OPTIMIZING FOR THE CLOUD

Facilitating use of challenging datasets using Kerchunk and Dask



I IOOS

P OFFICE OF WATER PREDICTION

> MAKING COMPLEX EASY





REACHING FOR THE CLOUD

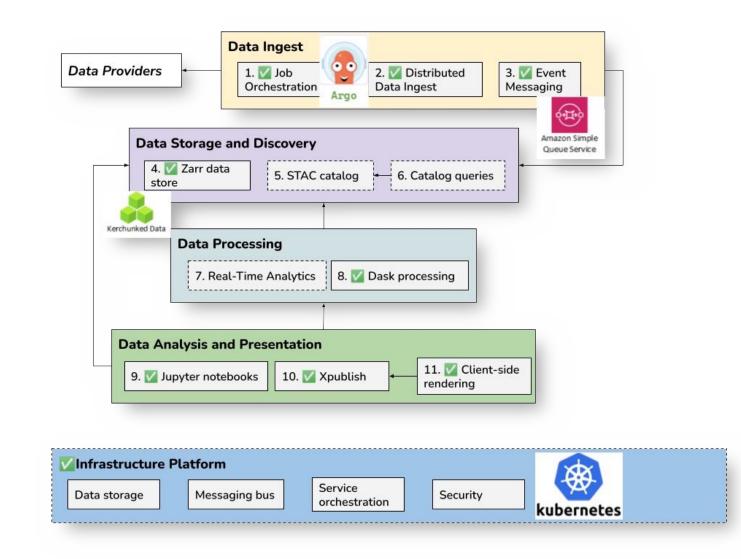
Architecting a Cloud-Native Service-Based Ecosystem for DMAC

- Goal: increase the use of IOOS data and promote connections to other disciplines by lowering the barriers for entry
- Objectives:
 - understand the current state, challenges, and opportunities
 - develop a roadmap and proposed architecture
 - prototypes and demonstration datasets

Prototype Roadmap

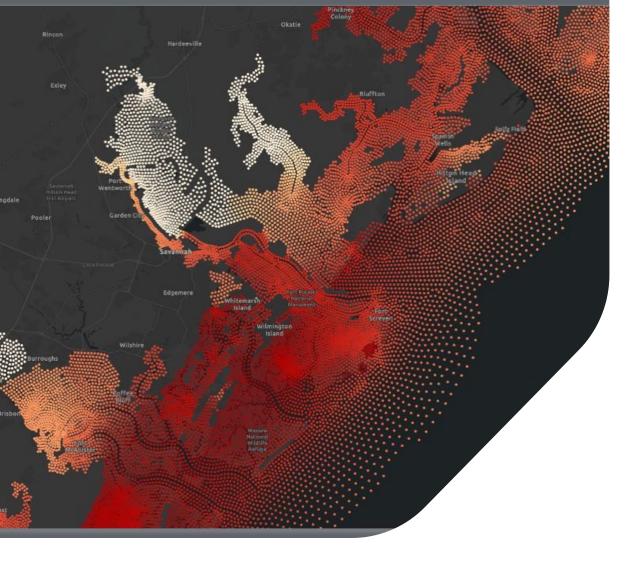
Workflow Components

- Ingest
- Storage and discovery
- Processing
- Analysis & Presentation



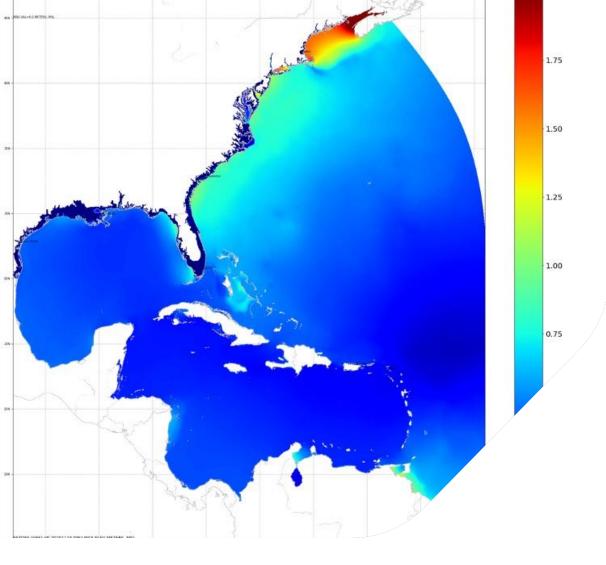
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Case Study #1



