Trials and Tribulations (and Joys) of Developing with Alternative Parallel Frameworks

Development of the Intermediate Complexity Atmospheric Research model and others

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Soren Rasmussen, Damian Rouson, and many others

November 13, 2023

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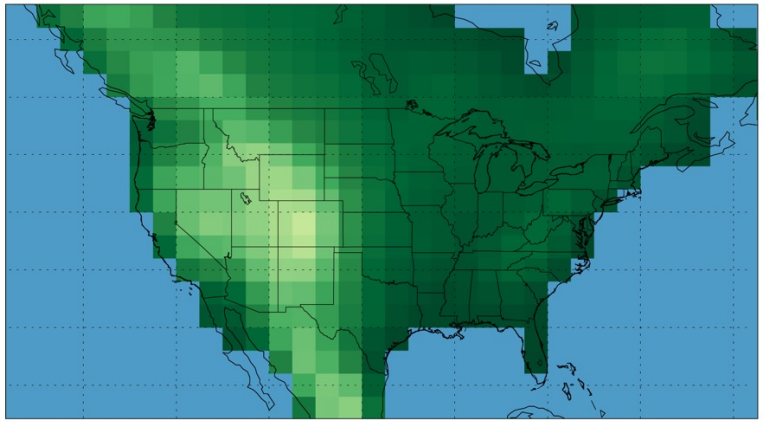
What I'm going to say

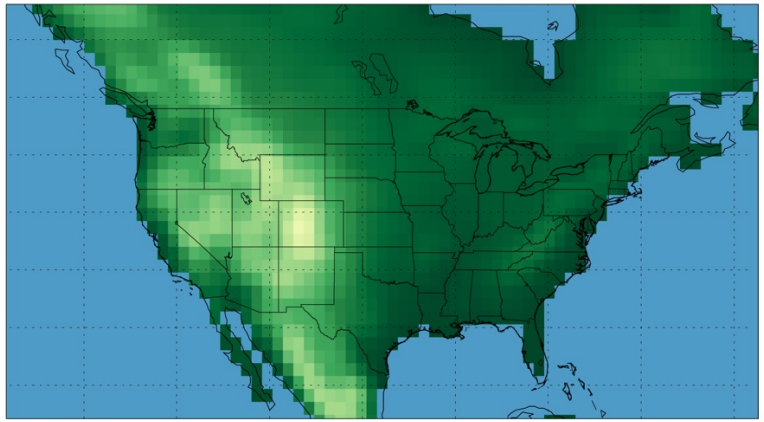
- Actionable use of Climate Projections
- Computing requirements / limitations
- Use of Coarray Fortran for rapid development
  - ICAR
  - SnowModel
- Scaling results
- Complications with Compilers and Computers
- Where might Parallel Applications be going?

Aren’t climate models useful already?

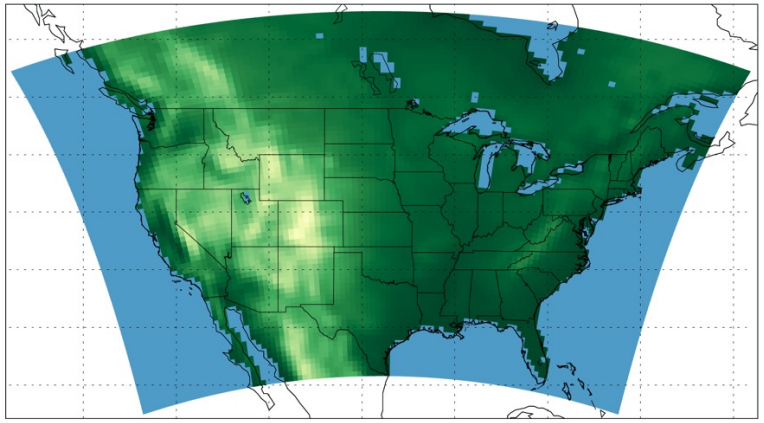
GFDL -CM3 2.5x2.0



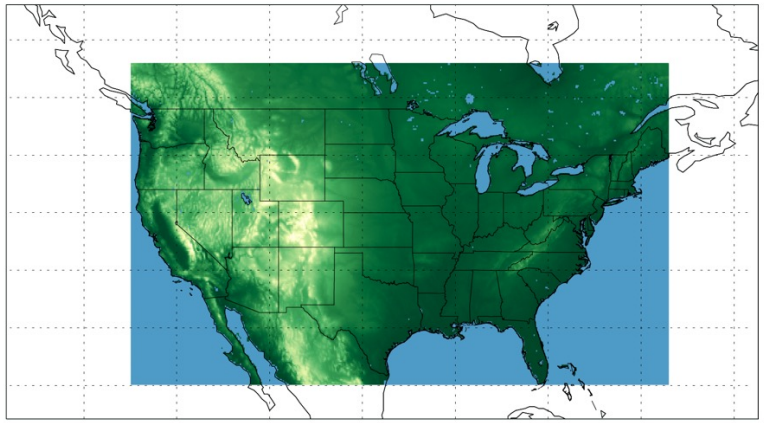
MRI-CGCM3 1.1x1.1



WRF 50x50 km



Reference 12x12 km



Terrain height (m)

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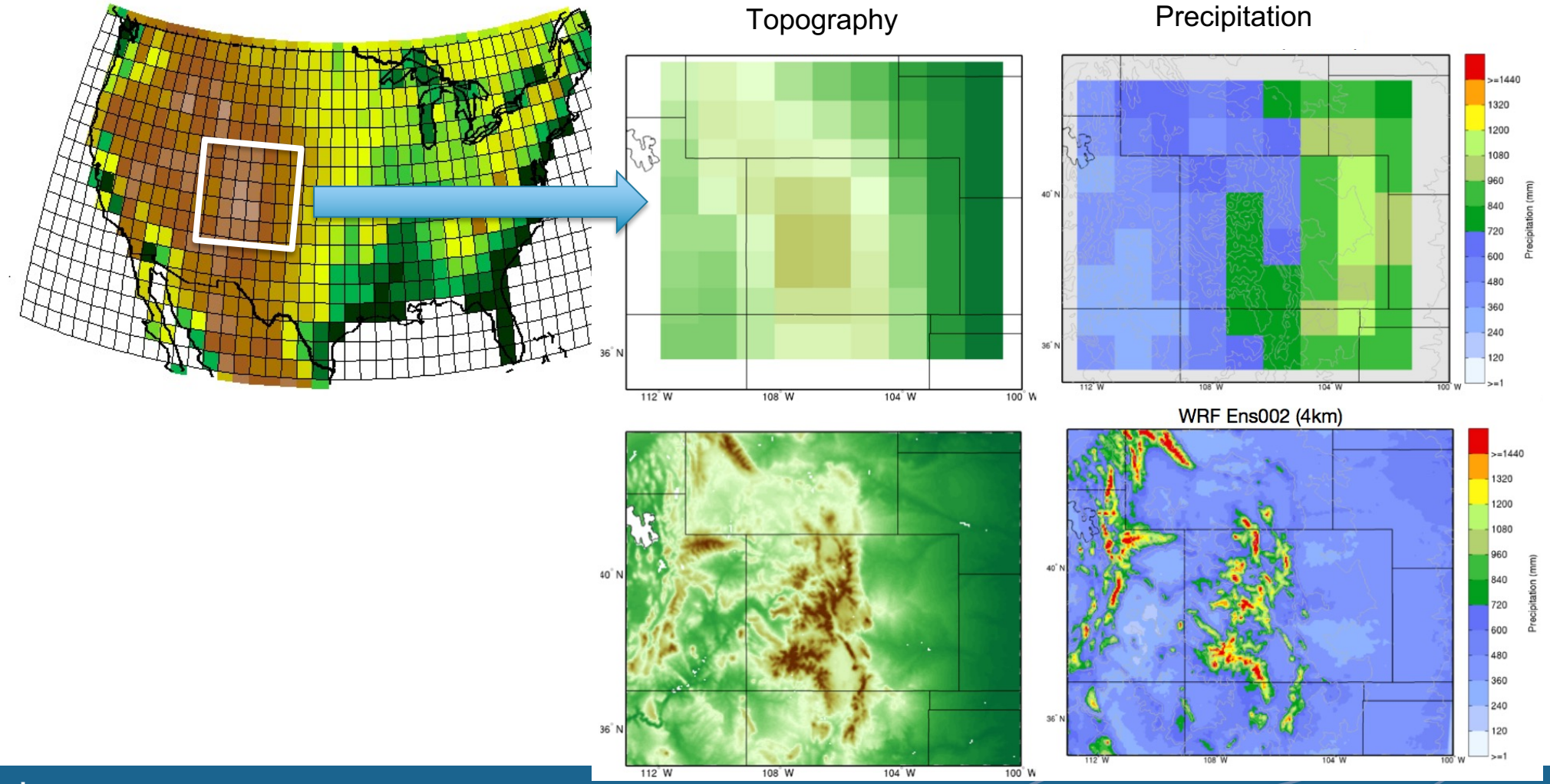
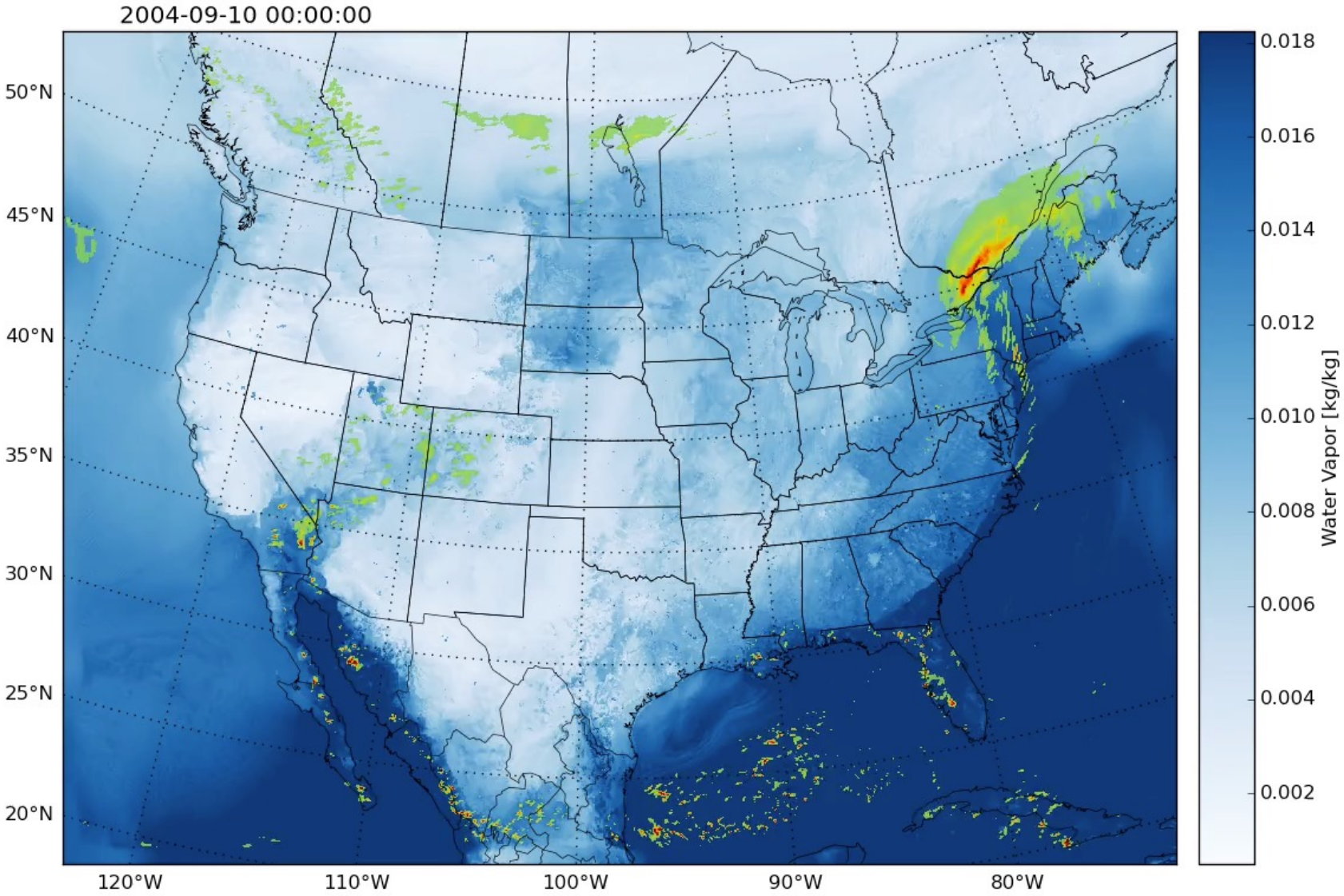
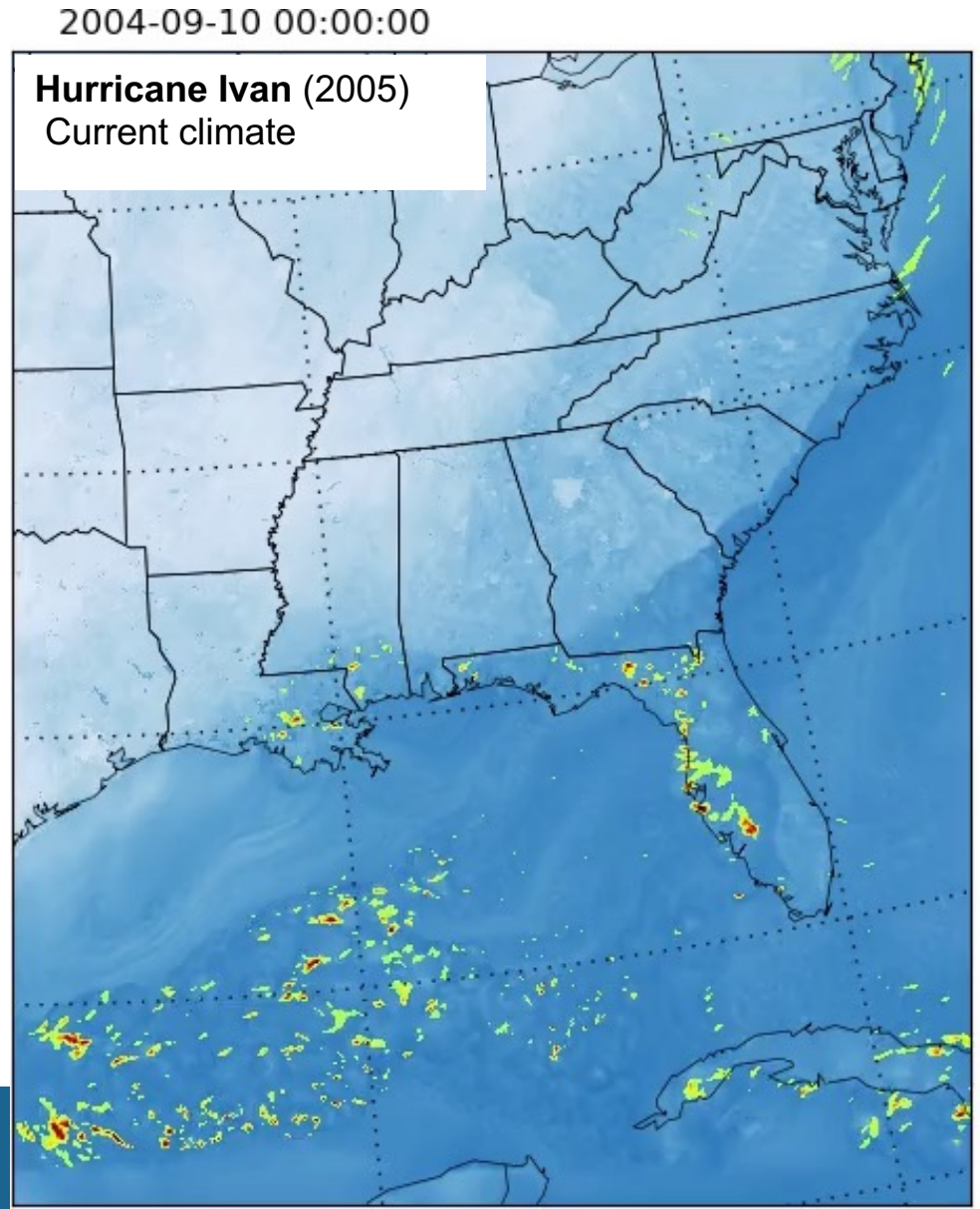
Climate Model Native Resolution and Application Resolution

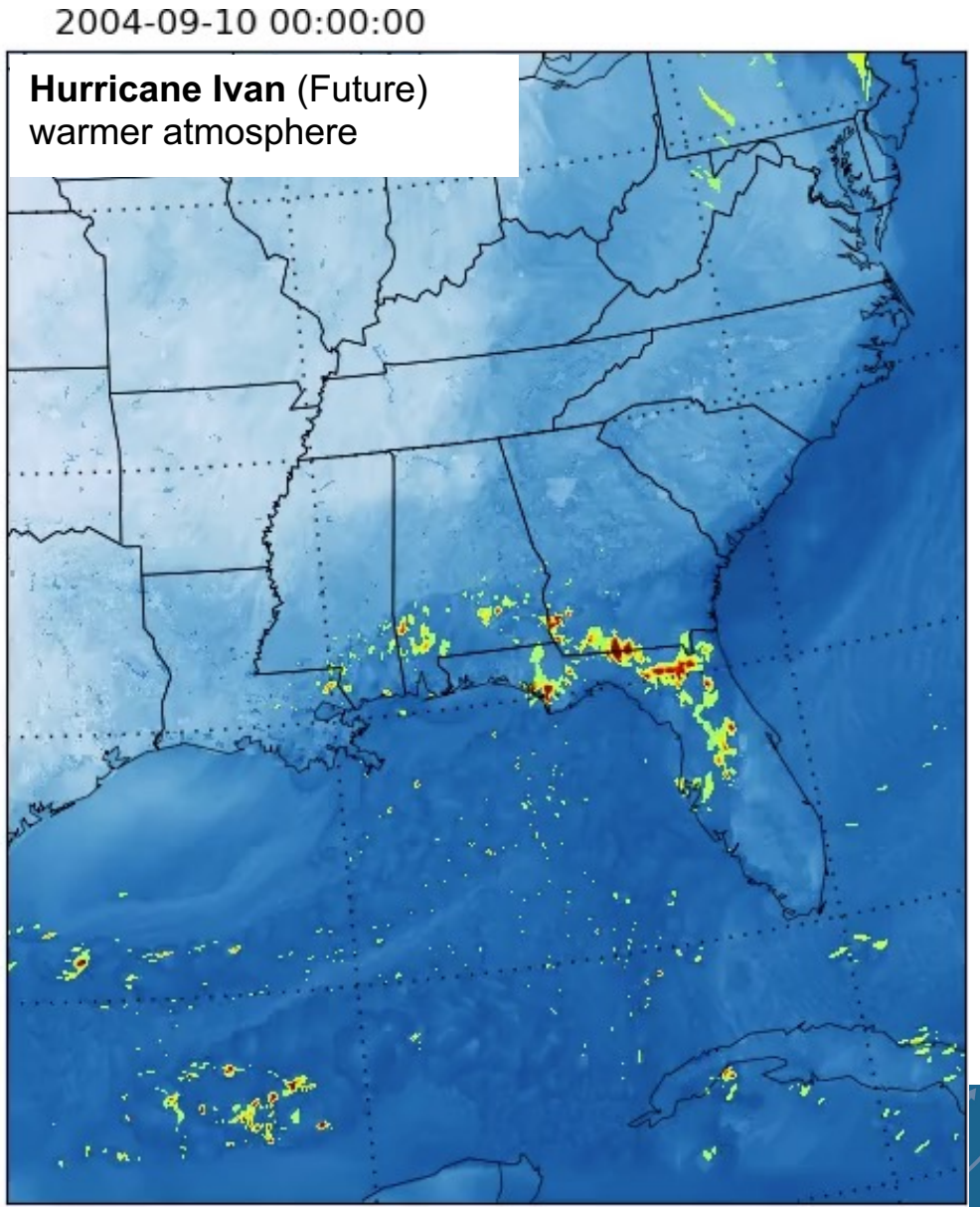


Dynamical Downscaling at Convection Permitting Scales



Hurricane Ivan





Gutmann et al. (2018)

A dichotomy of regional climate approaches

False

increasing physical representation

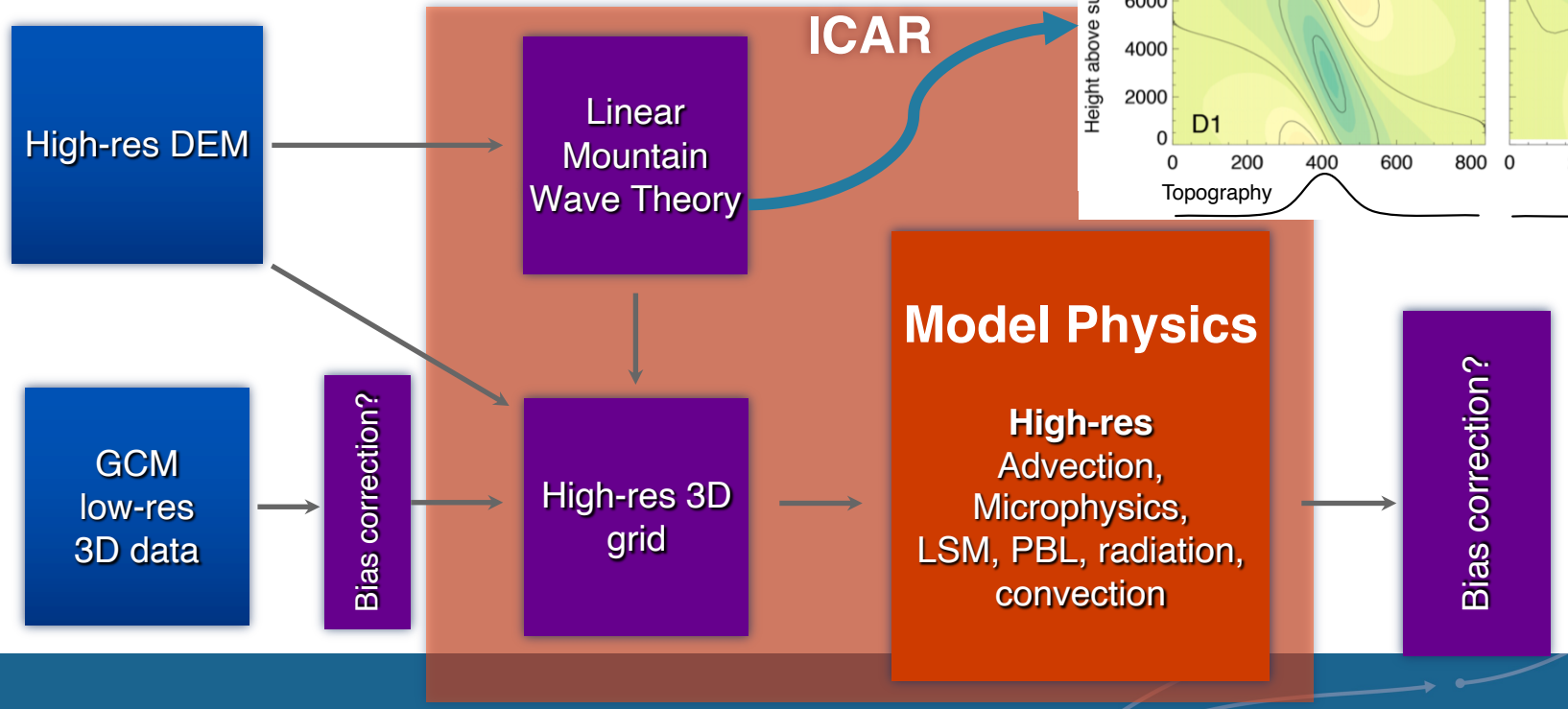
- Statistical downscaling based on rescaling GCM outputs
  - BCSD, BCCA, ARRM, LOCA

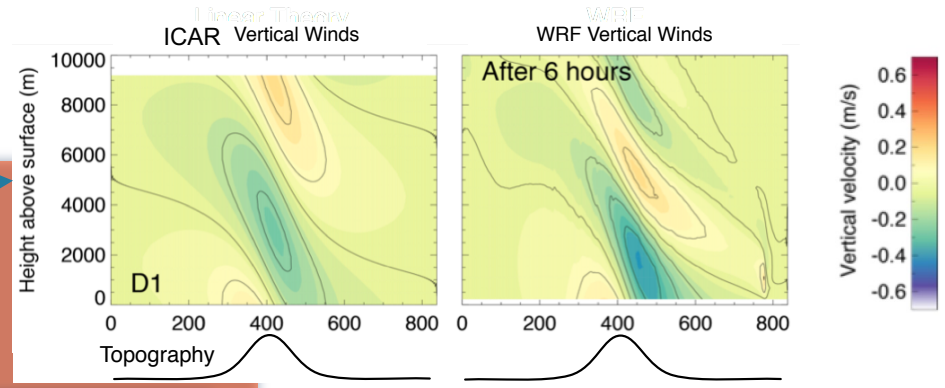
- Dynamical downscaling using state-of-the-art RCMs

