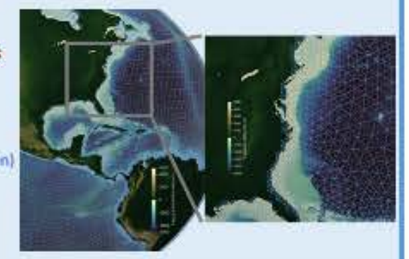


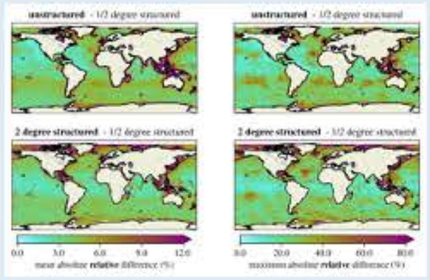
Unstructured, Mesh Grids

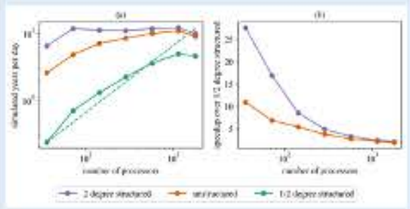
Why use unstructured mesh grids?

- Deep, open ocean, accurately simulated with low resolution
- Shallow, coastal areas require higher resolution
- *Variable meshes allow using high resolution ONLY where it is necessary thus saving computational costs **without degrading the results.***

Ocean mesh (grey polygons):
60km (mid latitudes) - 30km (equatorial and polar)
Wave mesh (blue triangles):
225km (open ocean) - 30km (coasts: matches ocean resolution)





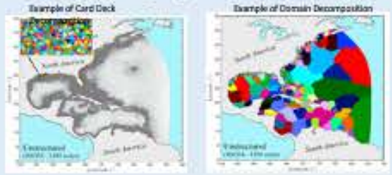


Brus et al. (2021) Geosci. Model Dev.

Parallelization Methods

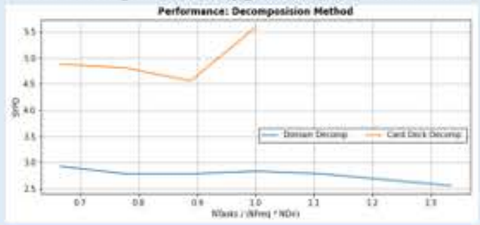
Does the parallelization method impact WW3 performance for our mesh grid?

- 'Domain decomposition' method groups neighboring grid cells on same processor
- 'Card deck decomposition' sequentially assigns grid cells to processors



From Figure 4. Abdolali et al. (2020)

- *For our global, unstructured mesh grid, implementing **domain decomposition parallelization is computationally more expensive (performs worse)** than the default card deck decomposition method*
- *We expect these results to depend on the size of the mesh grid used. Domain decomposition may be more efficient for meshes with larger numbers of grid cells (as seen in Abdolali et al 2020)*



Author Affiliations
1 Fluid Dynamics and Solid Mechanics (T-3), Los Alamos National Laboratory, Los Alamos, NM, USA
2 Mathematics and Computer Science Division, Argonne National Laboratory, Lemont, IL, USA
3 Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, GA, USA
3 Program in Ocean Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia, USA

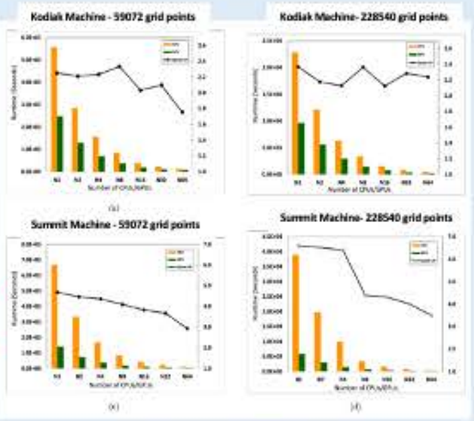
Key References

Abdolali, A. et al. *Large-scale hurricane modeling using domain decomposition parallelization and implicit scheme implemented in WAVEWATCH III wave model.* Coastal Engineering. 2020.
Brus, S., et al. *Unstructured global to coastal wave modeling for the Energy Exascale Earth System Model using WAVEWATCH III version 6.07.* Geosci. Model Dev. 2021.
Ikuyajolu, O. J., Van Roekel, L., Brus, S. R., Thomas, E. E., Deng, Y. and Sreepathi, S., *Porting the WAVEWATCH III (v6.07) Wave Action Source Terms to GPU.* Geosci. Model Dev. 2023.

Porting to GPU

What is the impact of using GPUs?

- Many supercomputer now have heterogeneous platforms (i.e. they contain both CPU's and GPU's)
- GPUs have low energy to performance ratio
- GPU programming is incompatible with CPU code, therefore, we focus on porting just "computationally expensive" components of WW3 to GPUs
- *Porting Wave Watch III wave action source terms (which consume ~78% of execution time) to GPUs results in **average speedup of 2x-4x** over serial CPU**
  **note: exact results vary depending on HPC machine used*

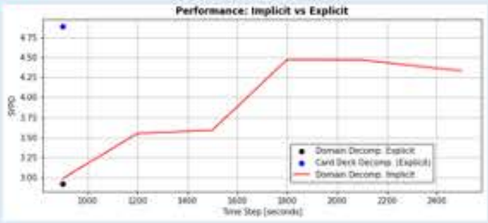


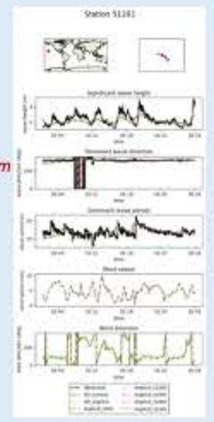
Ikuyajolu et al. (2022) Geosci. Model Dev. *In Review.*

Numerical Schemes

Can an implicit numerical scheme with large time steps out-perform an explicit scheme with shorter time steps?

- Implicit calculations are inherently more time consuming to perform than explicit calculations
- BUT they produce numerically stable results so you <u>can use large time steps</u> to improve computational efficiency (unlike explicit schemes which require small time steps to produce numerically stable results)
- *Implicit numerical scheme requires increasing the global time step from 900 seconds by over 2X (to at least 1800 seconds) before similar computational efficiency as the Card Deck Decomposition (with explicit time steps of 900 seconds) is obtained.*
- *Increasing time step beyond 1800 seconds does not further increase efficiency*





Conclusions

1) **Unstructured mesh grids used by E3SM give same accuracy as a high-resolution structured grid with the computational efficiency as a coarse-structured global grid.**
2) **Spectral resolution matters**
   - **For our grid, reducing the number of frequency bins from 50 to 36 has minimal impact on accuracy of results, yet increases throughput by 2X.**
3) **Domain decomposition slower for our mesh. May be worth it for very high res meshes (large numbers of grid cells)**
4) **Porting time consuming parts of code to GPU's results in average speed up of at least 2X**
5) **Implicit schemes produce numerically stable results – allowing WW3 to use very large time steps to increase efficiency.**