National Coastal Data Information System (NCDIS) Multi-decadal Year Reanalysis

- Long-term Reanalysis of Water Levels & Waves
- Integrating models & observations to predict flooding between tide stations
- Fills extensive gaps between observation locations



National Coastal Data Information System (NCDIS) 40 Year Reanalysis

- Atlantic reanalysis uses the HSOFS mesh (~1.8 million nodes)
 - 40 years of hourly data every 500m along the coast, including within bays, estuaries, and coastal river mouth entrances
 - ~70 TB of storage
- Pacific reanalysis uses the GSTOFS mesh (~450k-2.2m nodes)
 - Resolution down to 80 m for Hawaii and US West Coast
 - 90-120 m for Pacific Islands
 - ~300 TB of storage

Case Study #1: NCDIS Reanalysis

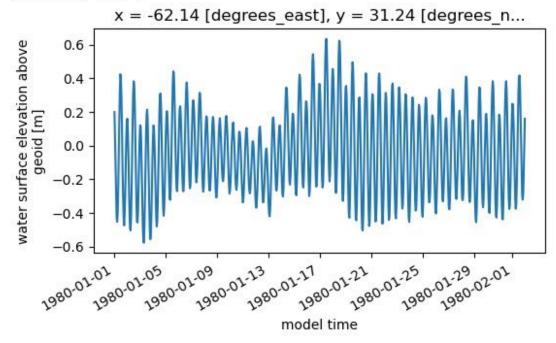
- ADCIRC output for ~1.8 million nodes over a 40-year period ~ 70 TB of data (5.5 TB for water level)
- Original data had a chunk size of ~1.8 GB which was leading to slow access times
- Rechunked the underlying netCDF to manageable chunk sizes
- Leveraging Kerchunk and intake catalogs
- Much faster access time for both extracting a timeseries and the entire grid

```
: catalog = intake.open_catalog('s3://ncdis-ra/ncdis_intake.yml')
  Intake Catalog
                                                                        ds = catalog['NCDIS-WaterLevel-1979-2021'].to dask()
sources:
                                                                        ds.zeta
 NCDIS-WaterLevel-1979-2021:
   driver: intake xarray.xzarr.ZarrSource
                                                                     xarray.DataArray 'zeta' (time: 376943, node: 1813443)
   description: 'NCDIS Water Level, 1979 - 2021'
   args:
     consolidated: False
                                                                       2
      chunks:
                                                                                               Array
                                                                                                             Chunk
       time: 240
                                                                                                                                        37694:
       node: 160000
                                                                                             4.97 TiB
                                                                                                         292.97 MiB
                                                                             Bytes
     urlpath: "reference://"
     storage options:
                                                                            Shape (376943, 1813443)
                                                                                                       (240, 160000)
       fo: 's3://ncdis-ra/jsons/fort.63_post_1979-2021.json'
                                                                                                                          1813443
       remote options:
                                                                                          18853 Tasks
                                                                                                       18852 Chunks
                                                                             Count
          anon: false
        remote protocol: s3
                                                                                              float64 numpy.ndarray
                                                                             Type
```

Case Study #1: NCDIS Reanalysis

%%time

CPU times: user 300 ms, sys: 16.7 ms, total: 317 ms Wall time: 2.24 s

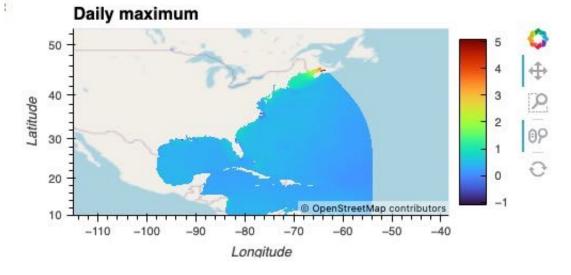


2 s to extra a one-month time series3 m to extract 141 annual time series6 s to compute the daily max for the grid

%time

zeta_sel = ds['zeta'].sel(time=slice('1985-01-01','1985-01-01'))
grid_max = zeta_sel.max(dim='time').load()
plot_gridded_output("Daily maximum", grid_max, "turbo", 500,250)