Intermediate Complexity Atmospheric Research model (ICAR)

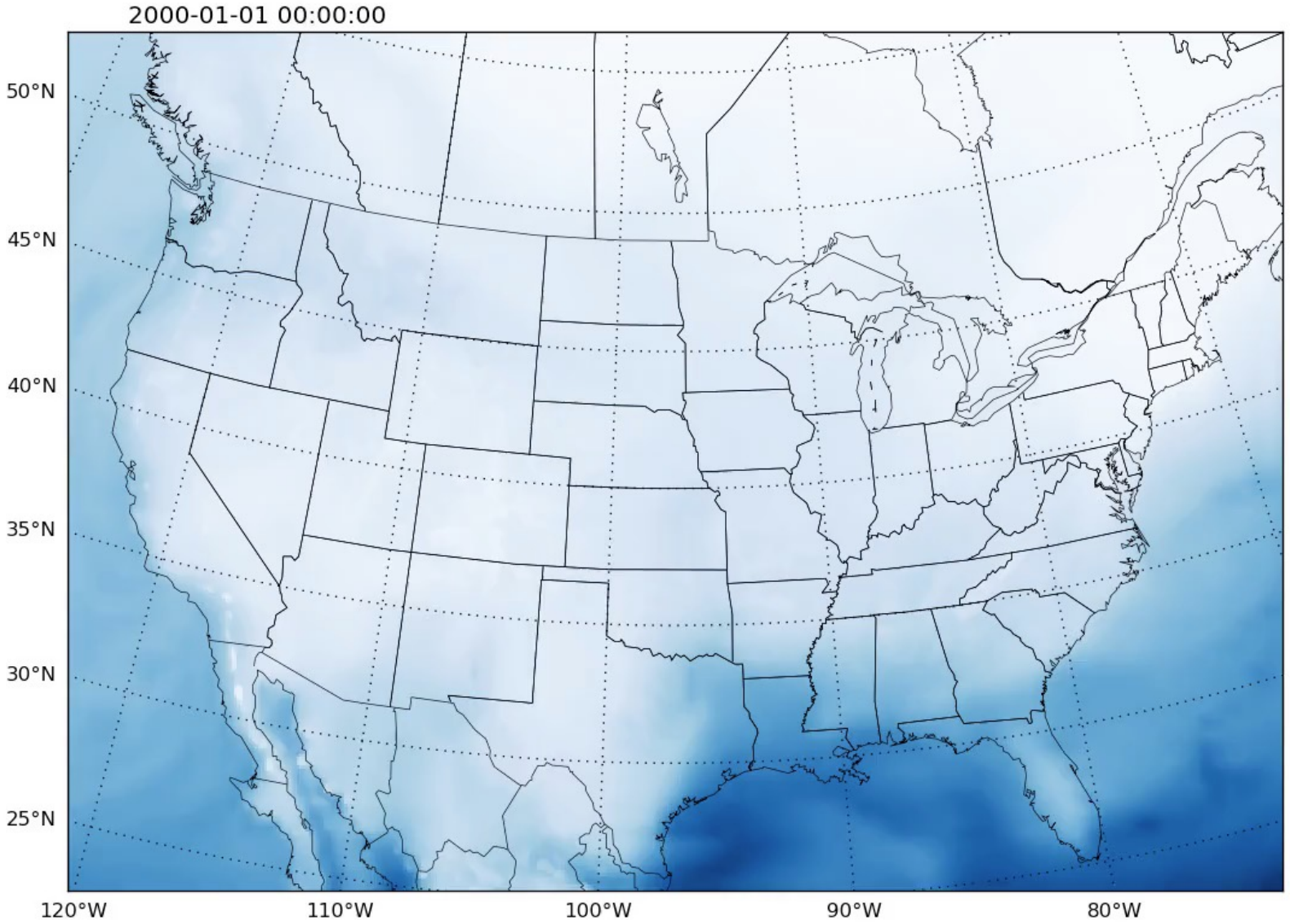
Identify the key physics and develop a simple model
GOAL: >90% of the information for <1% of the cost

http://github.com/NCAR/icar





ICAR simulation

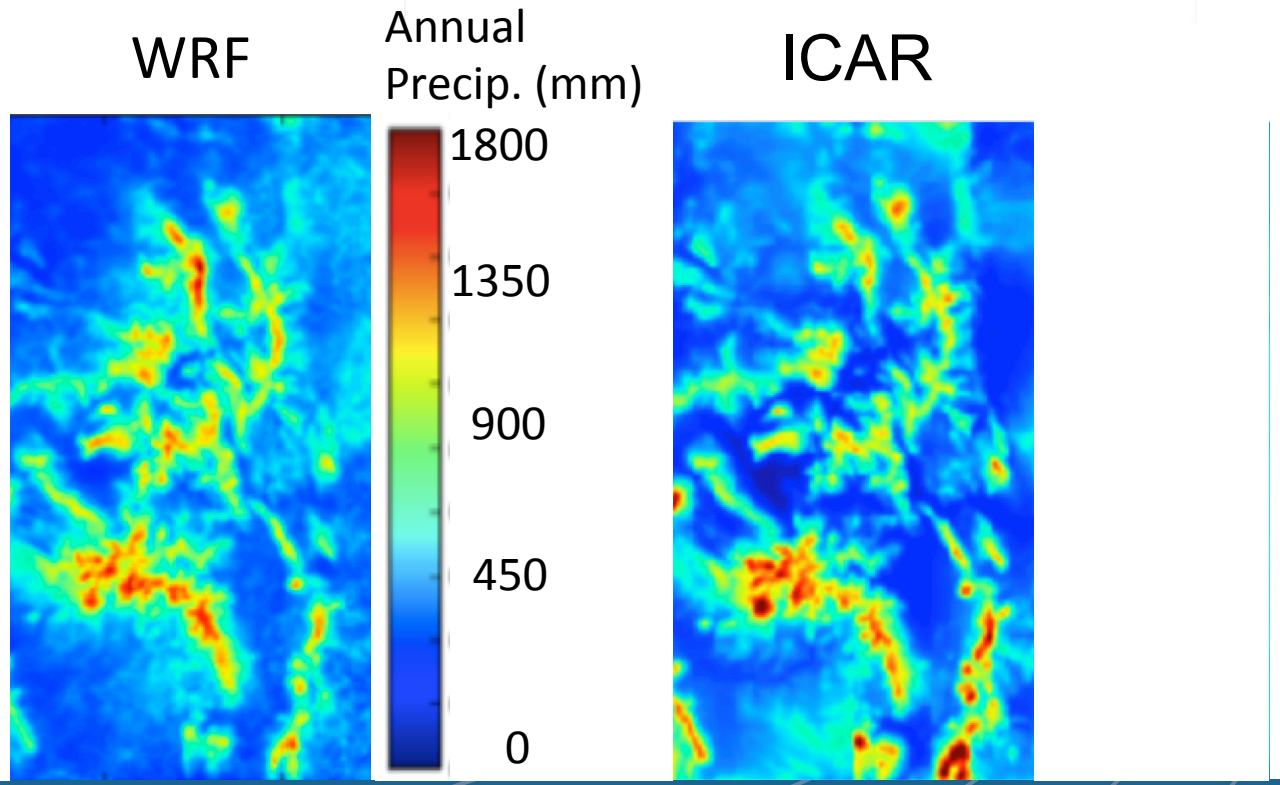


ICAR Precipitation

WRF and ICAR have very similar precipitation distributions.

ICAR requires ~1% of the computational effort of WRF.

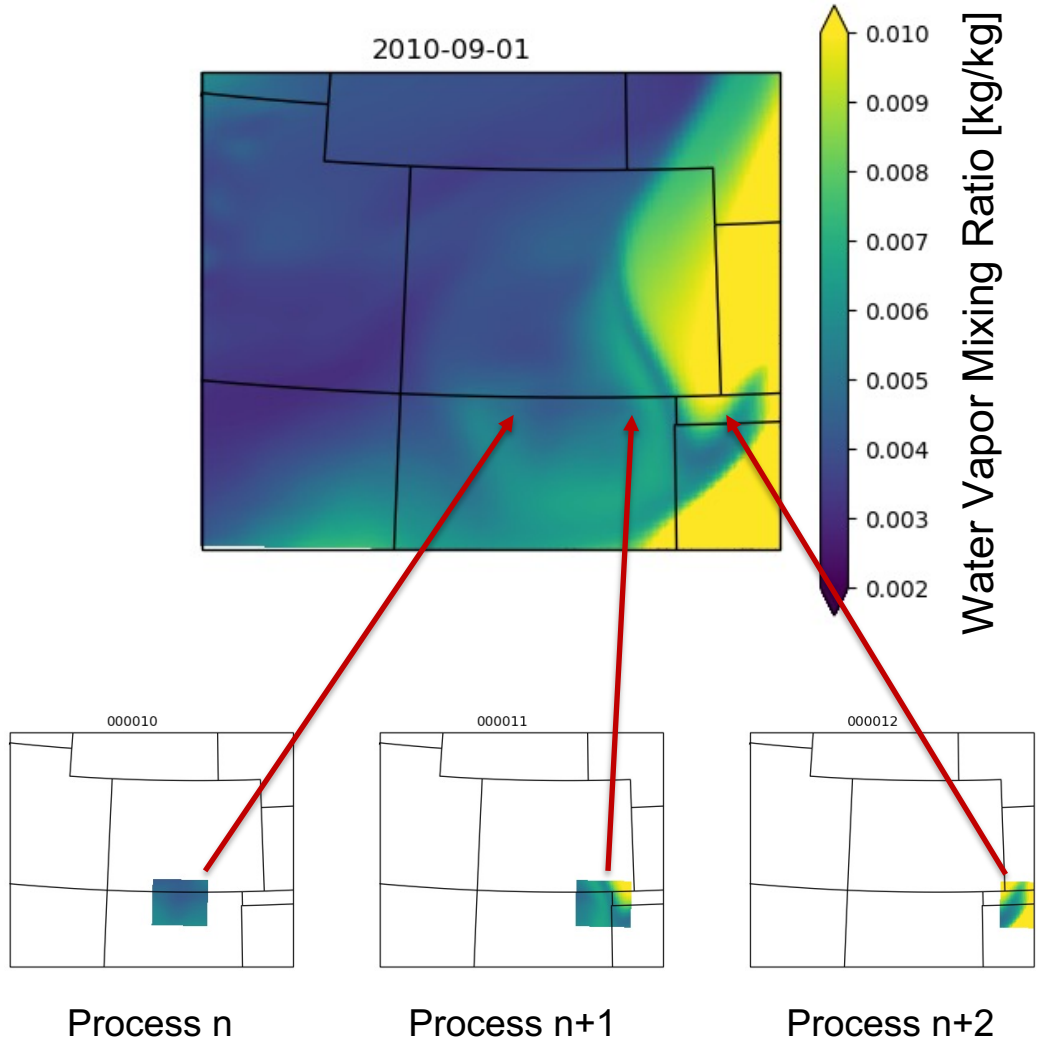
This enables a quasi-dynamical downscaling for a wide variety of GCM / scenario combinations



Partitioned Global Address Space

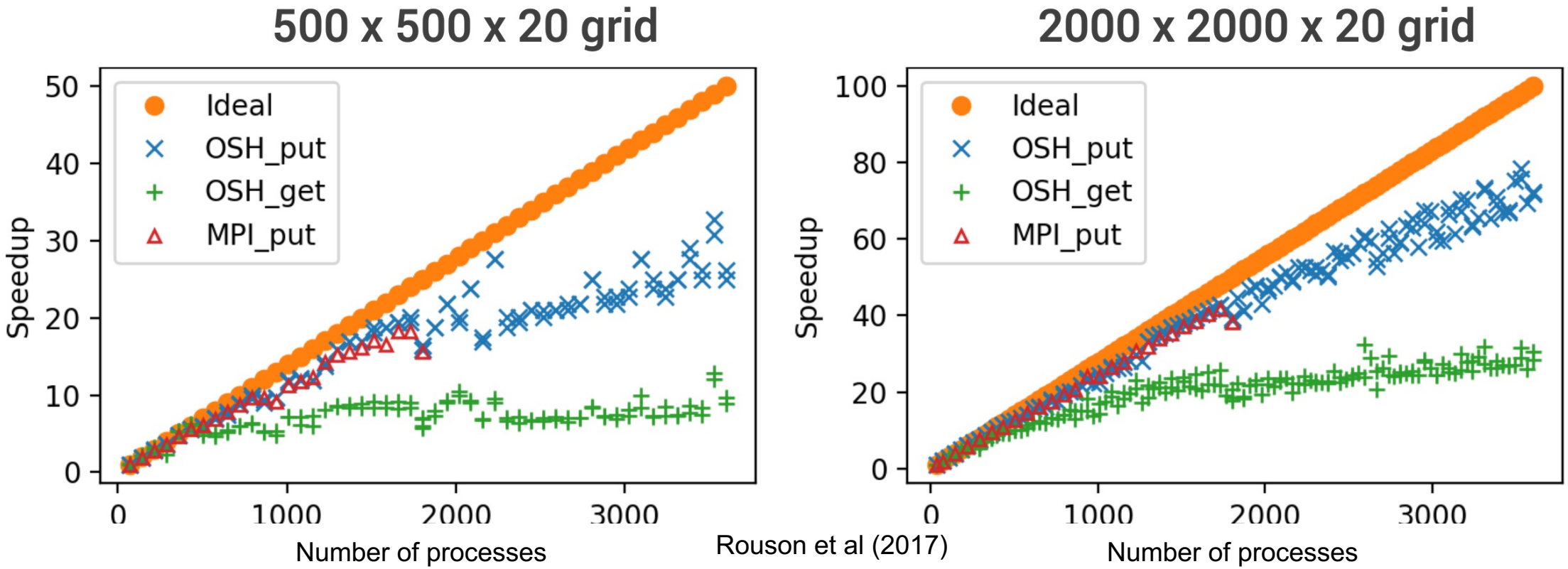
- Ideally, all variables would be coarrays
- Coarrays have costs and restrictions
- “Exchangeable” objects instead contain local data arrays and PGAS buffer coarrays

- Per time step:
  - Process edge grid cells
  - Send edge grid cells to neighbors **asynchronously**
  - Process inner grid cells
  - Sync with neighbors to update neighboring edges



Simple Scaling Results

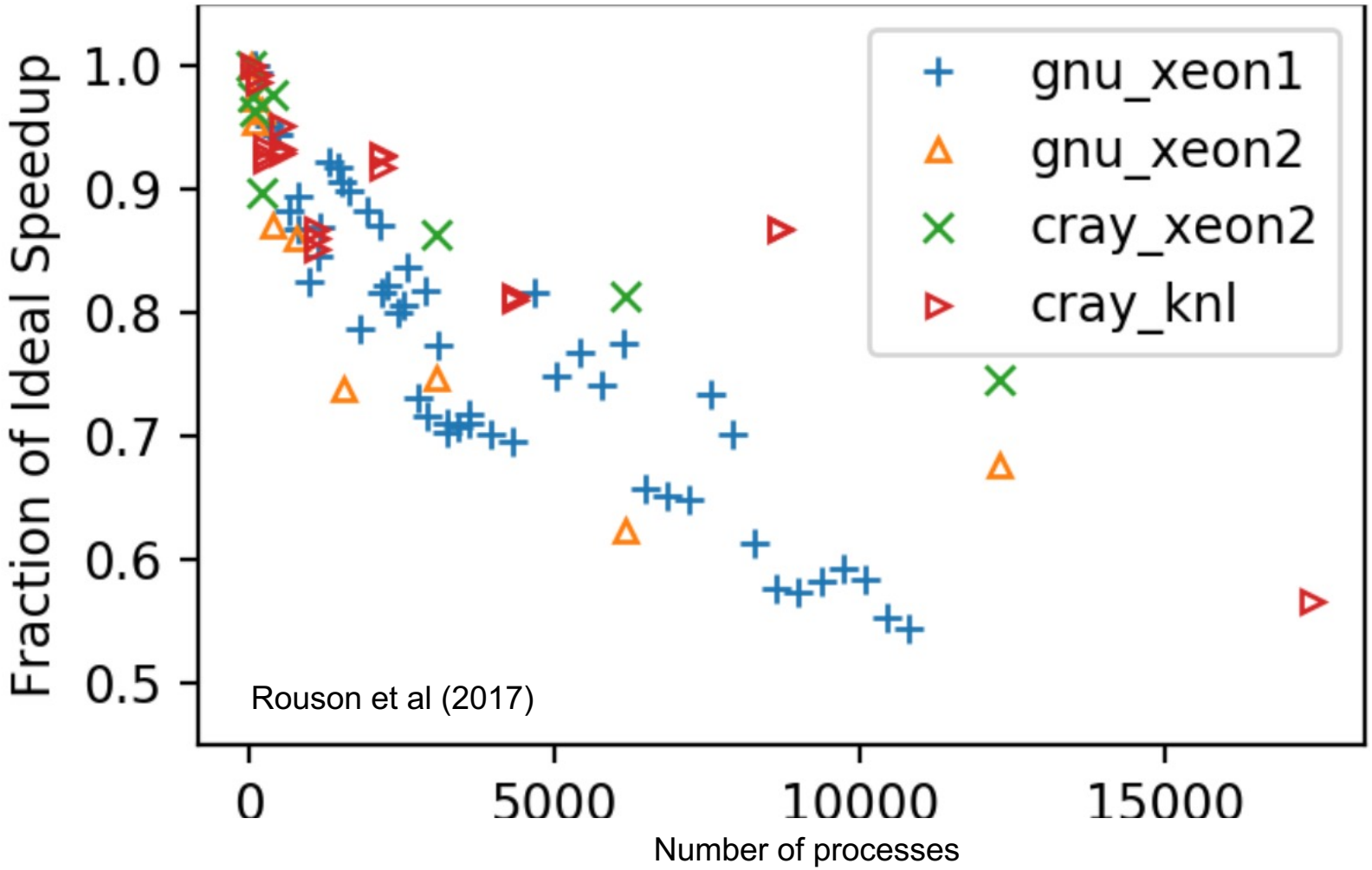
- Reduced syncs speeds up code
- Coarray fortran can leverage MPI, OpenSHMEM, GasNet,…



Rouson et al (2017)

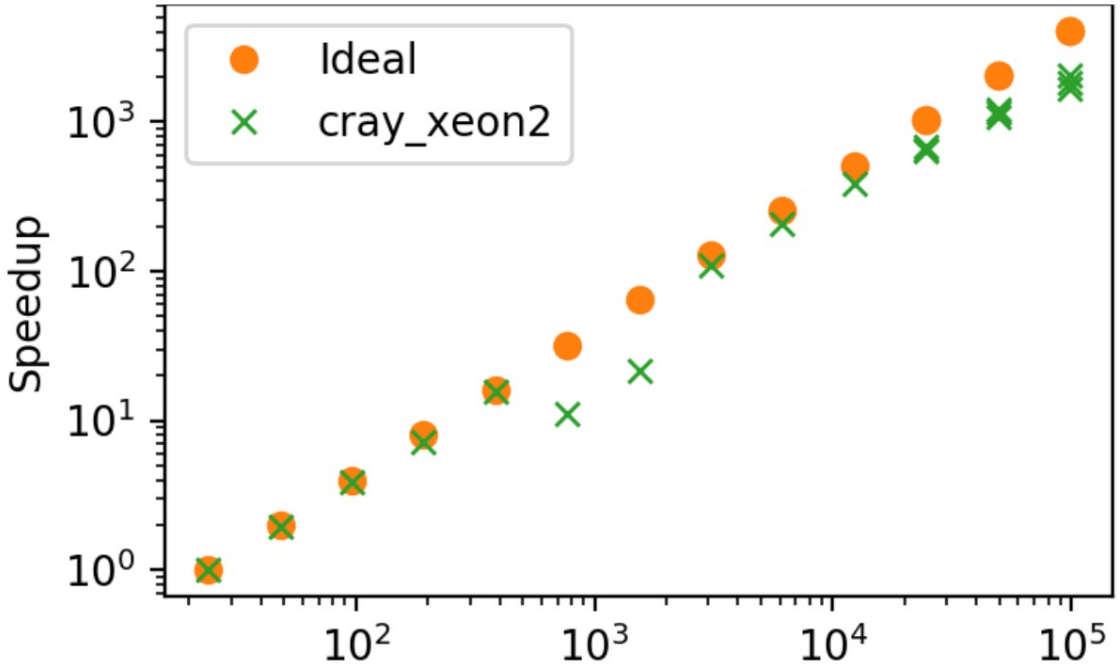
Scaling Across Computers

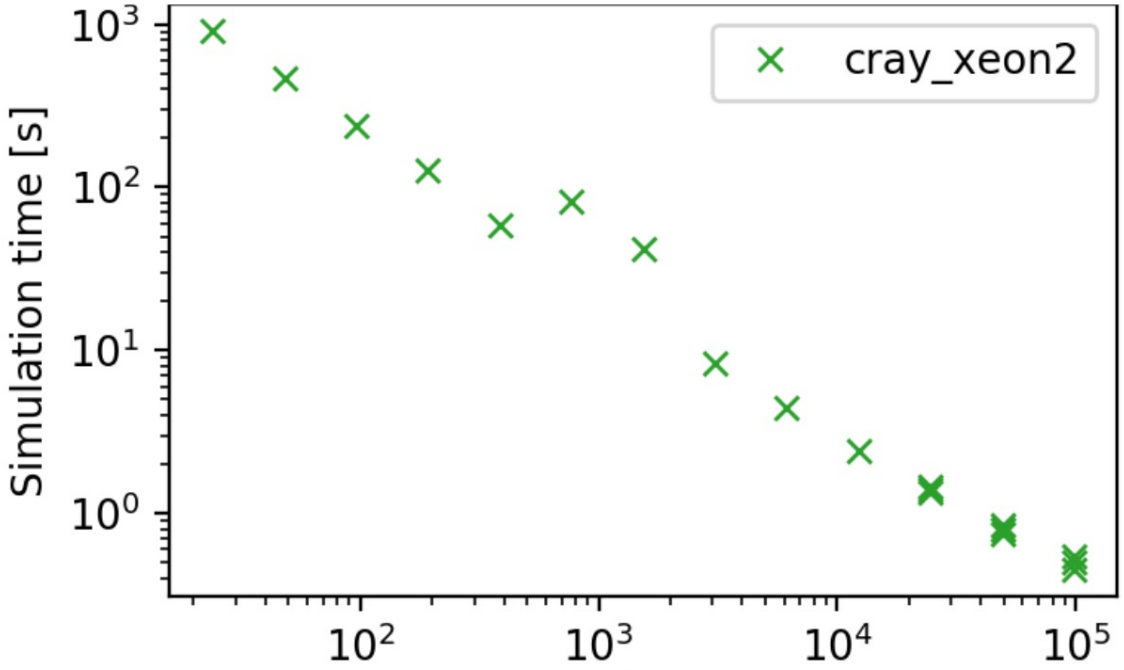
- Ideal = 1
- Cray compiler consistently outperforms GNU / opencoarrays
- Differences between computers (orange vs blue) smaller than between compilers (orange



Performance at Scale!

- Coarray fortran can scale extremely well
- Simplified code, physics only, no I/O…





Rouson et al (2017)

ICAR Users vs their Computers

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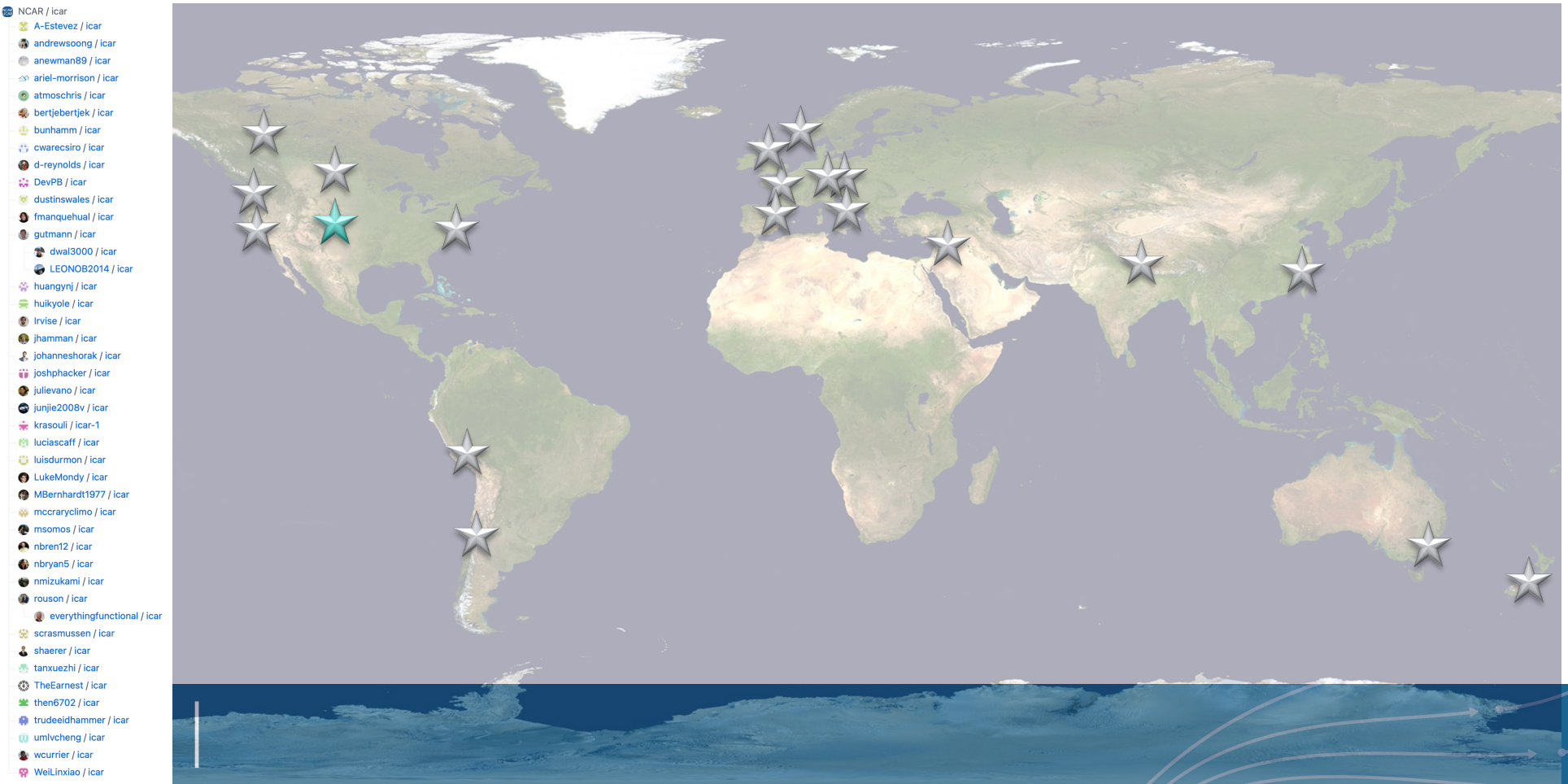
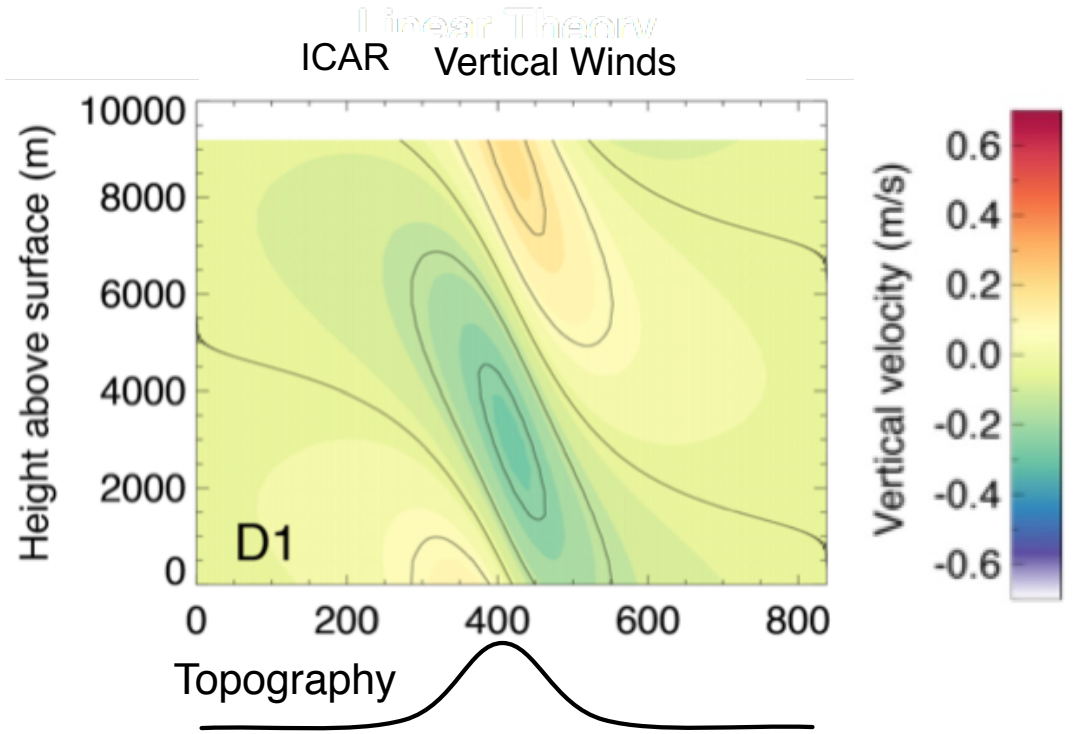
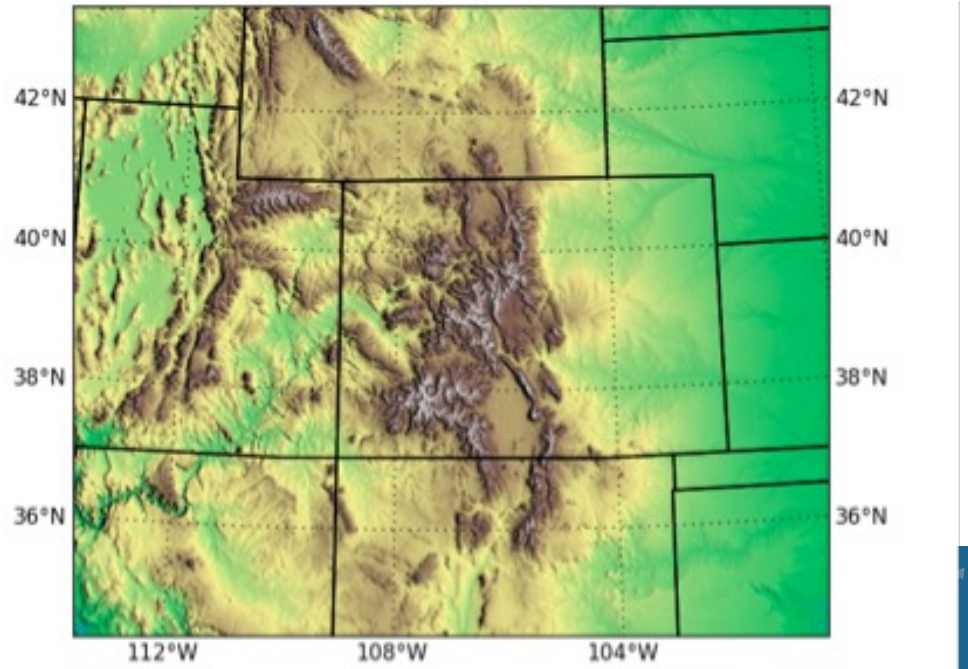
National Center for Atmospheric Research



Linear Wind Analytical Solution

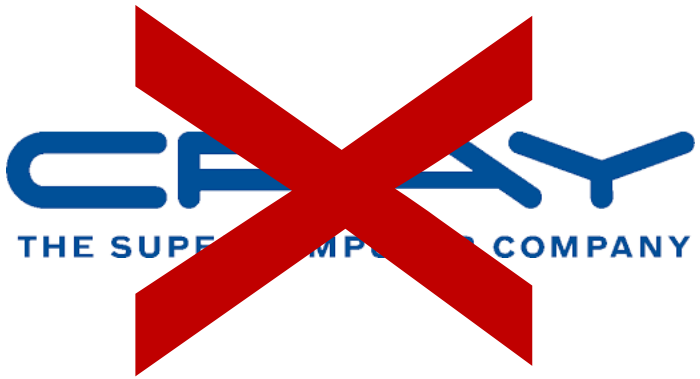
- Linear theory solution uses a global domain FFT
- Still expensive at run-time
- Create an enormous Look-up-Table
  - Typical LUT =
  - 500 x 500 x 20 x 2 x 36 x 10 x 10 = 134GB
  - nx * ny * nz * 2-vectors * ndirections * nspeeds * nstabilities
- In serial creation of LUT exceeds wall clock
- Great case for PGAS
  - Each process calculates a portion of the LUT over the global domain and sends the sub-domains to all other processes

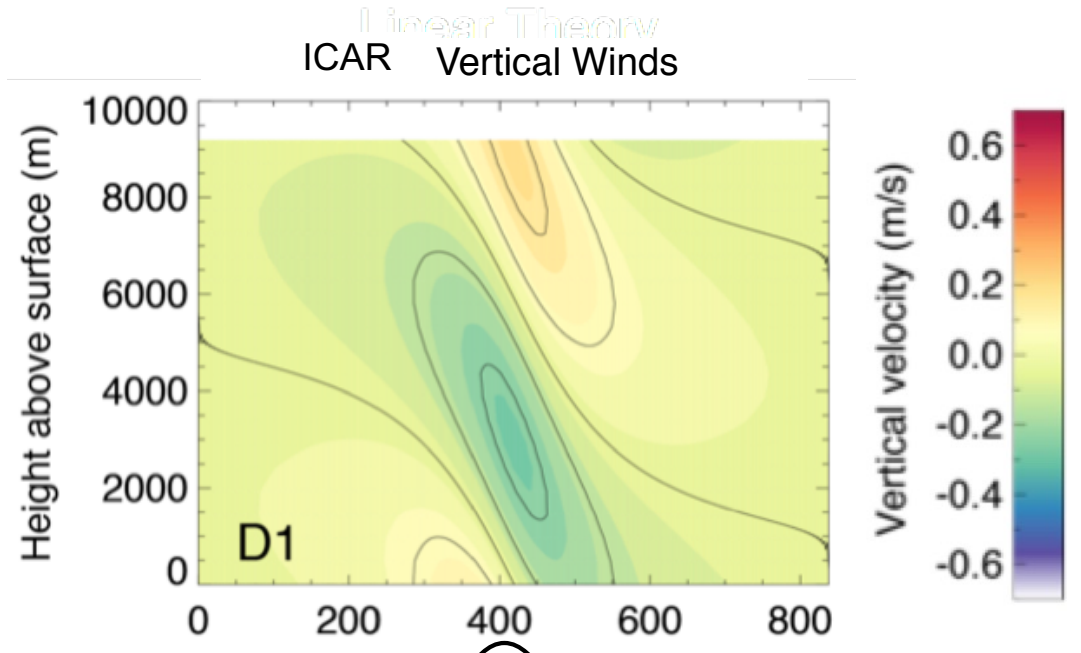


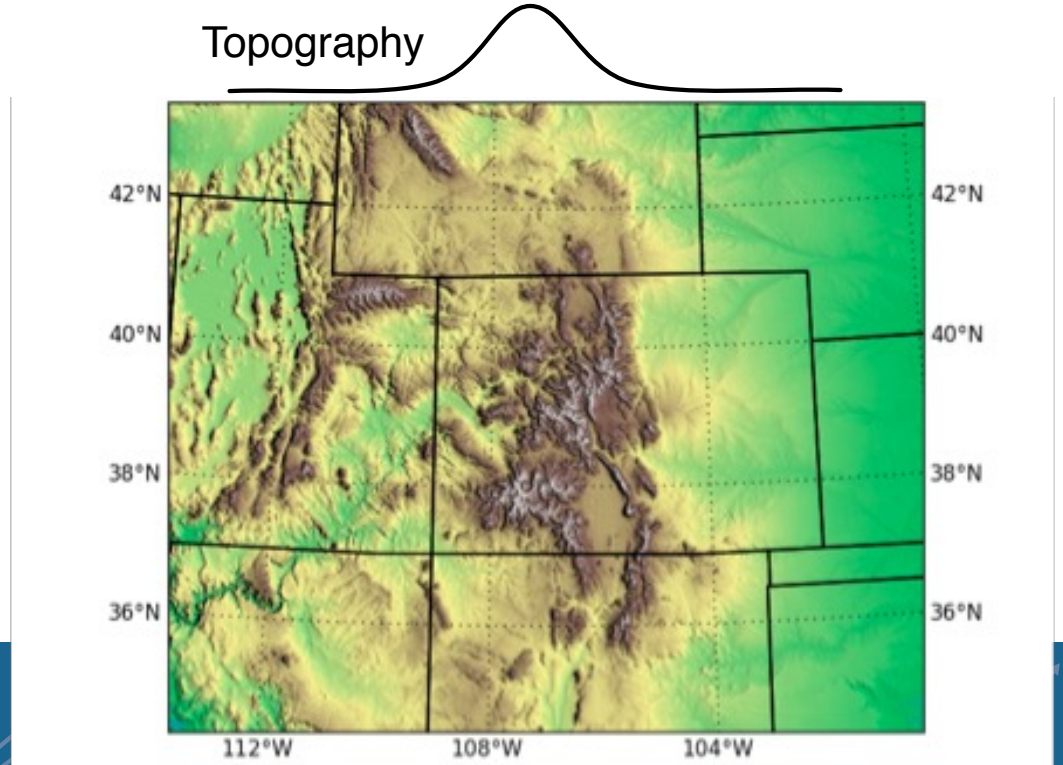


Linear Wind Analytical Solution

- Coarray LUT works great on GNU
- Crashes on allocation with Cray







Original Lookup Table (LUT)

```
subroutine copy_data_to_remote(wind, grids, LUT, i, j, k, z)
    implicit none
    real,           intent(in)  :: wind(:,:)
    type(grid_t),   intent(in)  :: grids(:)
    real,           intent(inout):: LUT(:,:,:,:,:,:)[*]
    integer,        intent(in)  :: i, j, k, z
    integer :: img

    do img = 1, num_images()
        associate(ims => grids(img)%ims, &
                  ime => grids(img)%ime, &
                  jms => grids(img)%jms, &
                  jme => grids(img)%jme)
        LUT(k,i,j, 1:ime-ims+1, z, 1:jme-jms+1)[img] = wind(ims:ime,jms:jme)
        end associate
    enddo
end subroutine copy_data_to_remote
```

No synchronization required!

Issue: one large coarray requires too much memory crashed Cray compiled code
Does Cray use special memory for coarrays allocated on NIC or other?

Non-Coarray LUT: step 1

Split large coarray into smaller buffer. Also need to send LUT indicies for each
First send then sync

```
! each image will communicate the wind values it has calculated for an ijkz
! location to the other images, the ijkz values are also sent so the receiving
! images know where to put the incoming values
do img = 1, num_images()
    associate(ims => grids(img)%ims, &
              ime => grids(img)%ime, &
              jms => grids(img)%jms, &
              jme => grids(img)%jme  &
        )
    LUT_co(1:ime-ims+1, 1:jme-jms+1, this_image())[img] = wind(ims:ime,jms:jme)

    LUT_index_co(this_image(), 1)[img] = i
    LUT_index_co(this_image(), 2)[img] = j
    LUT_index_co(this_image(), 3)[img] = k
    LUT_index_co(this_image(), 4)[img] = z
   end associate
enddo

sync all  Synchronization required!
```

Non-Coarray LUT: step 2

After sync, copy smaller coarray lookup table to large **non-coarray** table.
Need to use LUT_index variable to know where to copy

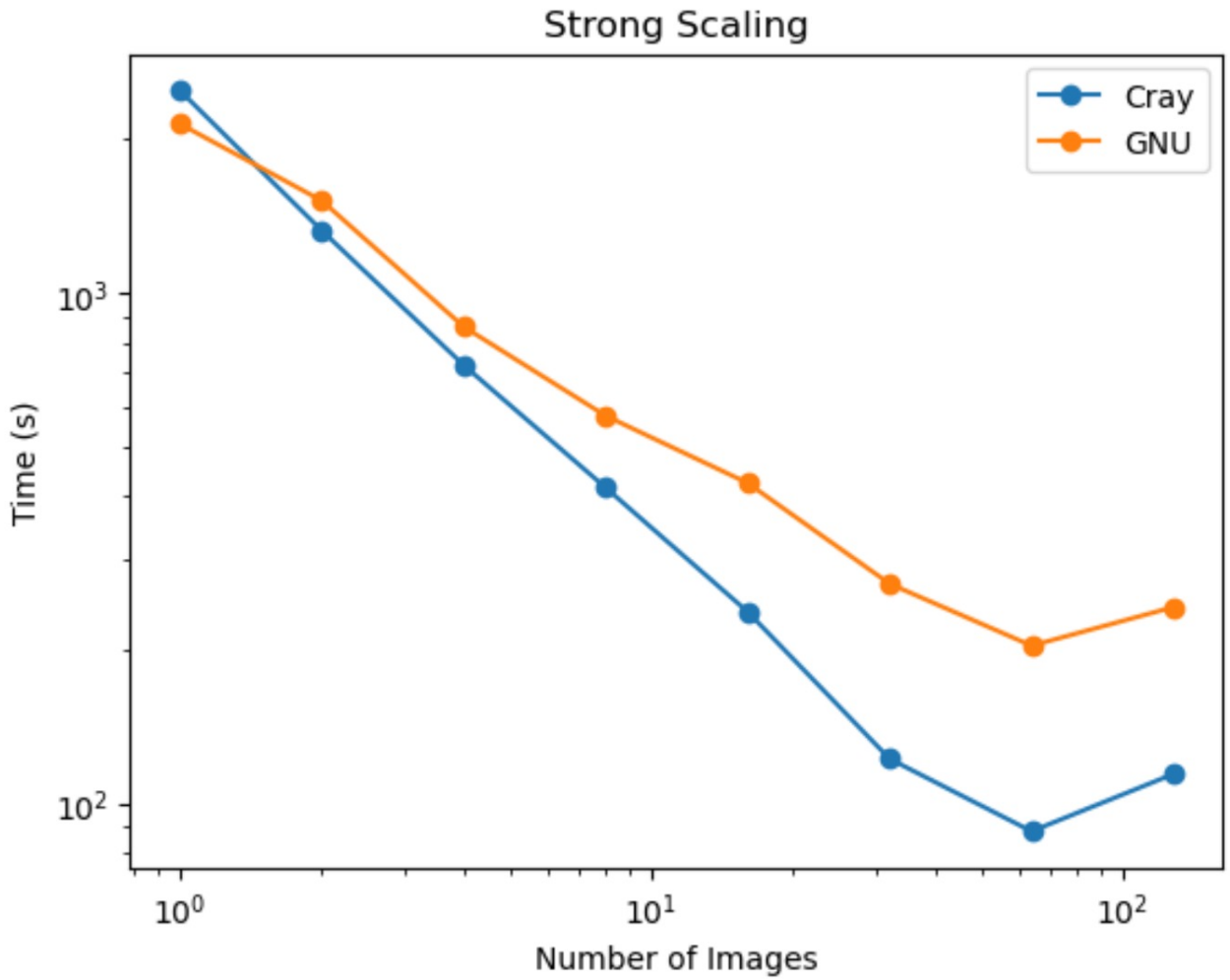
```
sync all

associate(ims => grids(this_image())%ims, &
          ime => grids(this_image())%ime, &
          jms => grids(this_image())%jms, &
          jme => grids(this_image())%jme)
    do img = 1, num_images()
        LUT_i = LUT_index_co(img, 1)
        LUT_j = LUT_index_co(img, 2)
        LUT_k = LUT_index_co(img, 3)
        LUT_z = LUT_index_co(img, 4)
        LUT(LUT_k, LUT_i, LUT_j, 1:ime-ims+1, LUT_z, 1:jme-jms+1) = &
             LUT_co(1:ime-ims+1, 1:jme-jms+1, img)
    end do
end associate
sync all
```

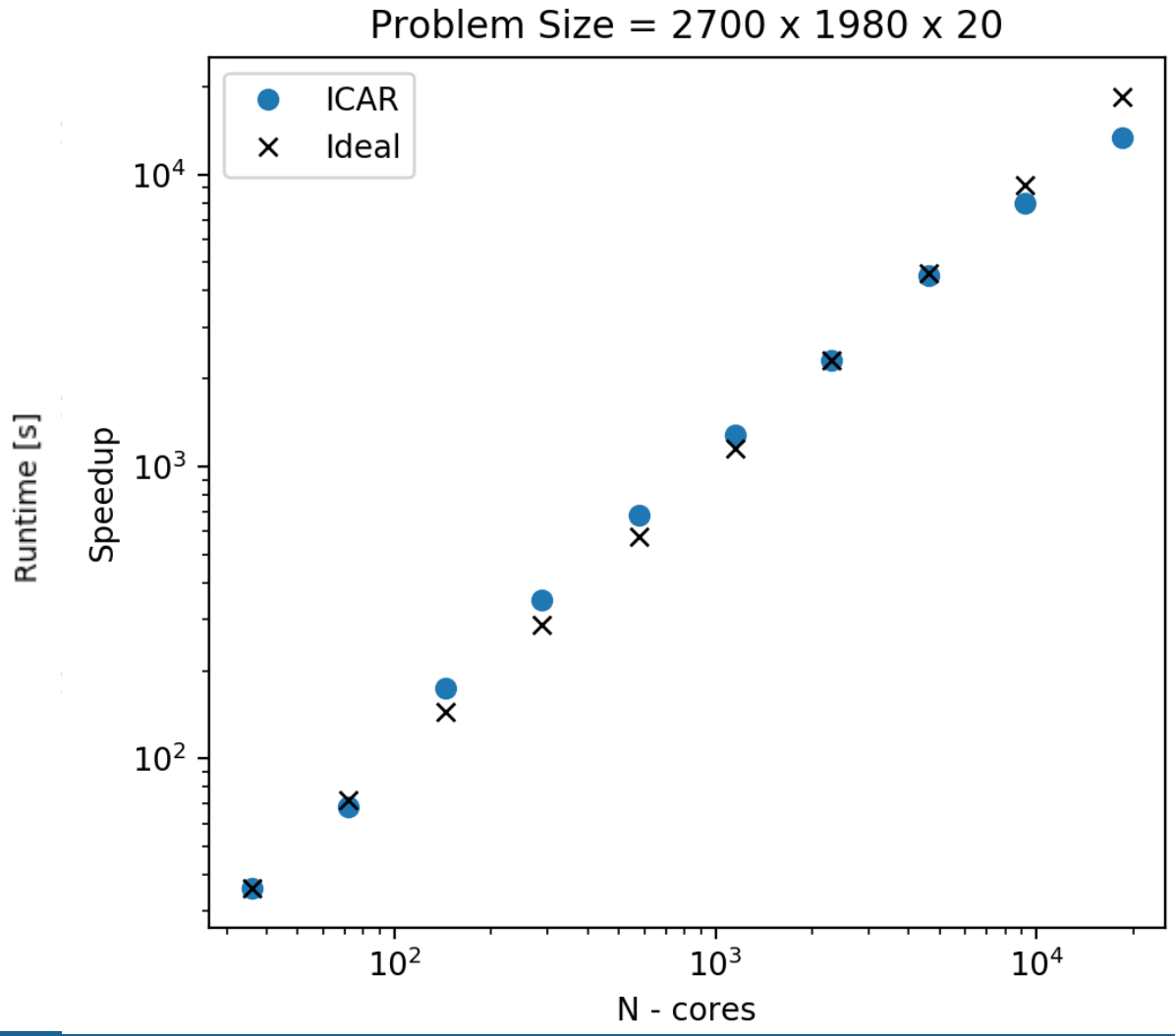
Two synchronizations required! (other approaches possible)

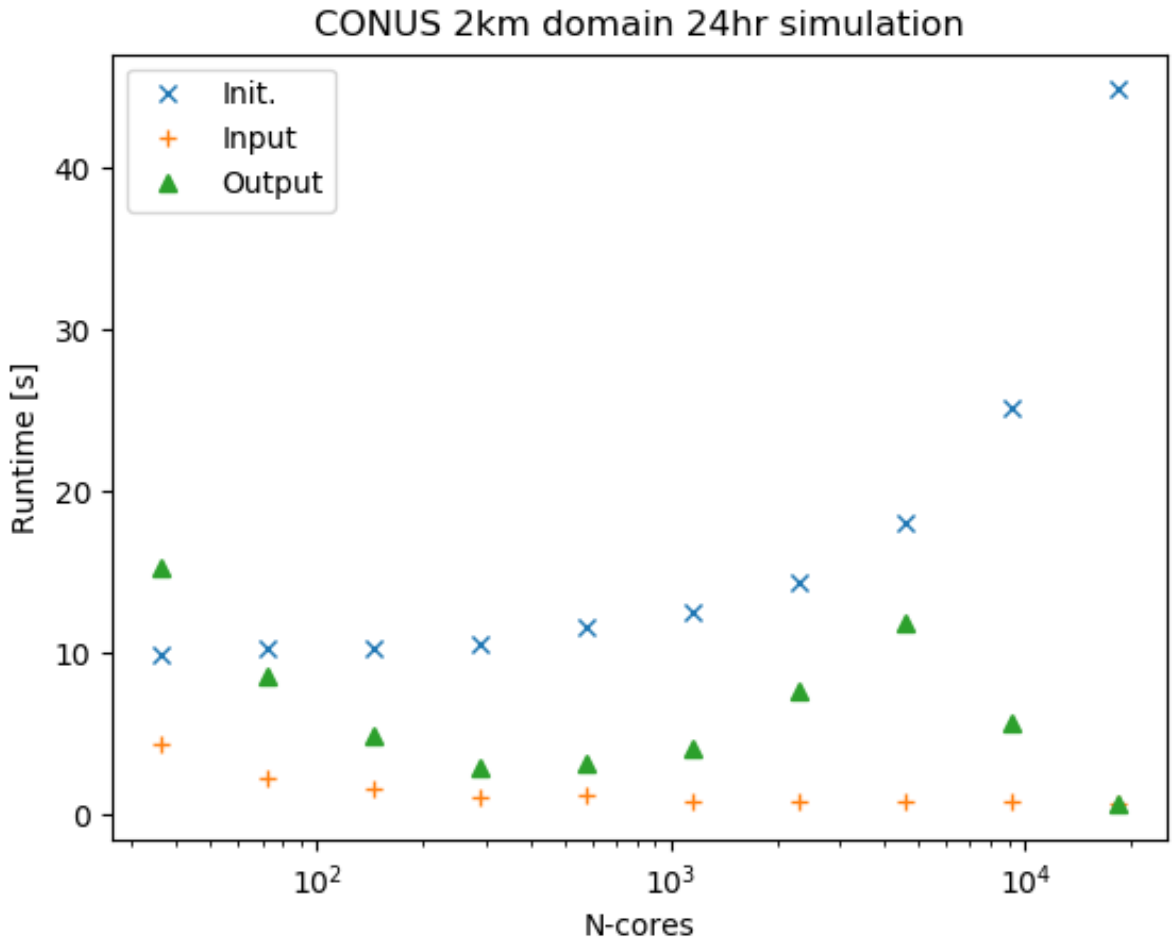
Strong scaling on smaller domains

- 210 x 160 grid cell domain
- Cray ~2.5x faster than GNU! (90s v 220s)
- Primarily due to coarray communication, GNU is faster than Cray on a single process
- Odd performance drop when node is full



Real Applications

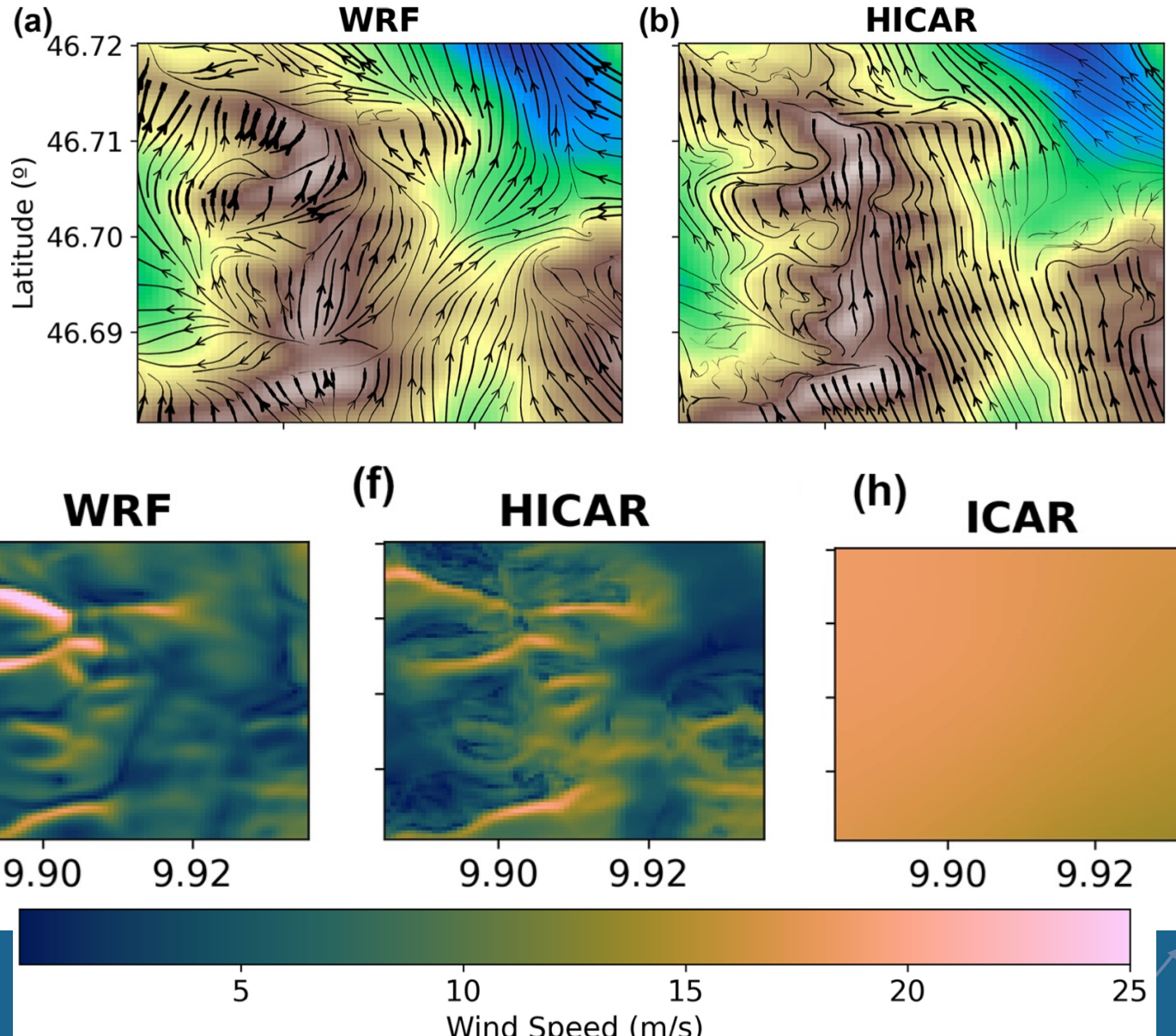




Coarrays makes parallel easy!

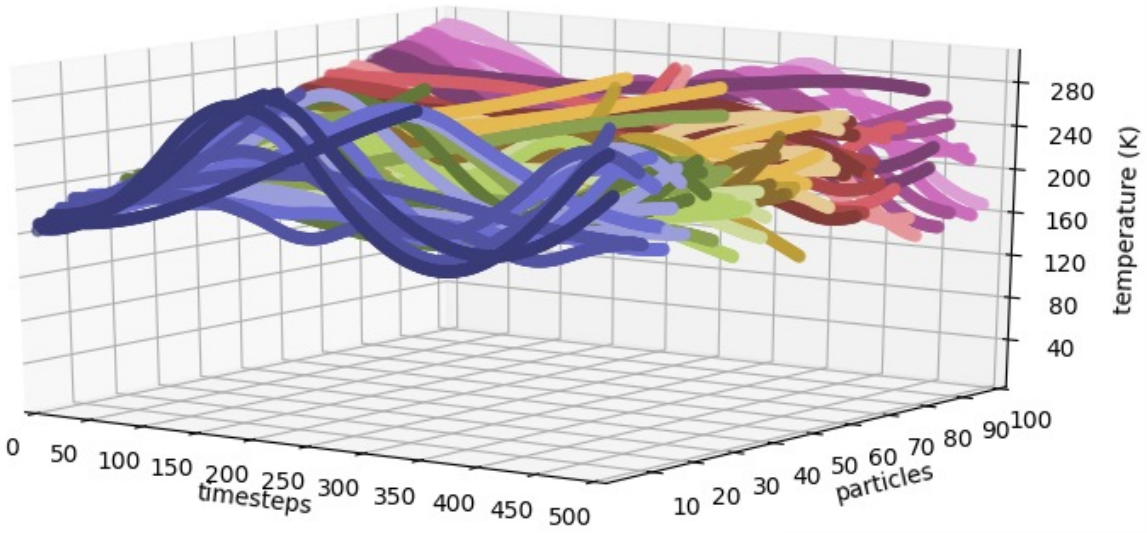
- New iterative wind solver added to ICAR by grad student
  - Dylan Reynolds at SLF
  - no computer science or atmospheric science background!

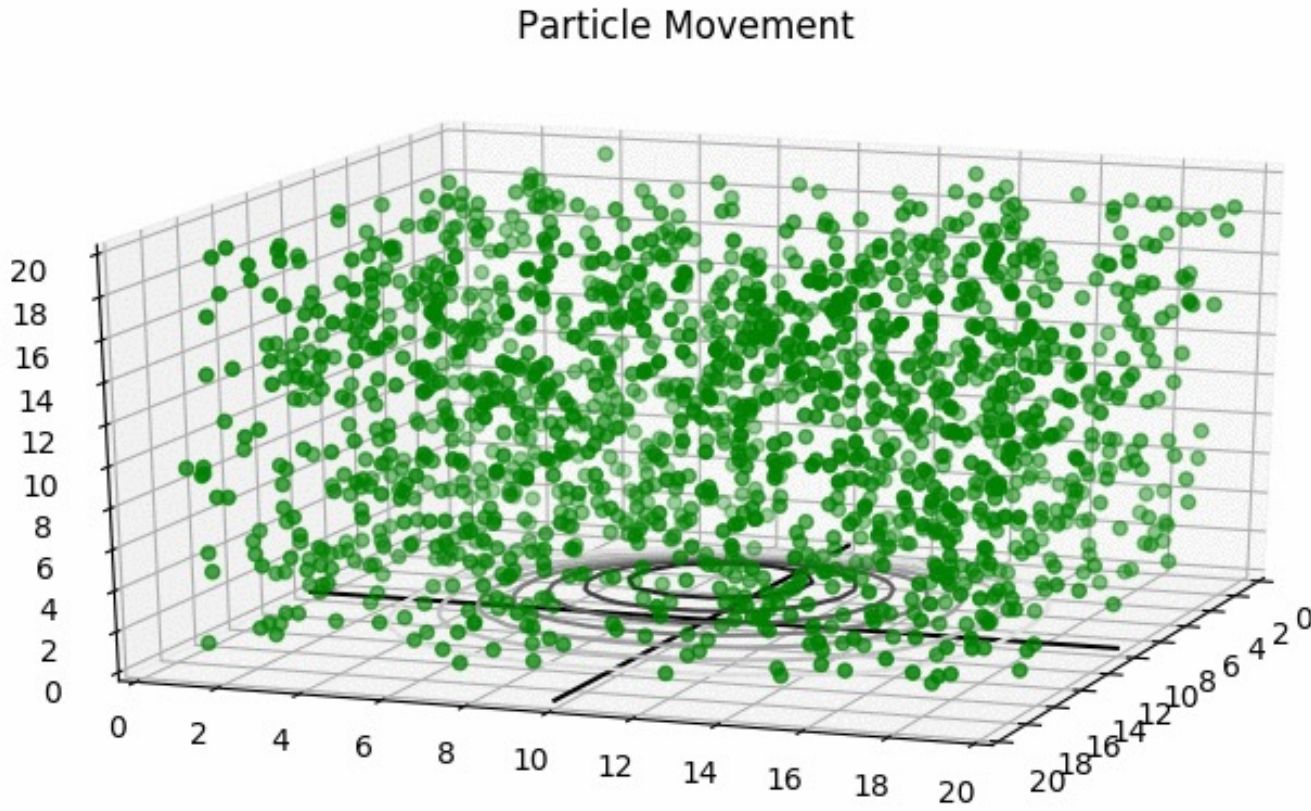
- Adds surface wind adjustments
- ICAR linear theory only adjusts upper level winds



Coarrays makes parallel easy!

- New lagrangian air parcels added by Grad Student
  - Soren Rasmussen, Cranfield (now NCAR)
  - Fortran objects as coarrays
  - Passing entire object between processes





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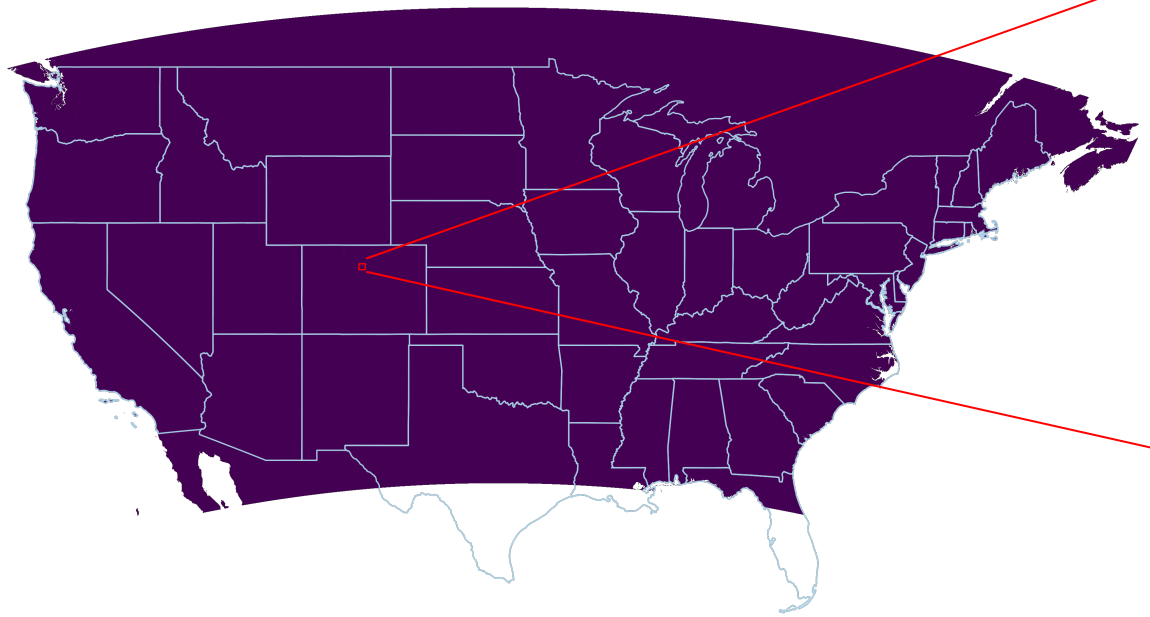
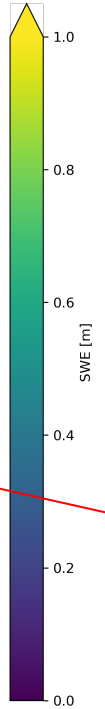
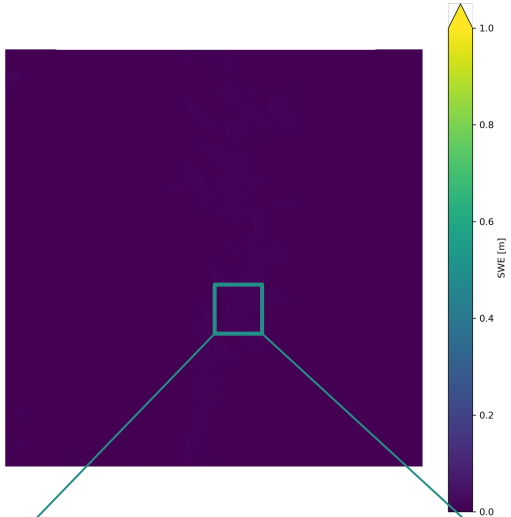
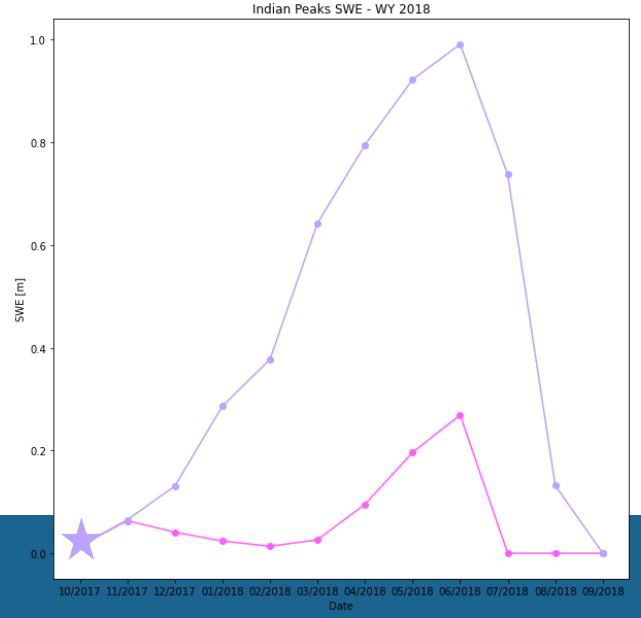


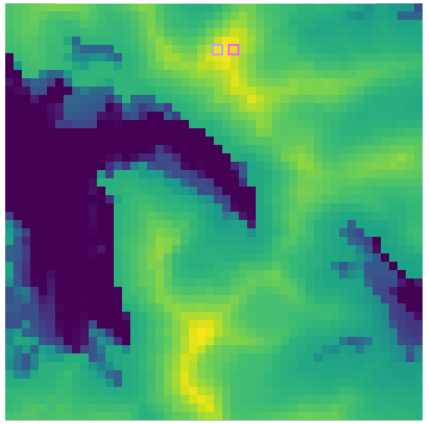


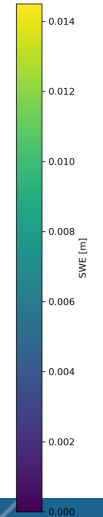
Domain Zoom 2500 km²





Domain Zoom 25 km²





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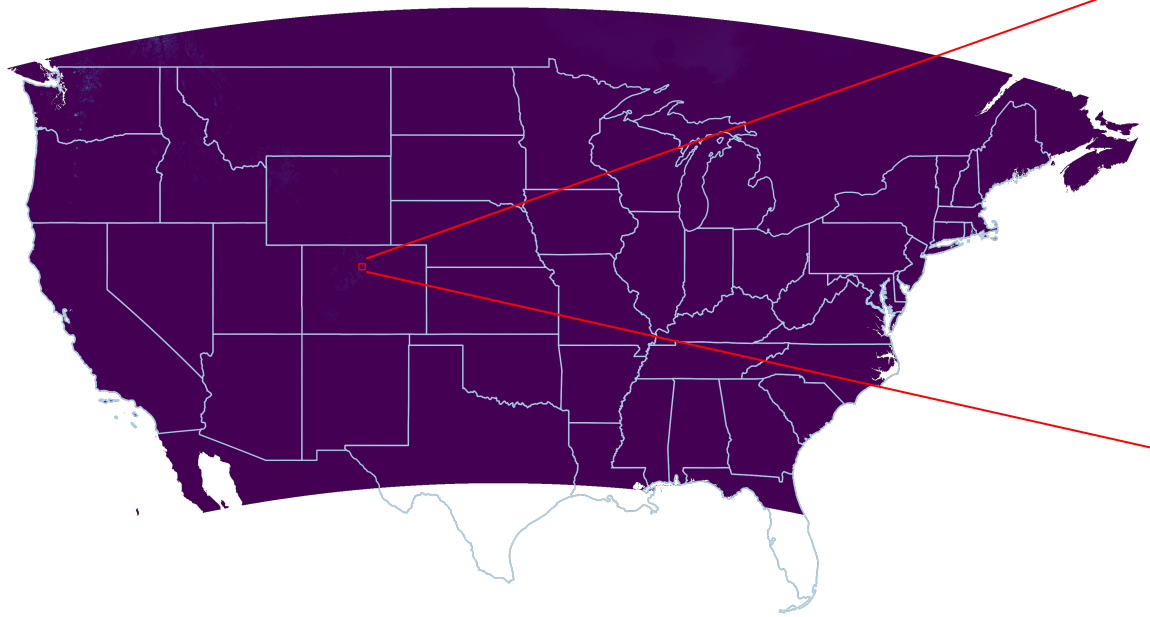

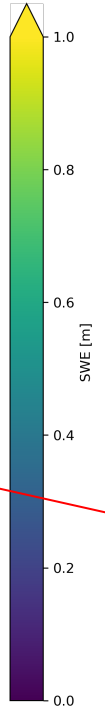

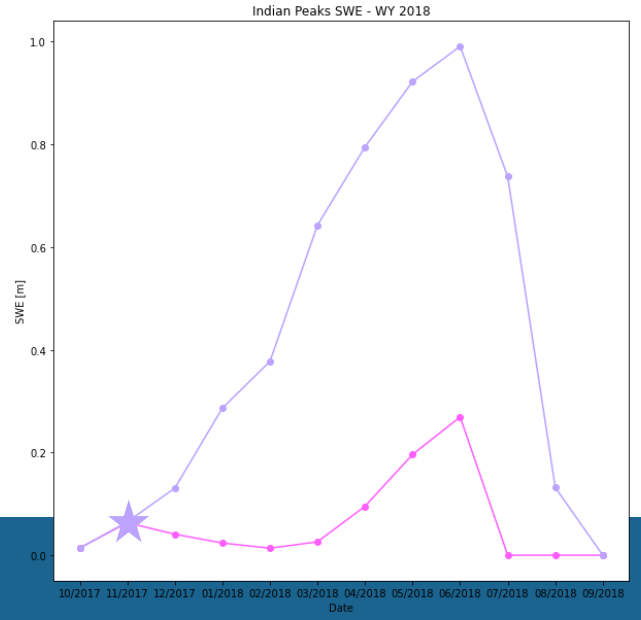

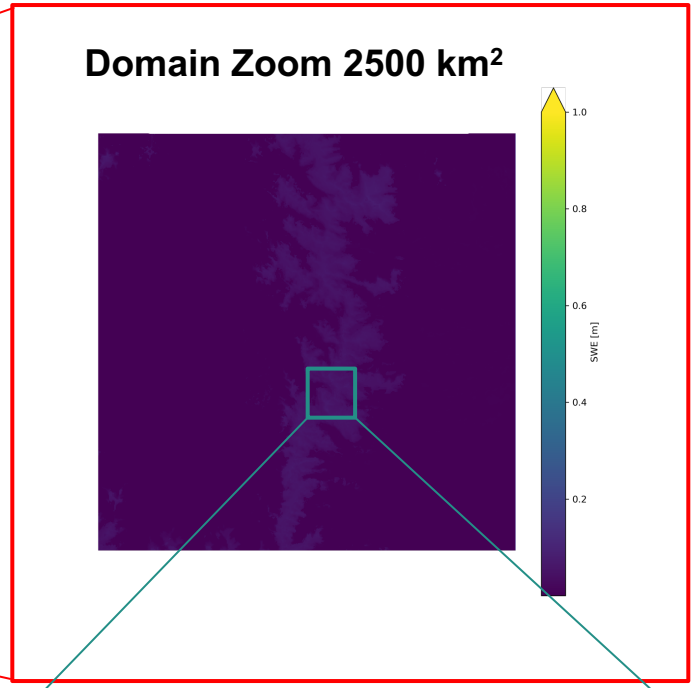

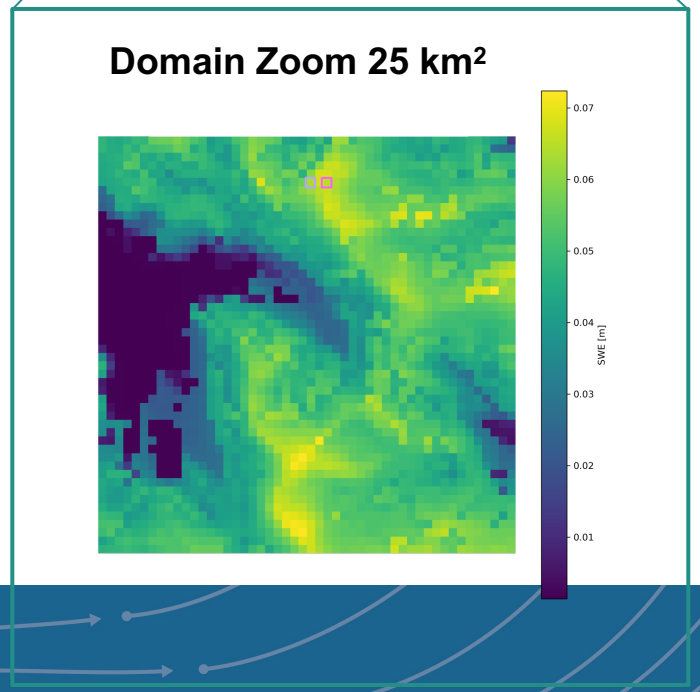

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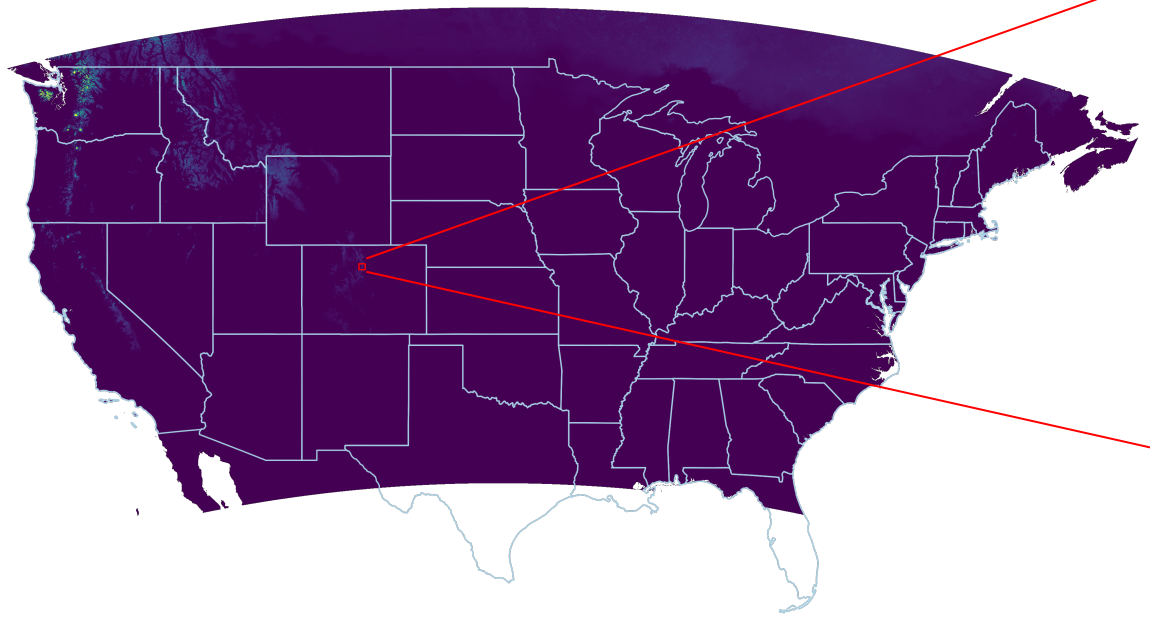
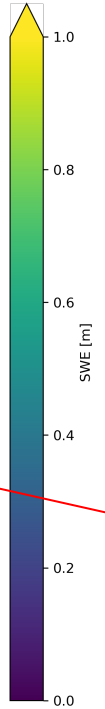
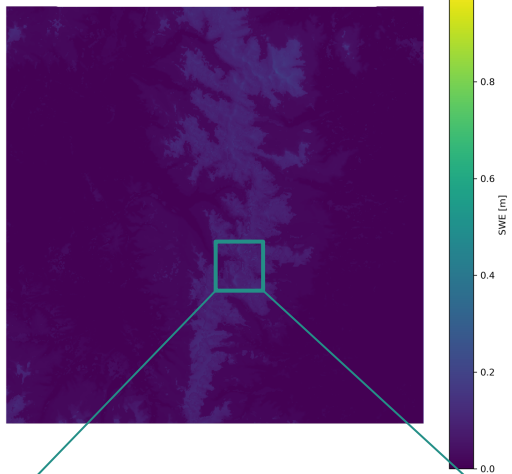
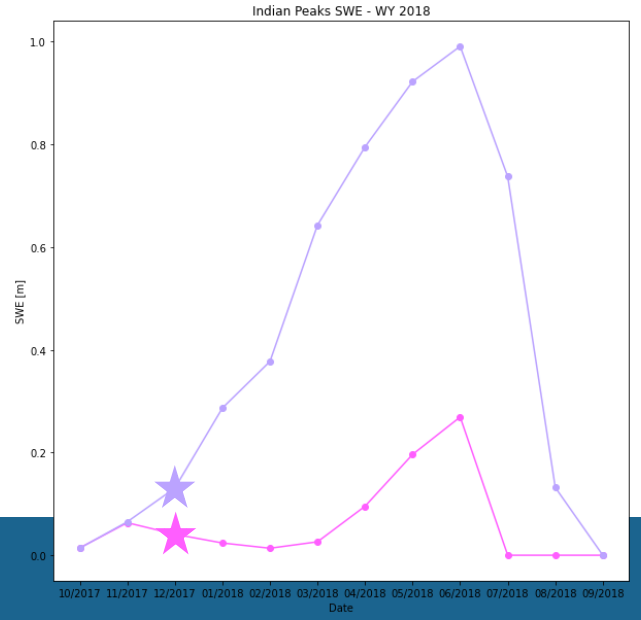




Domain Zoom 2500 km²





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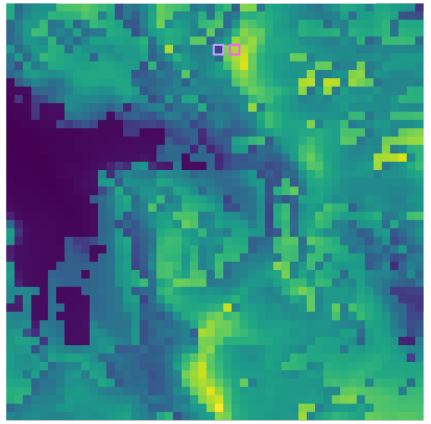

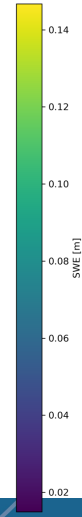

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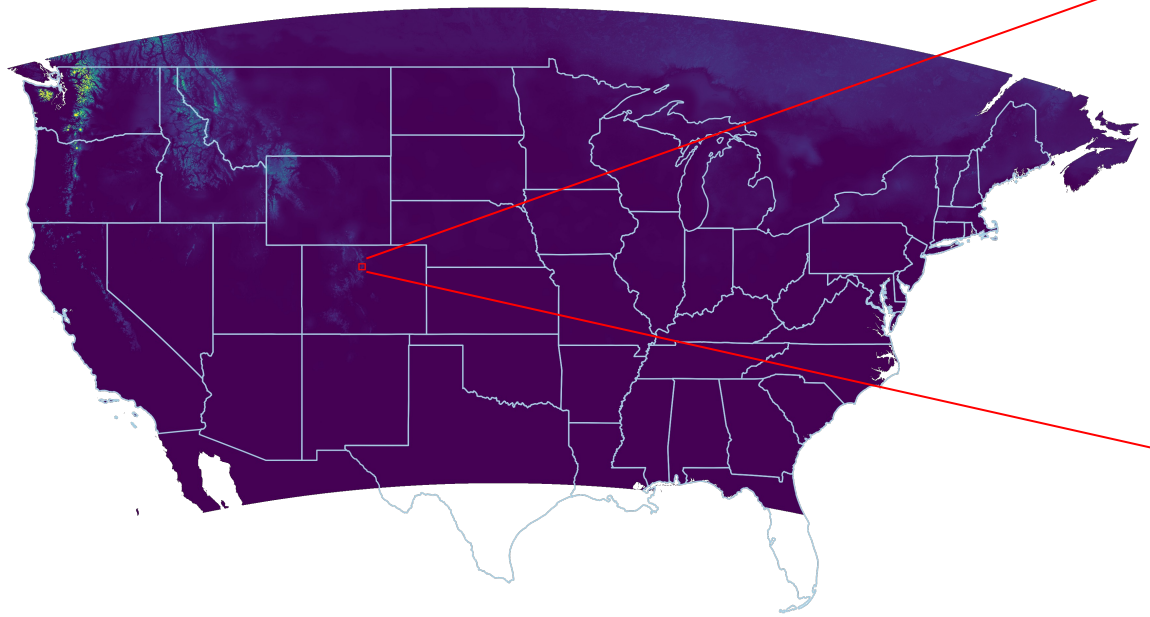
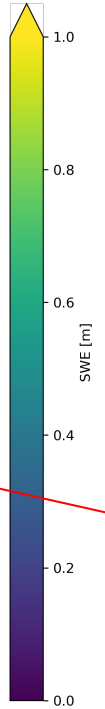
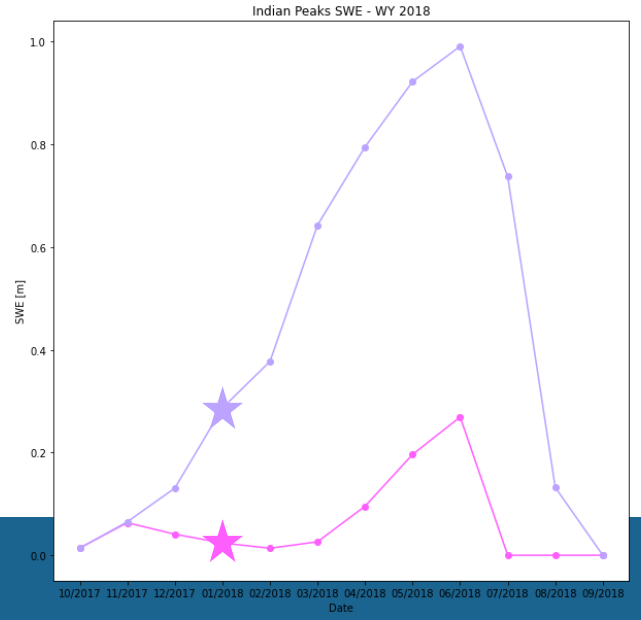
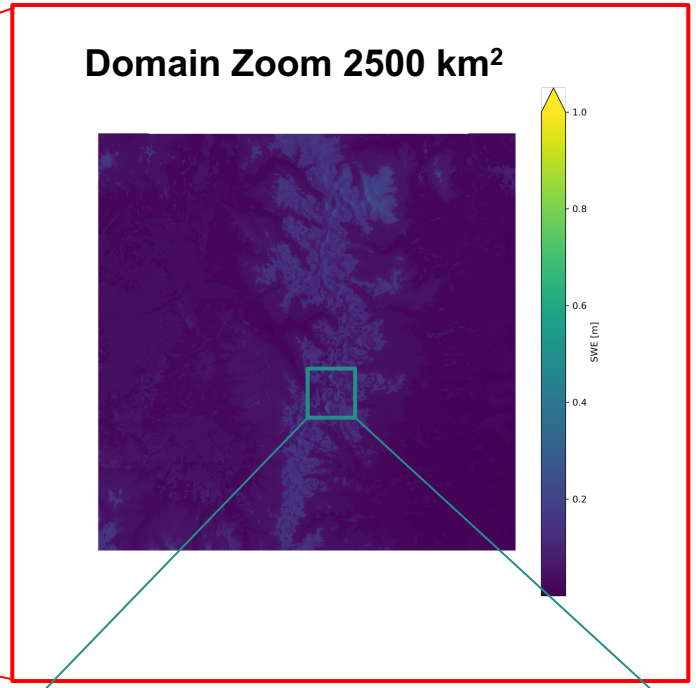
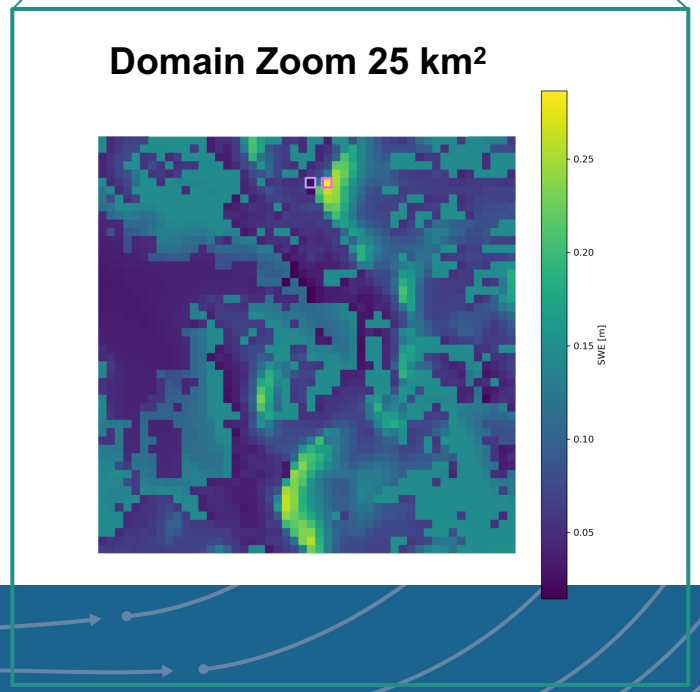
CONUS SWE January 1st , 2018











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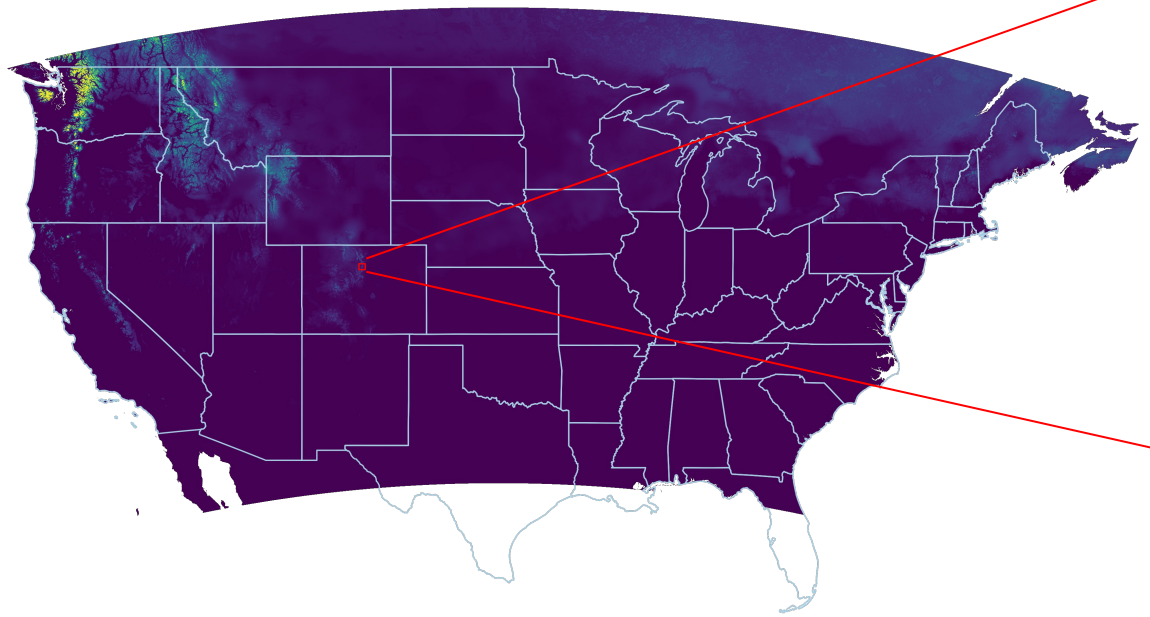
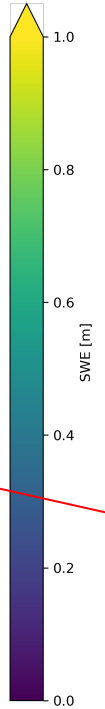
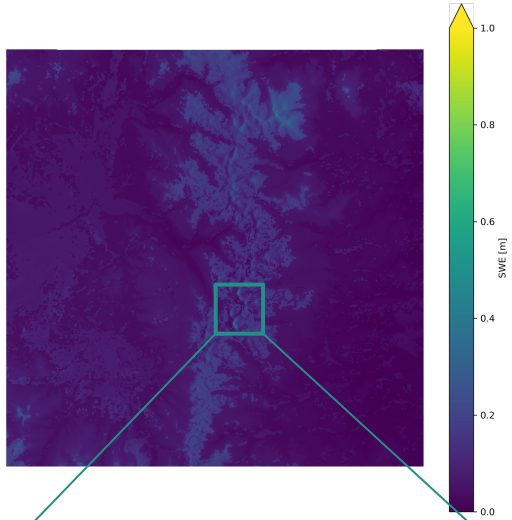
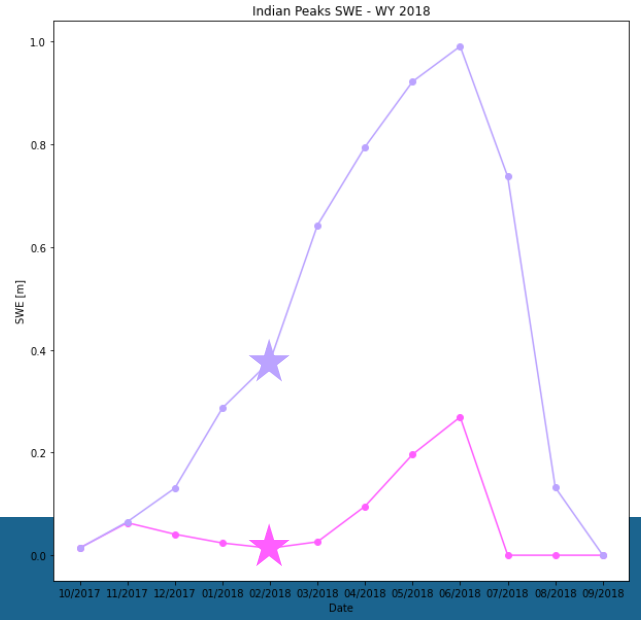
CONUS SWE February 1st , 2018





Domain Zoom 2500 km²





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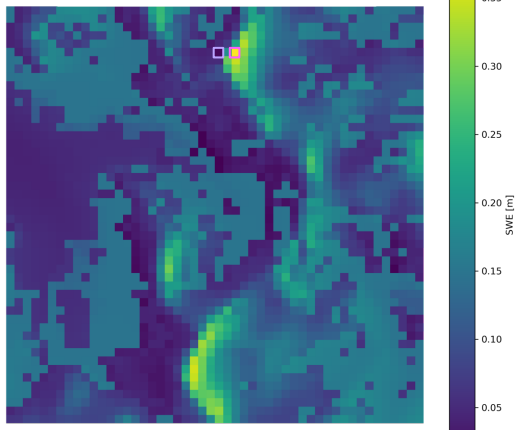

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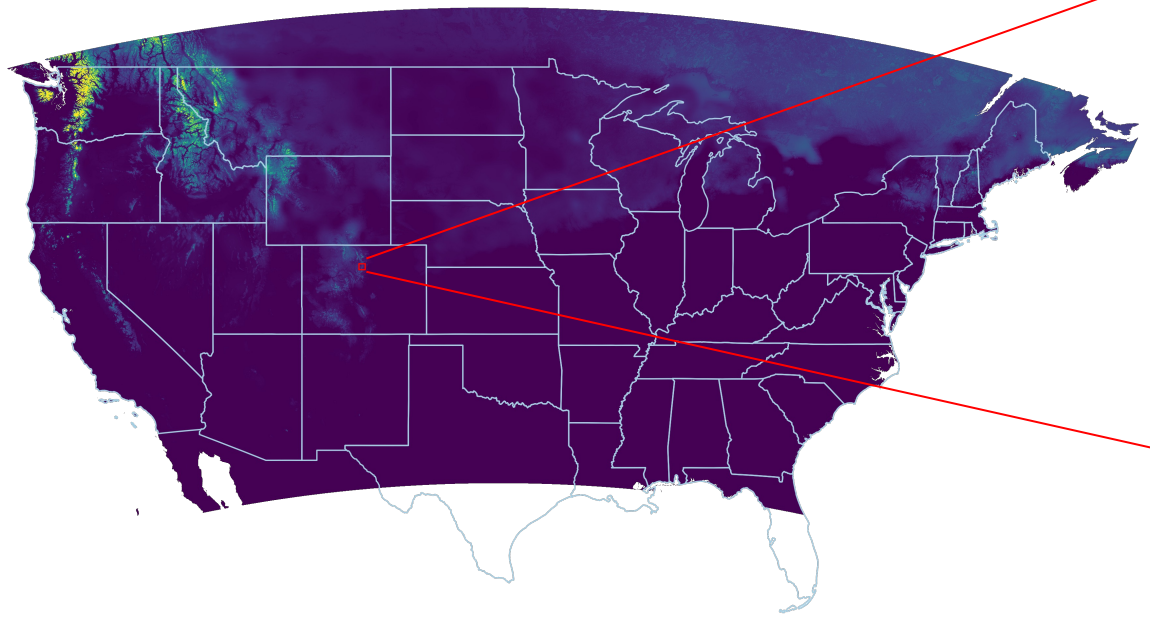
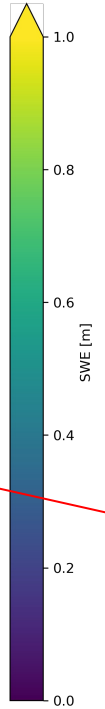
CONUS SWE March 1st , 2018





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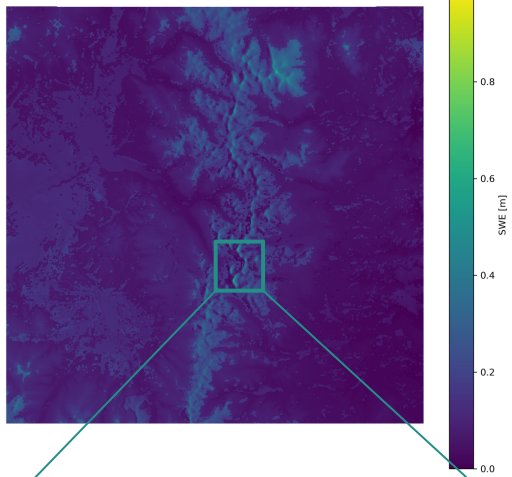

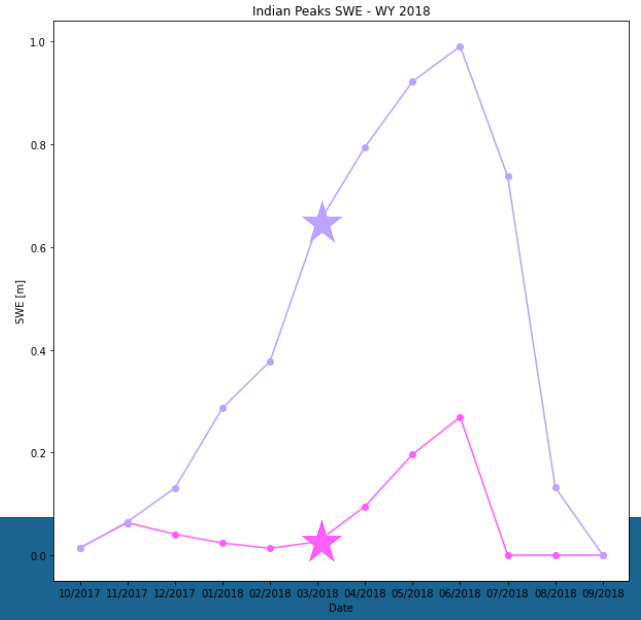

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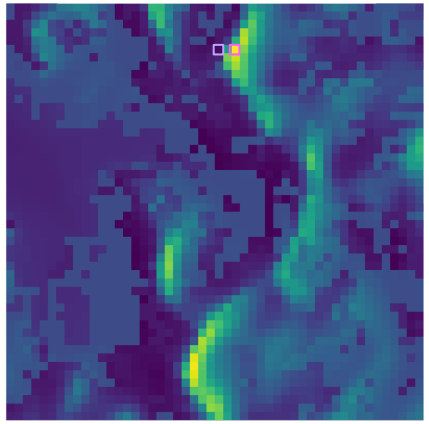
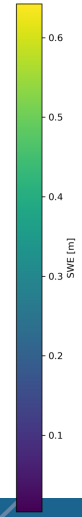
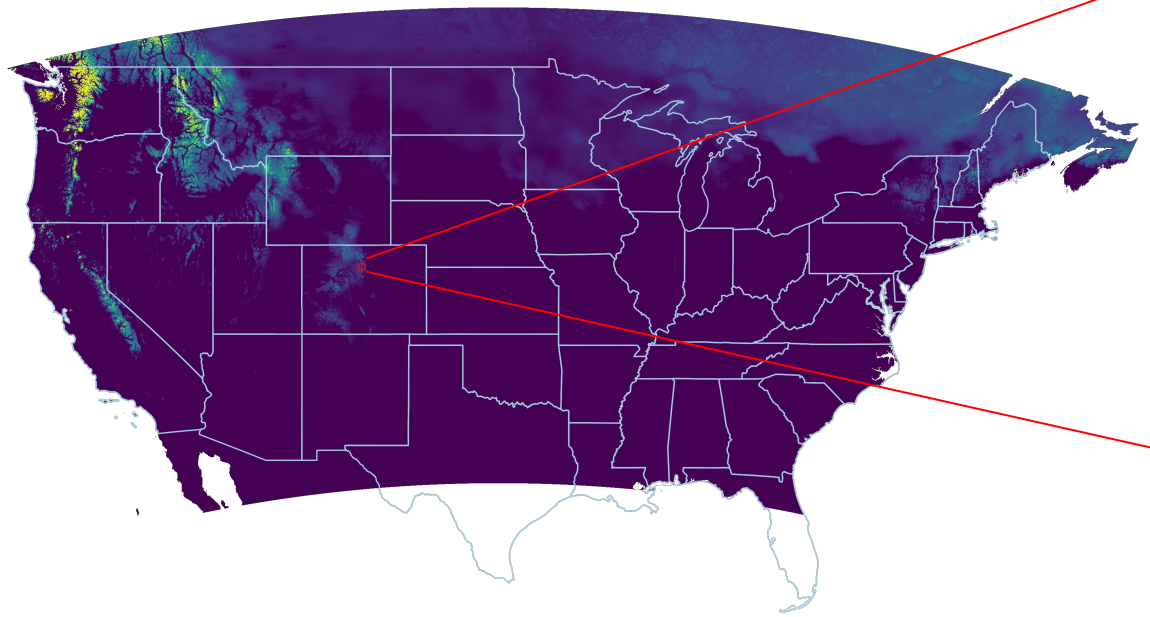
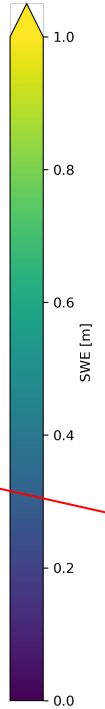




CONUS SWE April 1st , 2018





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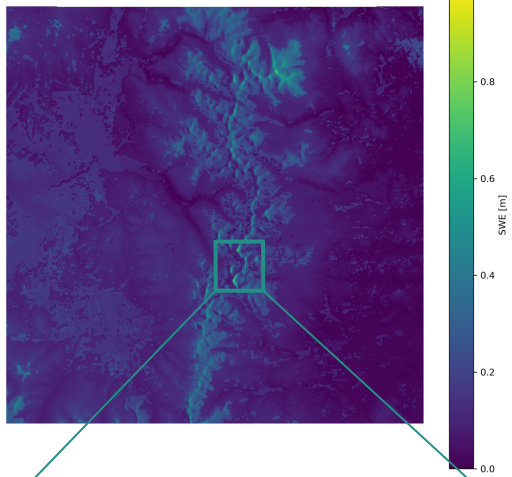

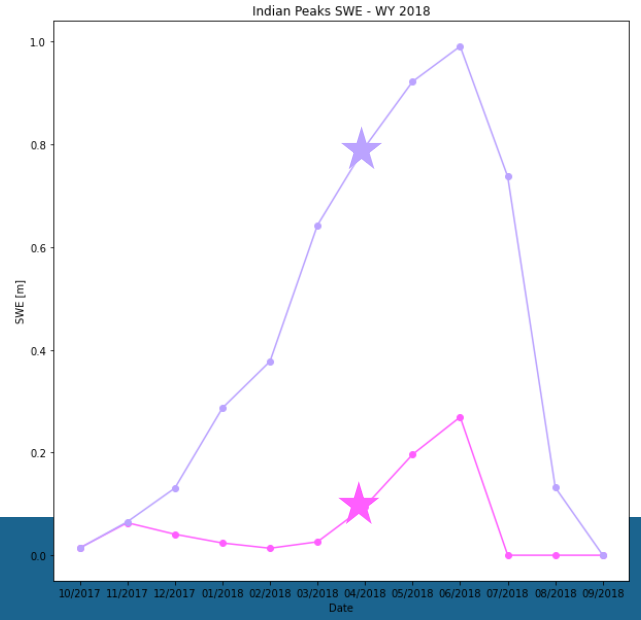

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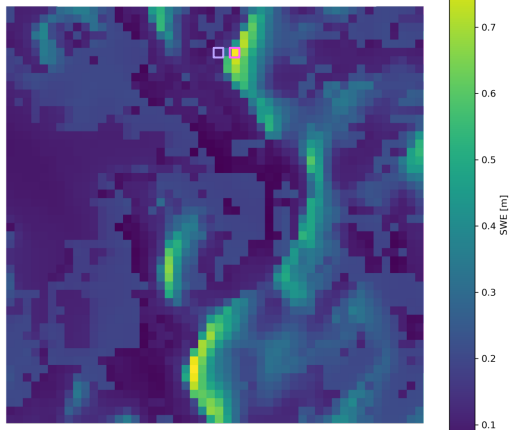

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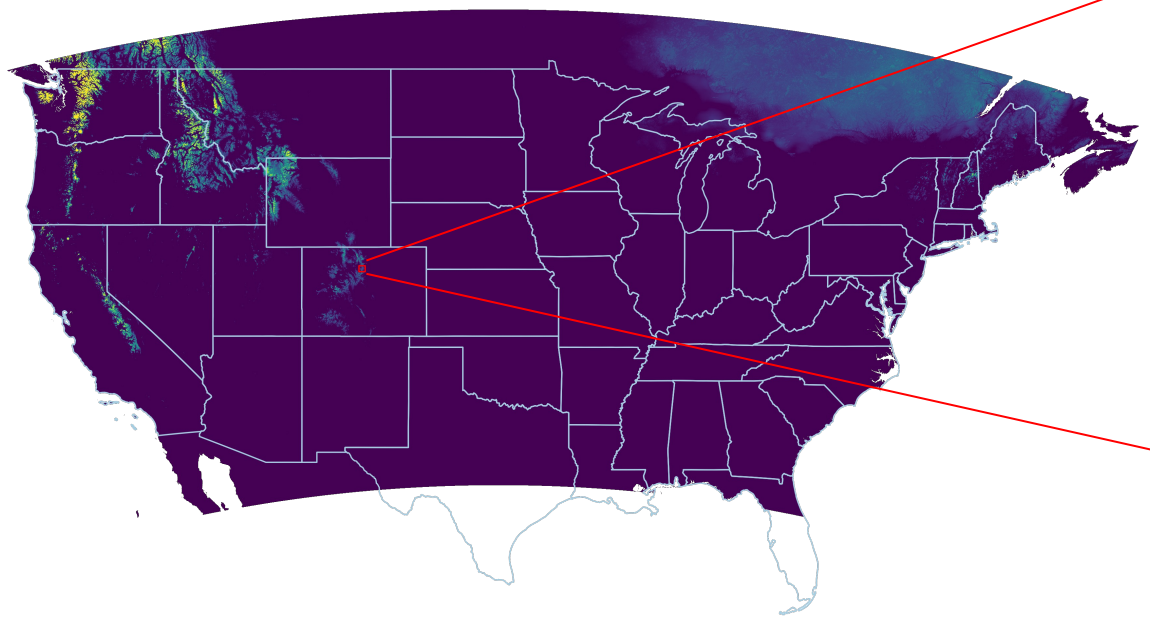
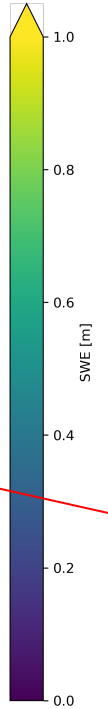
CONUS SWE May 1st , 2018





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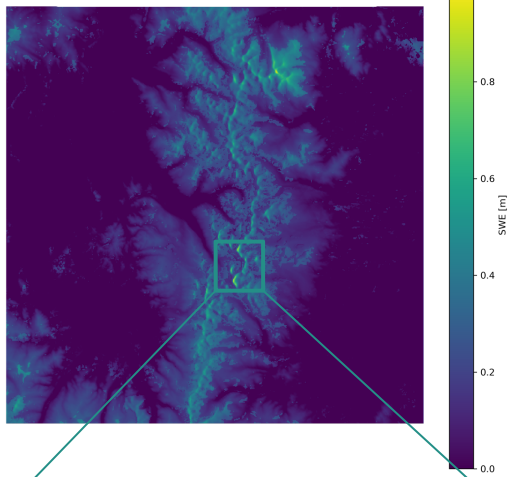

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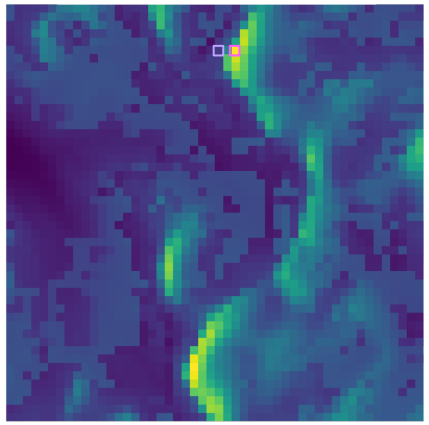

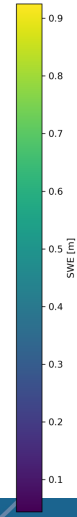

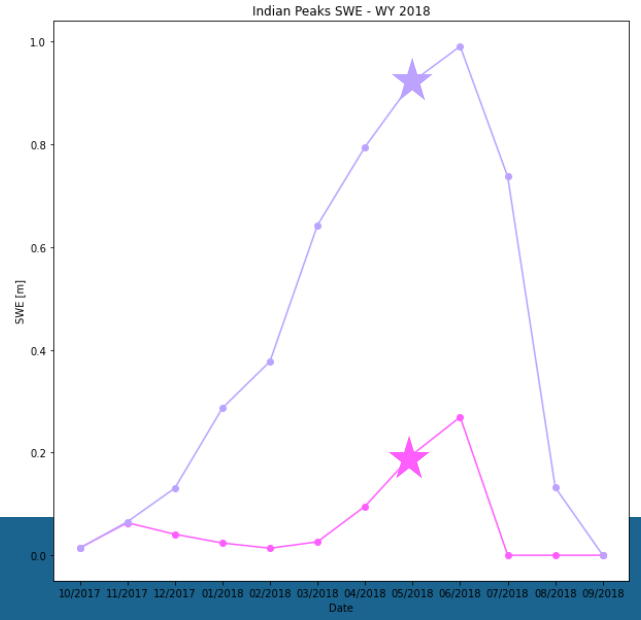

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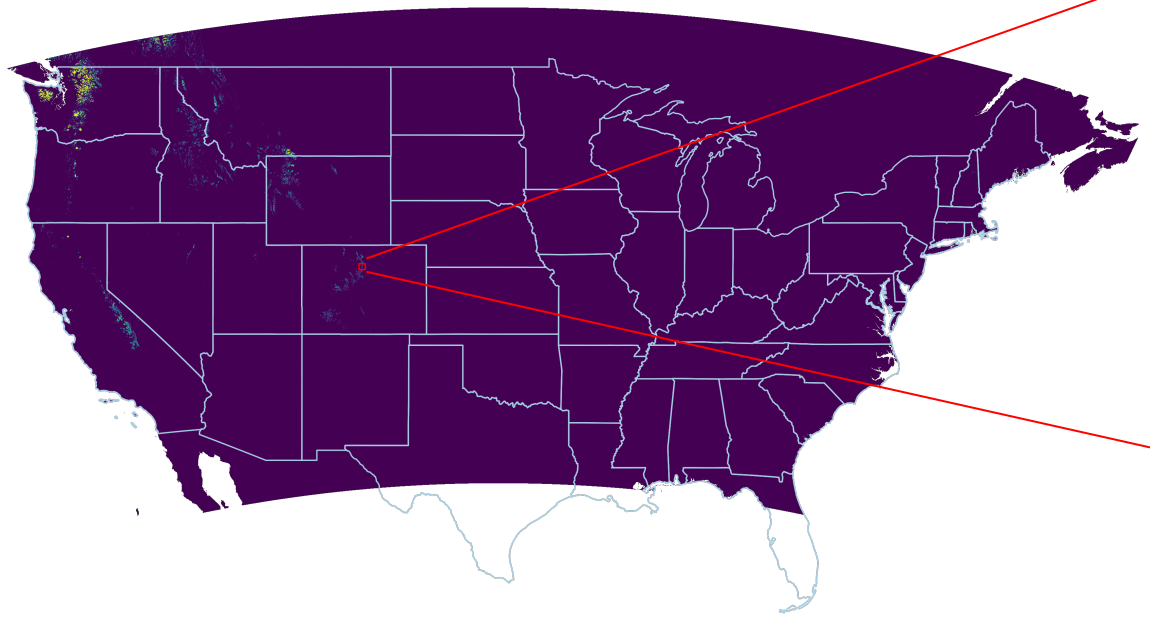
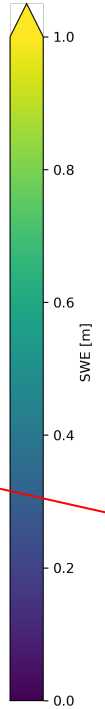
CONUS SWE June 1st , 2018





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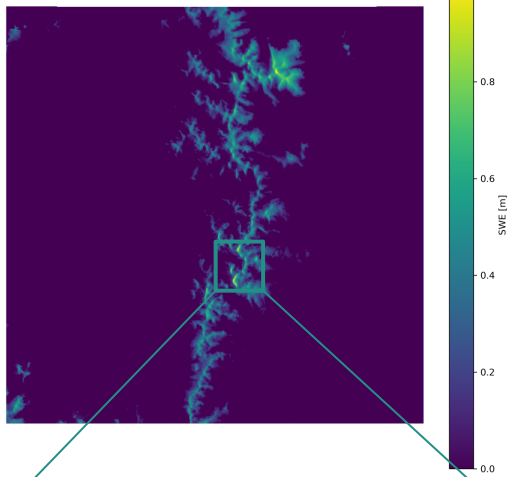

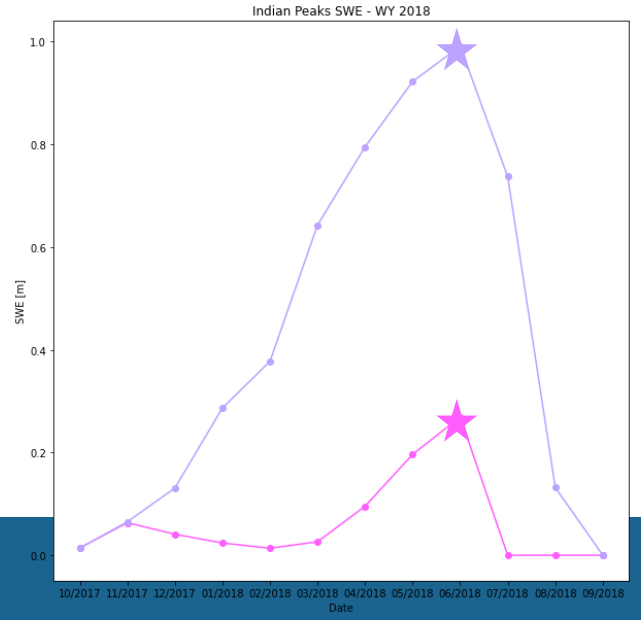

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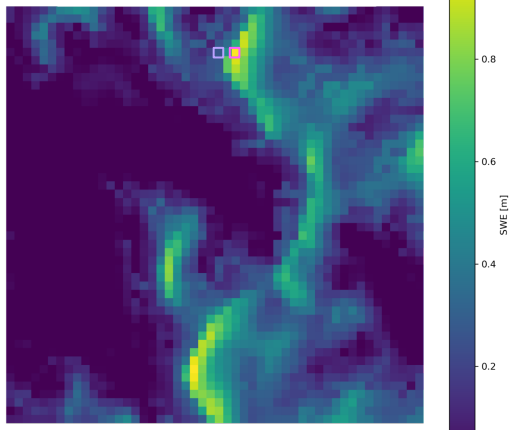

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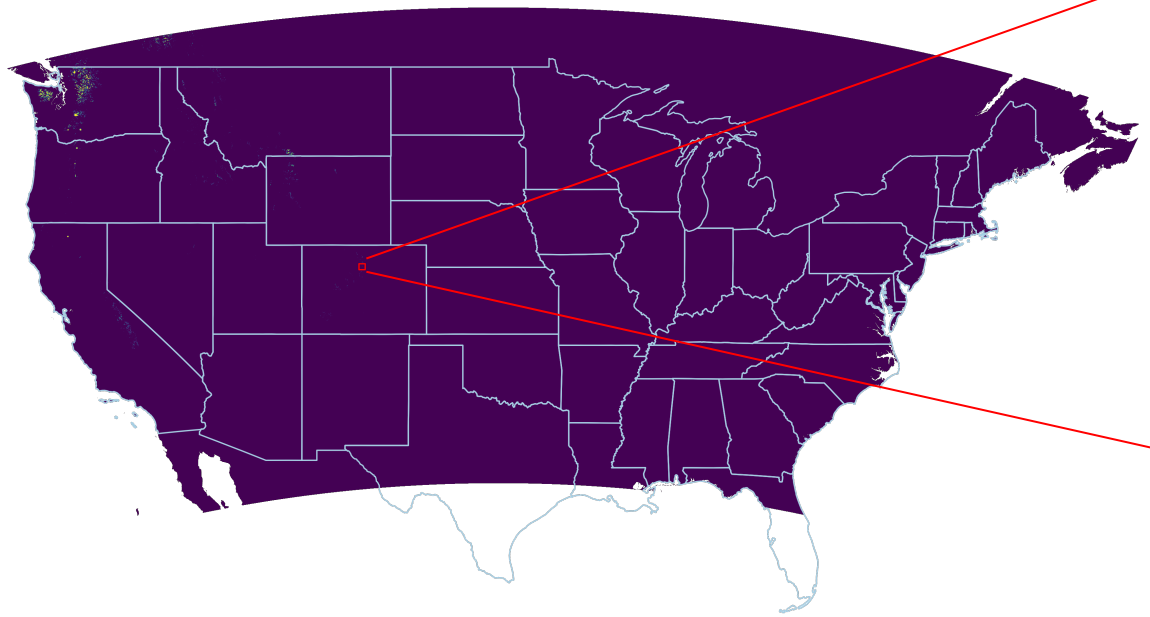
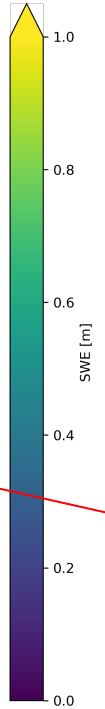
CONUS SWE July 1st , 2018





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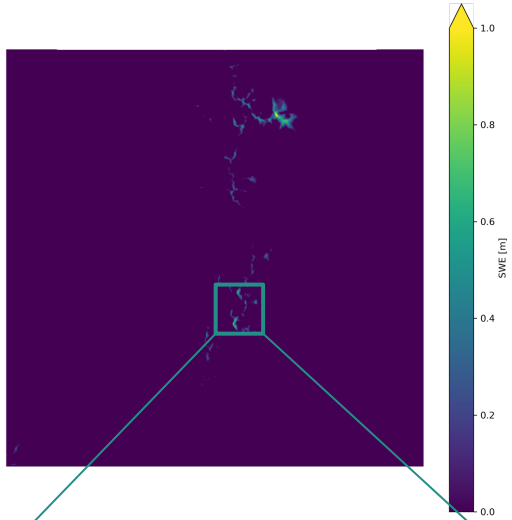
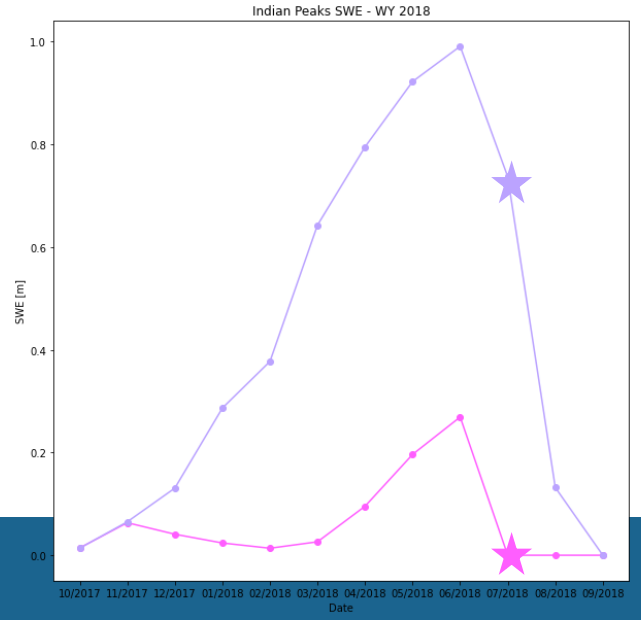
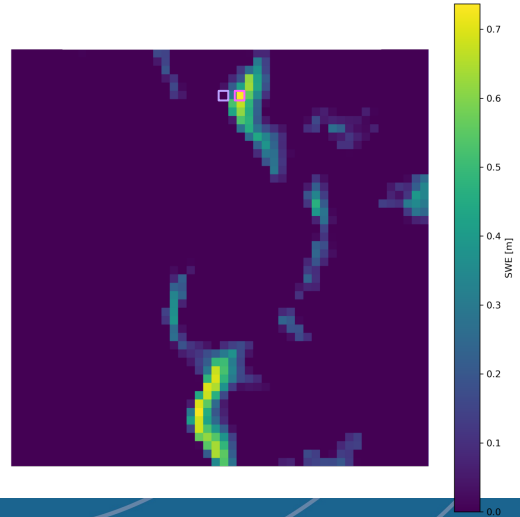




Domain Zoom 25 km²



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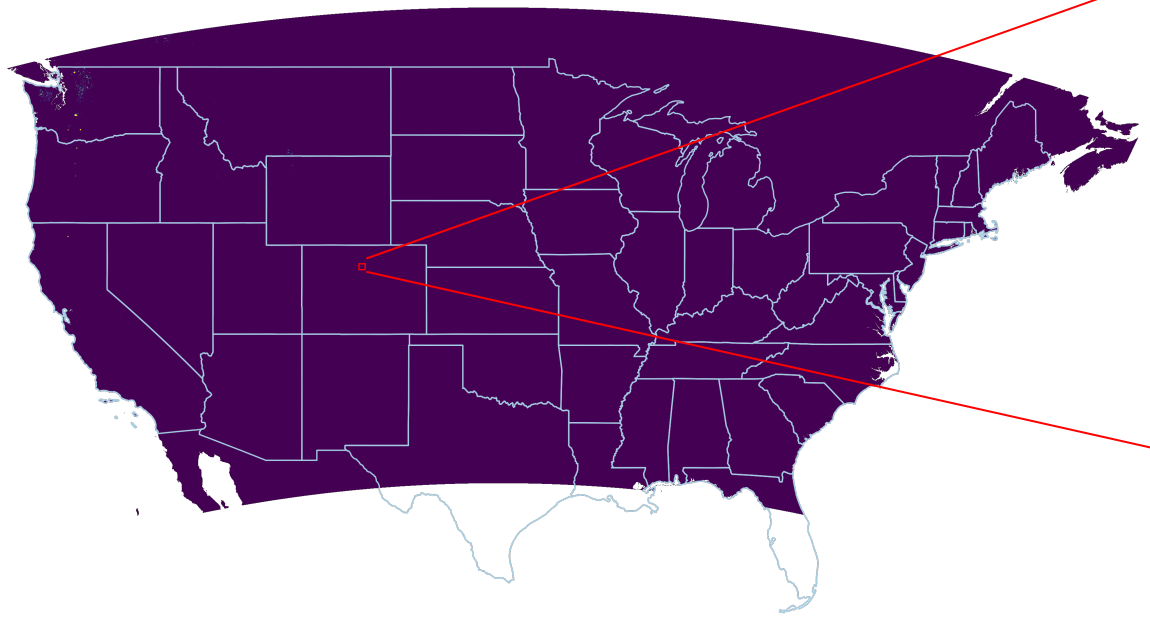
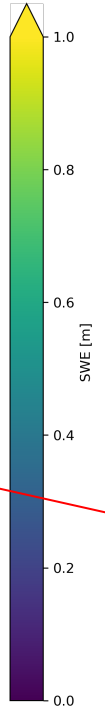
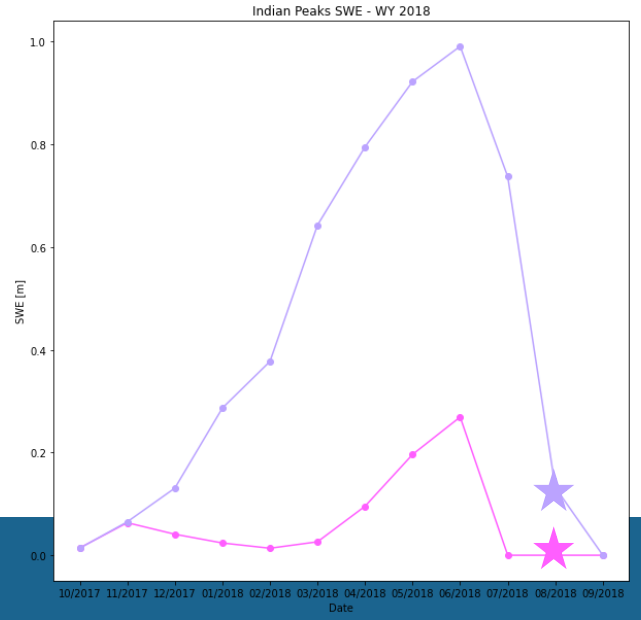
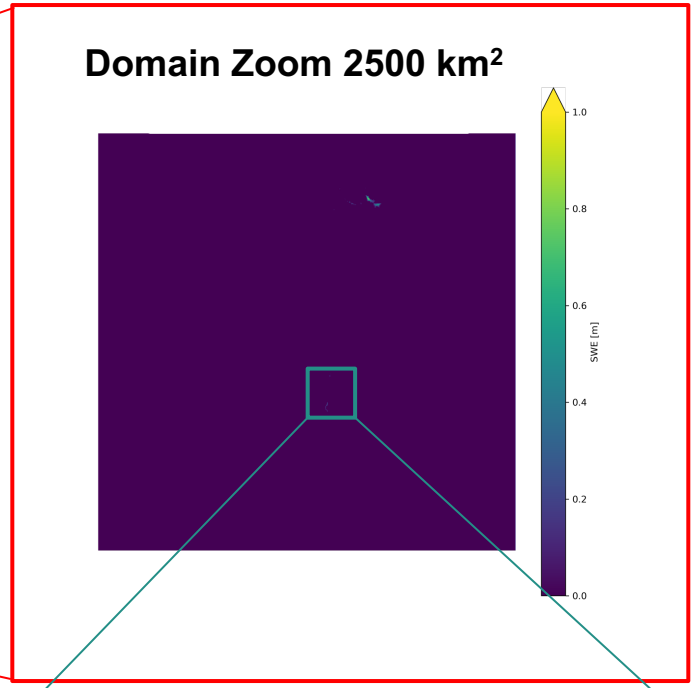
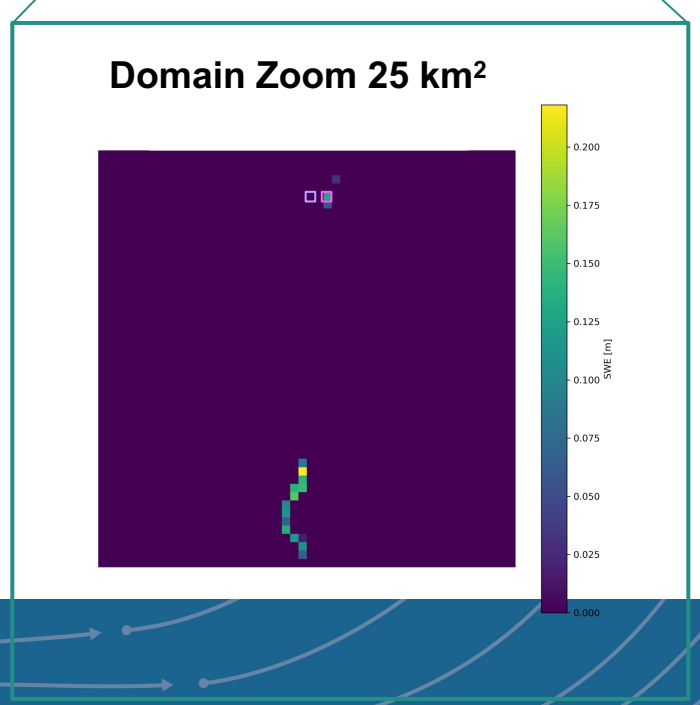
CONUS SWE August 1st , 2018











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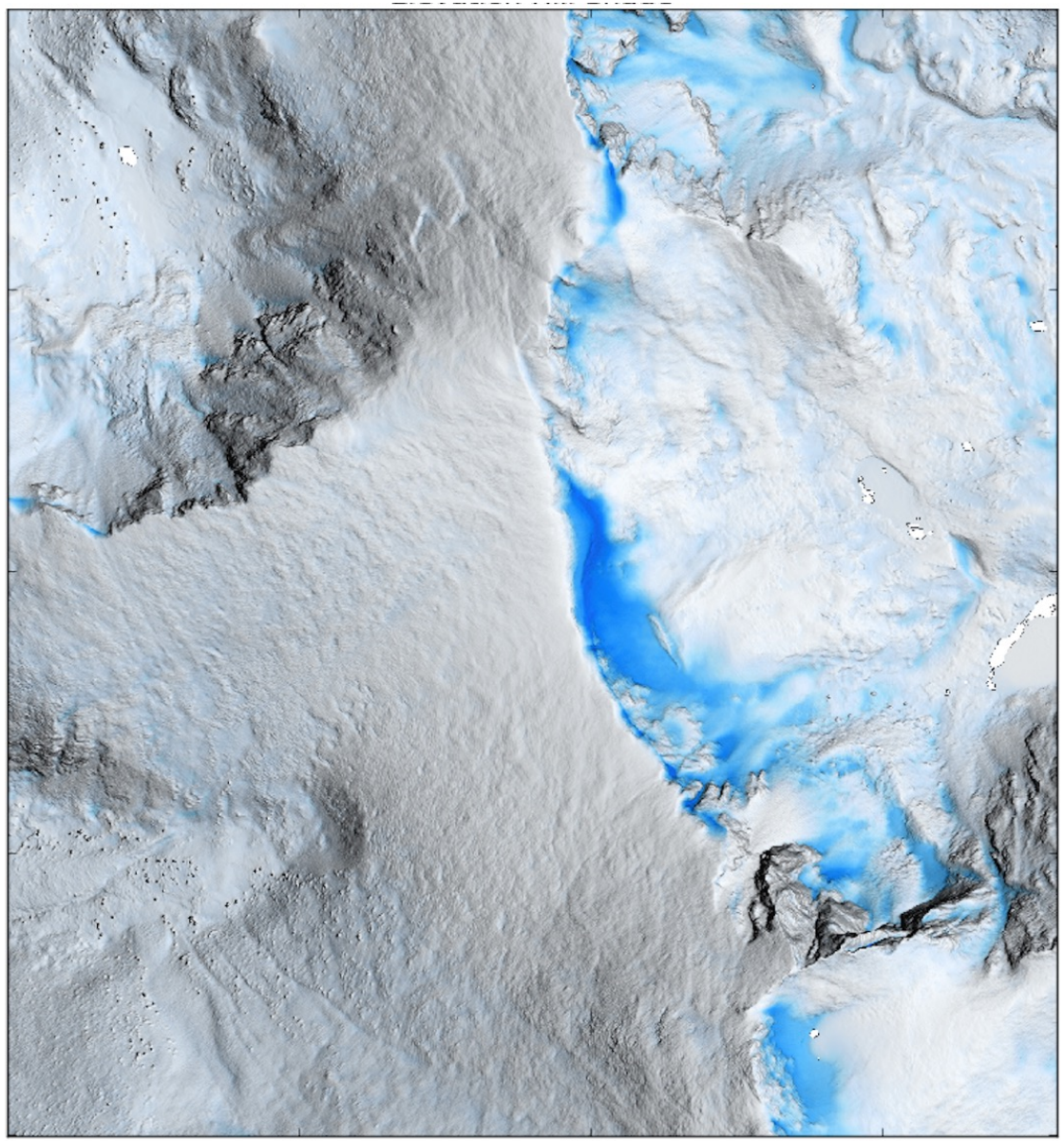

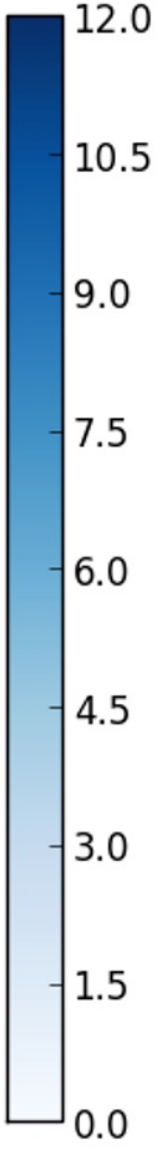
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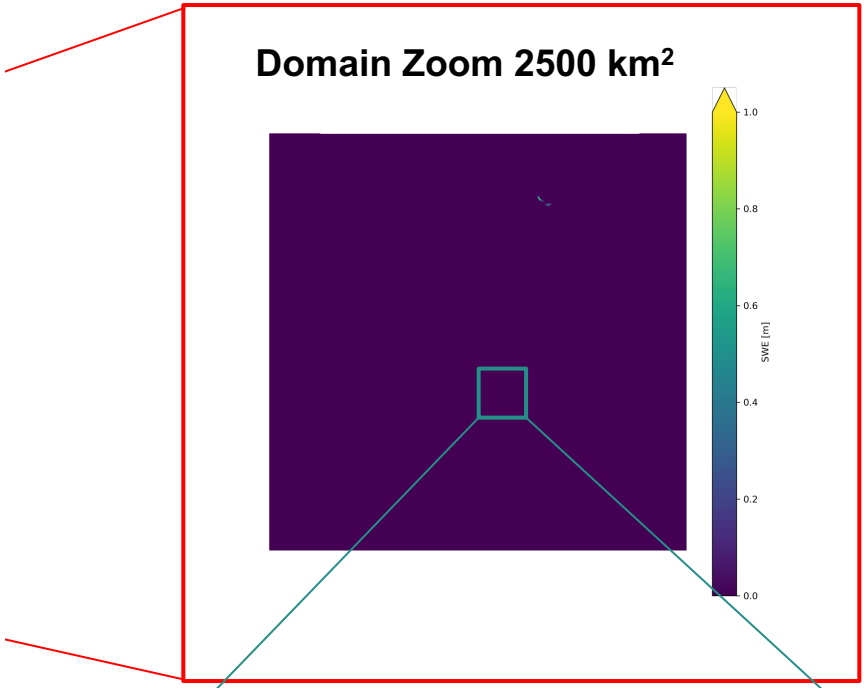
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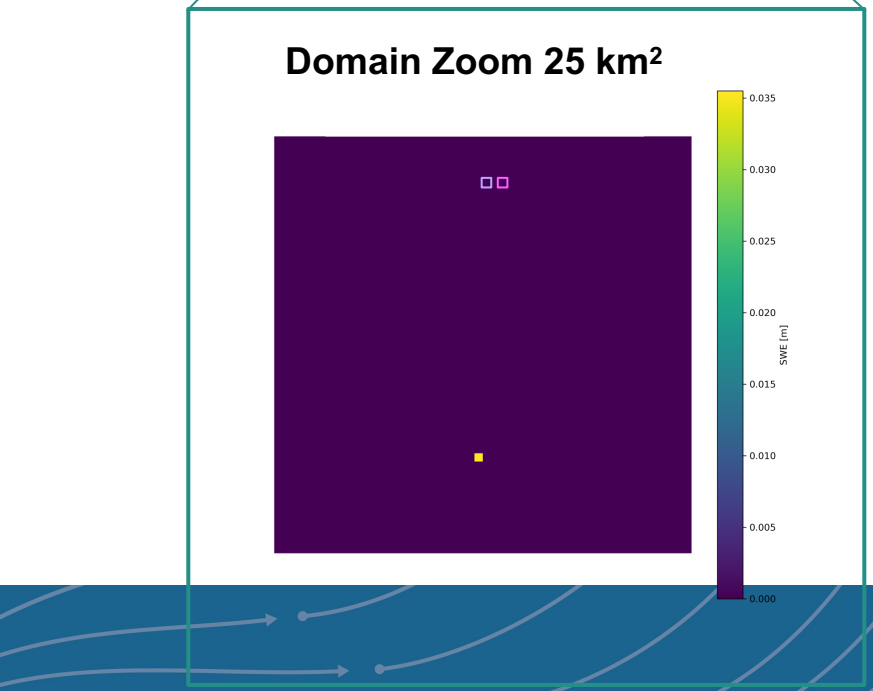
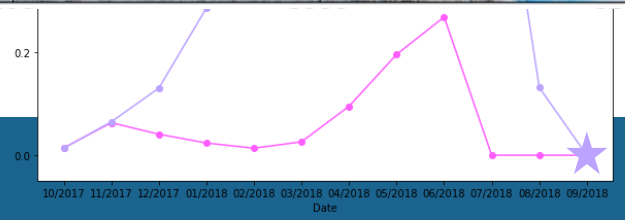
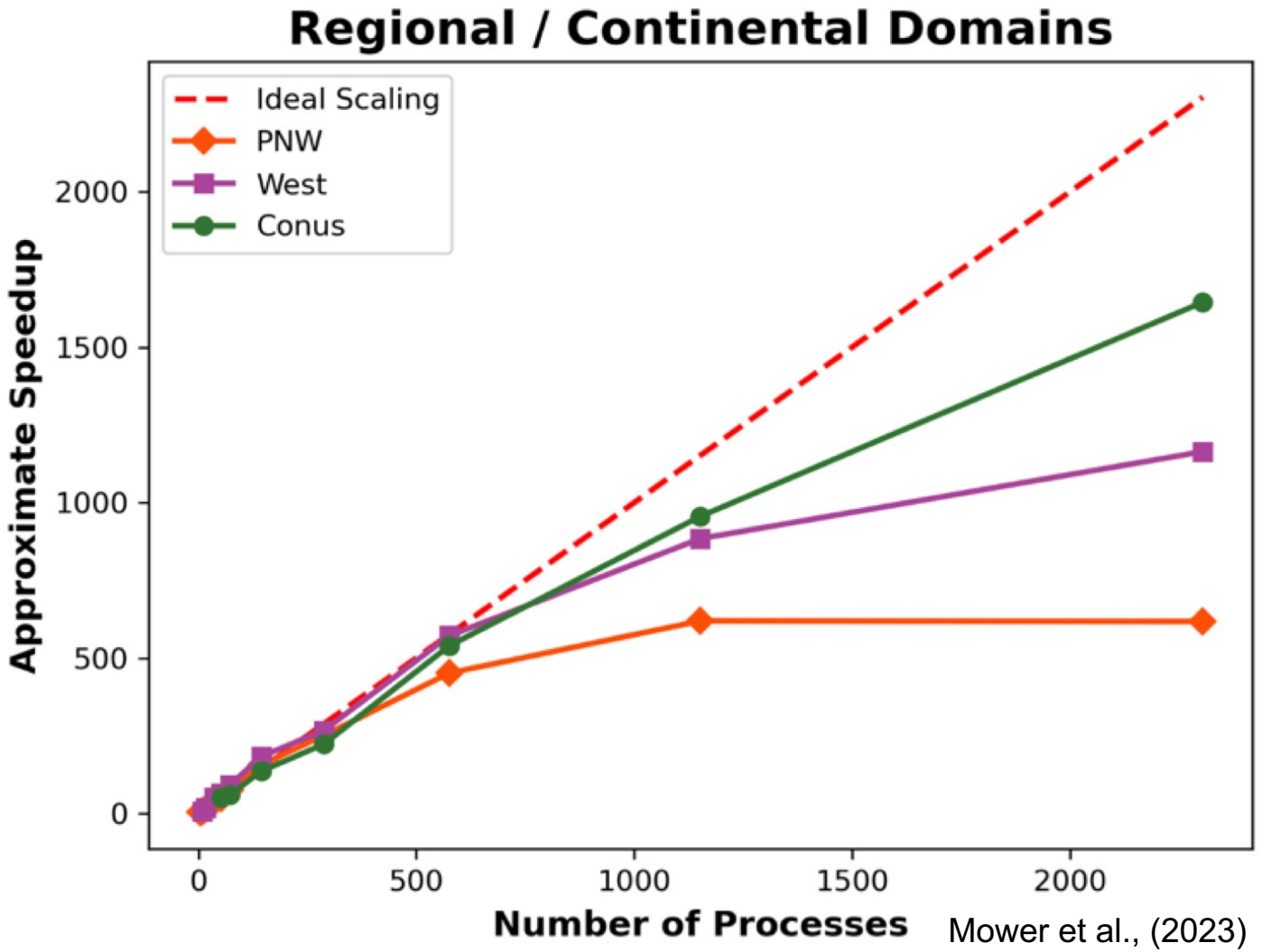

Domain Zoom 25 km²
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0.000
SWE [m]


0.2
0.0
10/2017 11/2017 12/2017 01/2018 02/2018 03/2018 04/2018 05/2018 06/2018 07/2018 08/2018 09/2018
Date

NCAR
UCAR

Parallelization of SnowModel

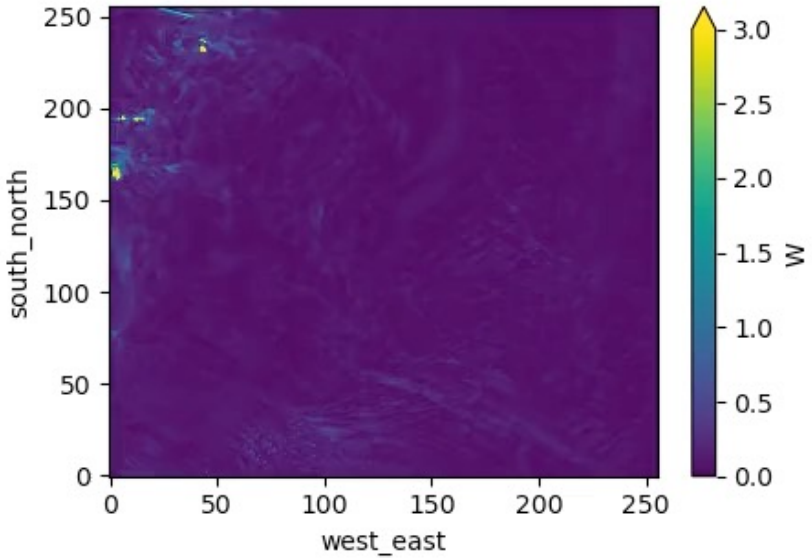
- One of the best high-res snow models in the world
- One of the only snow models that transport snow in the wind
- Parallelization of legacy fortran code
- Mix of F77-F90
- Use of coarray fortran enabled an early career scientist (and now PhD student) to parallelize code efficiently



Mower et al., (2023)

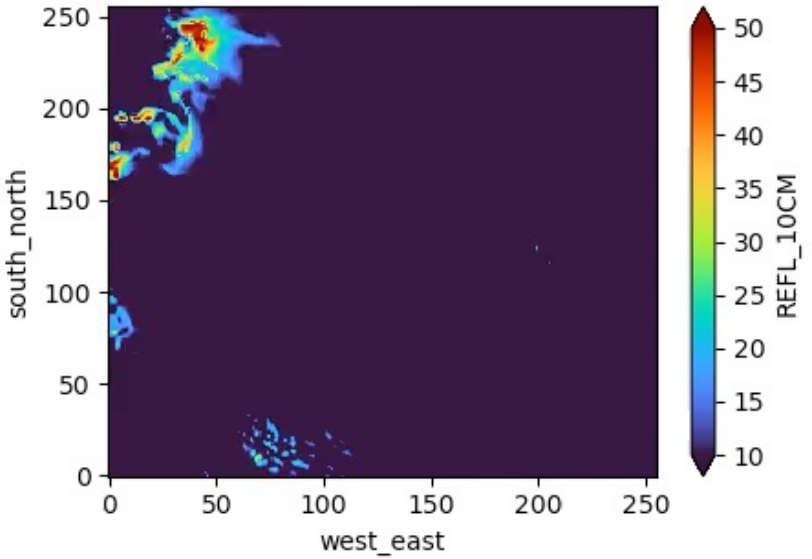
Learning from Radar data

- Radar spatial patterns contain information about storm dynamics
- Radar observations are assimilated into state of the art atmospheric models
  - But they don't know what the patterns mean
- Leveraging HPC or ML should enable greater information



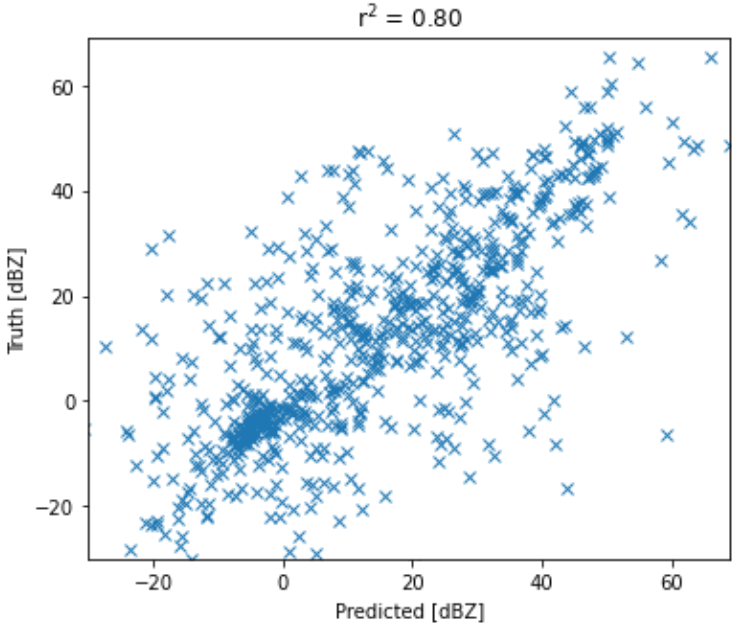
Simulated Radar Reflectivity

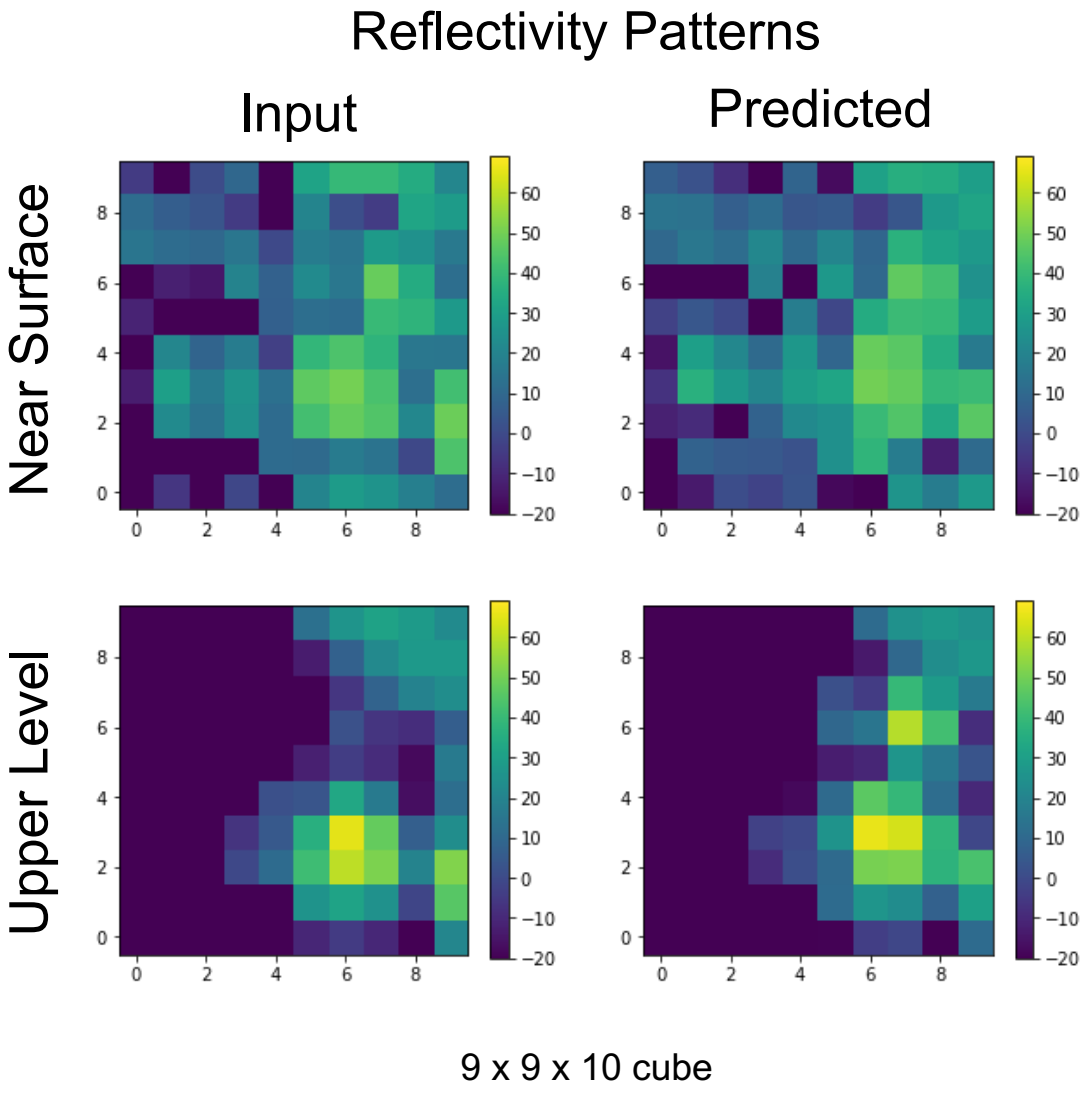
Simulated Vertical Wind Speed



Spatial Analog Machine-Learning Approach

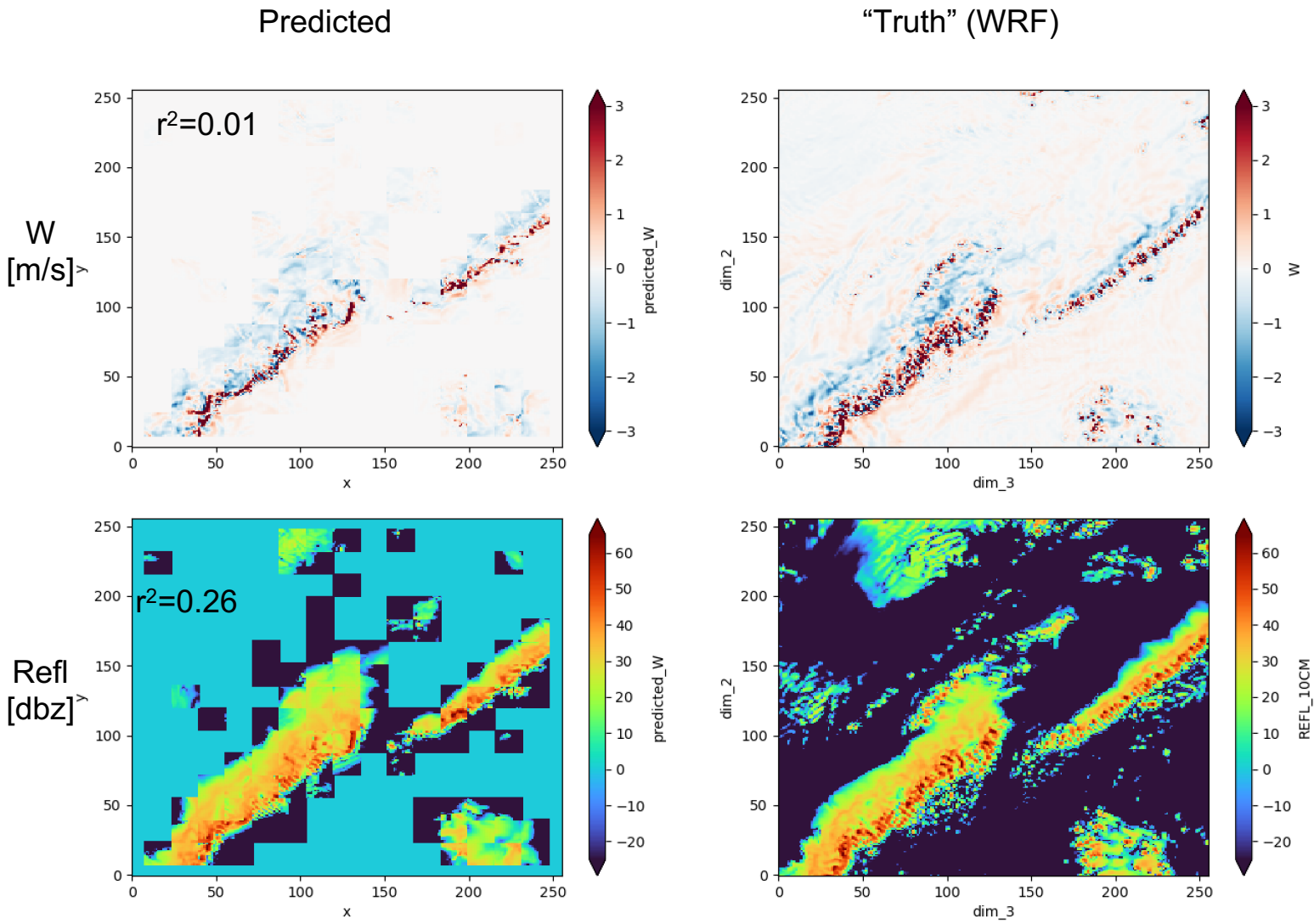
- Benefits from **big** data
- Selecting using 3-D spatial patterns
- Chop domain into 9x9x10 data cubes
- Search for best matches from archive
- Single cases promising but scaling is challenging





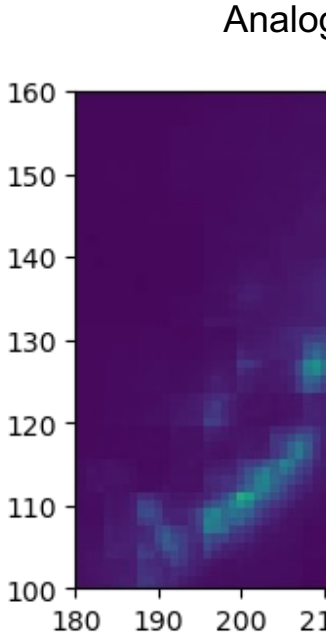
Scaled up Shallow Learning Approach

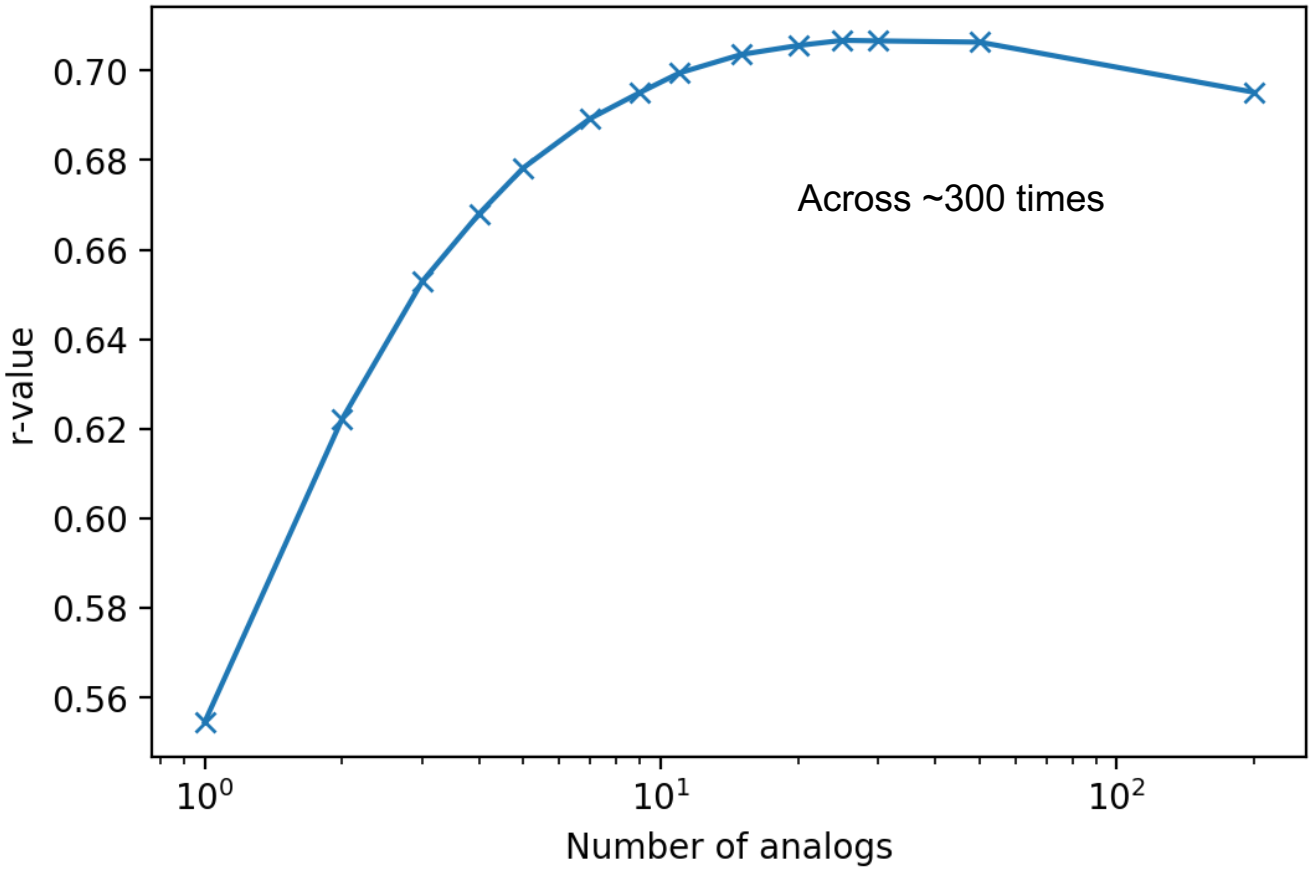
- Scaling across multiple nodes to process
  - Searching ~500,000 possible matches for each of ~500,000 16x16x5 patches
- Initial analog patch investigation
  - Note “blocky” nature
  - No predictions outside of blocks
  - W-field has strong isolated updrafts with associated trailing subsidence
- Error derived from goodness of fit in reflectivity only
  - Even so, where errors are larger, W-fields disagree more
- Need to scale up further… now running ~100,000,000 possible patches

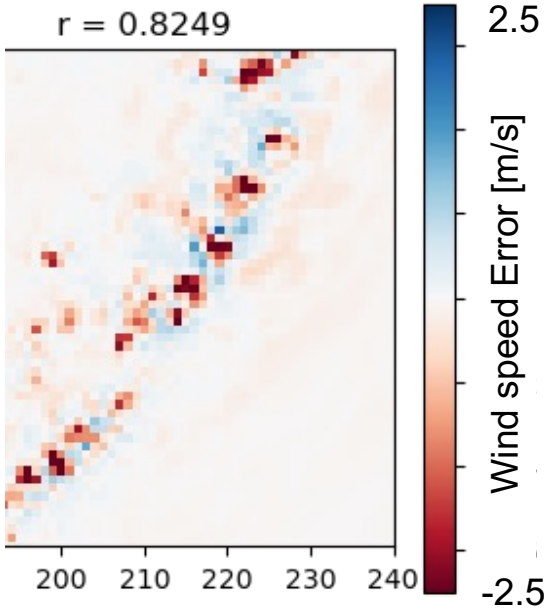


Skill of spatial analogs

- Increasing
- Increasing magnitudes

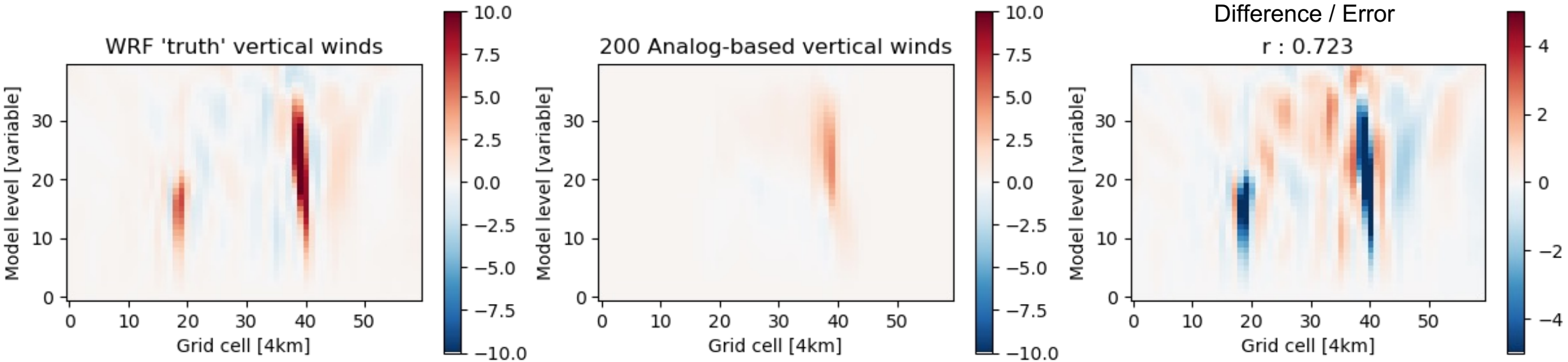


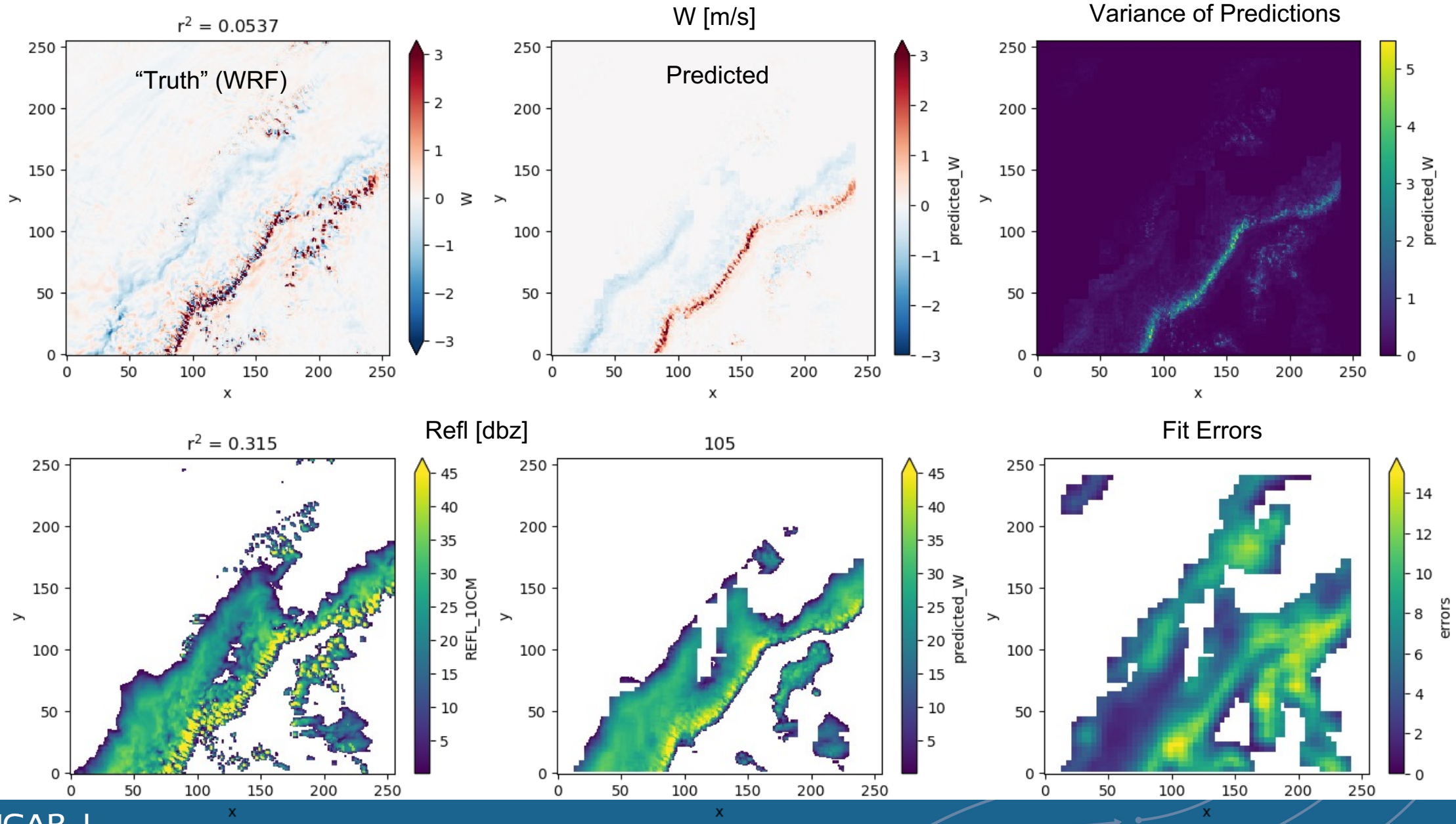




Spatial Analog 3D wind field

- Spatial analogs can provide 3D wind fields
- But DA tests with 3D w from WRF did bad things…

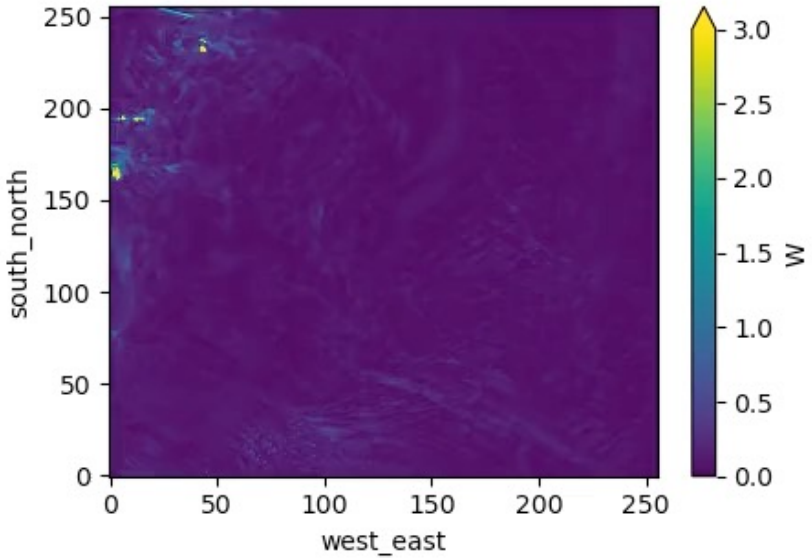



W [m/s]
Variance of Predictions
r^2 = 0.0537
"Truth" (WRF)
Predicted
Refl [dbz]
Fit Errors
r^2 = 0.315
105
x
y
W
predicted_W
REFL_10CM
errors

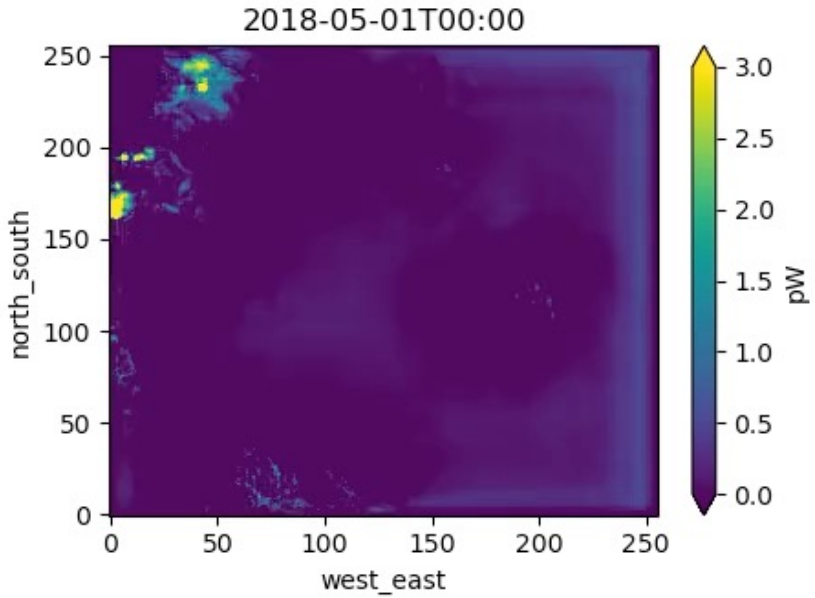
Unet results

- WRF extremes are larger
- UNET is smoother (larger areas with “high” values)
  - Same problem as shallow ML model

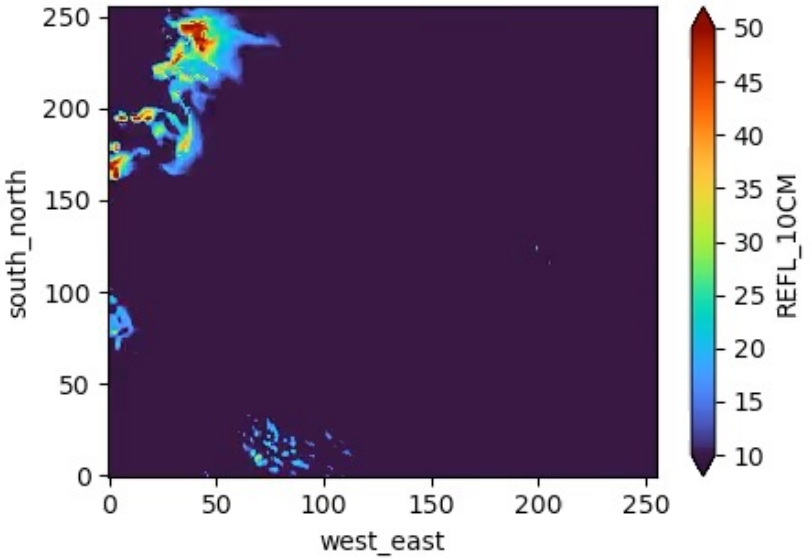
WRF w



UNET predicted-w



WRF reflectivity



Whither PGAS / ATM in an AI world?

- As ML advances, more HPC applications are “written” in Pytorch / Keras
- ML applications “easy” to port to GPUs, TPUs, WaferscaleEngine, and other accelerators
- Multi-node GPU utilization can remain challenging
- ~~Young~~ programmers are lazy
  - Adapt ATM techniques for their world
- ~~Young~~ ~~ML~~ programmers like python
  - Push ATM paradigms for ~~fortran, c++, chapel,~~ python?
  - Think outside the box, no longer “just” communication, e.g. Dask task-graphs

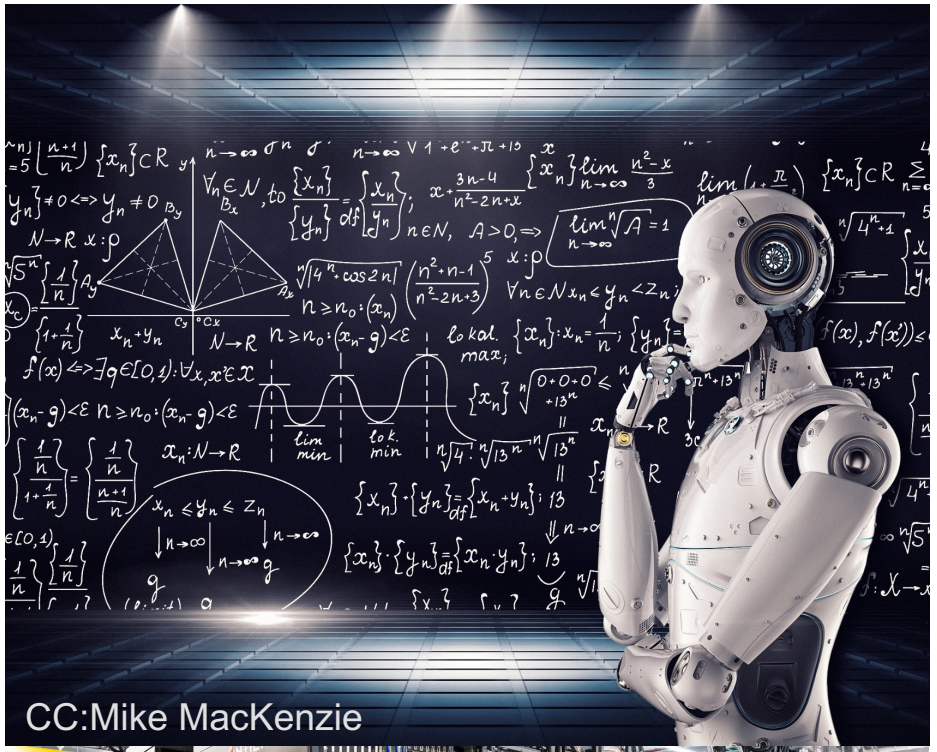
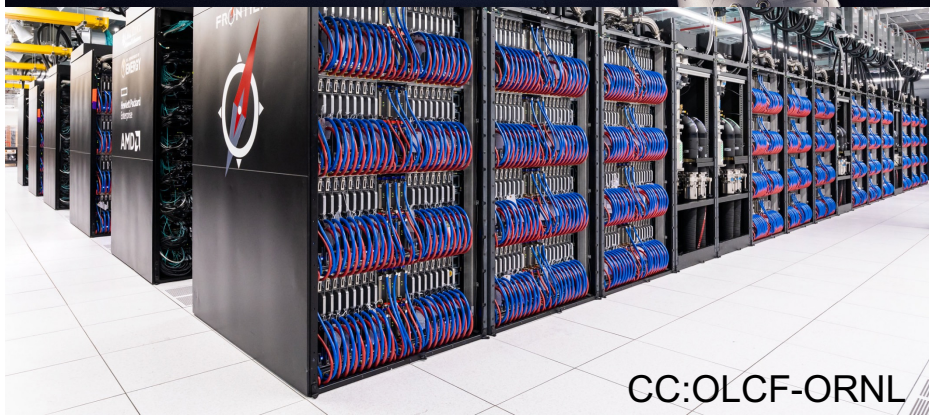


Image via www.vpnsrus.com



Trials and Tribulations (and Joys) of Developing with Coarray Fortran

- Simple communication API
- Early career scientists / students have parallelized real-world applications that perform at scale (thousands of cores)
- Not all compilers support coarrays
- Those that support coarrays have issues
  - Memory limits
  - Speed
  - Documentation
- Issues getting support from HPC centers leaves a bad taste in the mouth