CPU times: user 1.18 s, sys: 285 ms, total: 1.46 s Wall time: 6.31 s



Case Study #1: NCDIS Reanalysis

- Requirements for post-processing and product generation
 - Pull 40-year variables (time series or max values) on the 500-m grid
 - Pull 40-year variables (time series or max values) on the nodes
 - Validate model output alongside NWLON, USGS, and USACE water level observations
 - Calculate daily maximums and monthly means
 - Regression analysis, histograms, trends,
- Dask and Nebari
 - Deployed Nebari in AWS
 - Gives access to a Kubernetes cluster without having to manually configure it
 - Utilizes Dask Gateway so work can be scaled across the cluster

National Water Model

Case Study #2

Case Study #2: National Water Model

- Supplements traditional NWS river forecasts
- Streamflow and discharge forecast for 2.7 million reaches
- Additional hydrologic information on 1km, 250m, & 100m grids
- Updated hourly
- ~5 GB of data per day
- NOT gridded...networked

Current River Forecast Points (~3,600)



- Released original API c. 2019
 - Queries the NODD S3 bucket
 - Temporal, spatial, and variable subsetting
 - Terminal point and feature ID filters

NWM Streamflow Output Points (~2.7 mil)





National Water Model Forecast

- Make access easier and more performant
- Use the files that are already stored in the NODD AWS bucket
 - Avoid duplicating the data
 - Each forecast hour is written to a different netCDF file in the AWS bucket
 - Latitude / longitude information not stored with the model output
 - Network information not stored with the model output



National Water Model Forecast

Completed Tasks

- Transform model output in NODD bucket to cloud optimized format
- Create a net CDF file with the lat/lon info
- Create virtual dataset by merging Kerchunked output and lat/long data
- Create intake catalog to allow data access w/o knowledge of underlying data file format

Remaining Tasks

- Workflow to automatically kerchunk files when they arrive in the NODD AWS Bucket
- Directed graph to allow stream tracing

Case Study #2: National Water Model

Example 1:

- Open the dataset with python and view structure

```
catalog = intake.open_catalog('s3://nextgen-dmac/nwm/nwm_intake.yml')
ds = catalog['NWM_Data'].to_dask()
```

ds

xarray.Dataset

▶ Dimensions:	(time: 18, feature	e_id: 2776738, re	ference_time: 1)	
Coordinates:				
feature_id	(feature_id)	float64	101.0 179.0 1.18e+09 1.18e+09	8
latitude	(feature_id)	float32	dask.array <chunksize=(2776738,), met<="" td=""><td>8</td></chunksize=(2776738,),>	8
longitude	(feature_id)	float32	dask.array <chunksize=(2776738,), met<="" td=""><td>8</td></chunksize=(2776738,),>	8
reference_time	(reference_time)	datetime64[ns]	2023-06-12	89
time	(time)	datetime64[ns]	2023-06-12T01:00:00 2023-06	8
Data variables:				
crs	(time)	object	dask.array <chunksize=(1,), meta="np.nd</td"><td>8</td></chunksize=(1,),>	8
nudge	(time, feature_id)	float64	dask.array <chunksize=(1, 2776738),="" m<="" td=""><td>8</td></chunksize=(1,>	8
qBtmVertRunoff	(time, feature_id)	float64	dask.array <chunksize=(1, 2776738),="" m<="" td=""><td>8</td></chunksize=(1,>	8
qBucket	(time, feature_id)	float64	dask.array <chunksize=(1, 2776738),="" m<="" td=""><td>8</td></chunksize=(1,>	8
qSfcLatRunoff	(time, feature_id)	float64	dask.array <chunksize=(1, 2776738),="" m<="" td=""><td>8</td></chunksize=(1,>	8
streamflow	(time, feature_id)	float64	dask.array <chunksize=(1, 2776738),="" m<="" td=""><td>8</td></chunksize=(1,>	8
terminal	(feature_id)	float64	dask.array <chunksize=(2776738,), met<="" td=""><td></td></chunksize=(2776738,),>	
velocity	(time, feature_id)	float64	dask.array <chunksize=(1, 2776738),="" m<="" td=""><td>8</td></chunksize=(1,>	8

Example 2:

- Extract all data in an AOI at a specific time and compute the maximum value

- Cloud optimized data makes accessing the data very performant
- This example took less than 2 seconds to complete

8	%time
10	on_min= -90.5777
la	at_min=35
10	on_max=-75
la	at_max=37
t	ime_s='2023-06-12T15:00'
i	ds = np.where((ds.longitude>=lon_min) &(ds.longitude<=lon_max) & (ds.latitude>=lat_min) & (ds.latitude <= lat_max))[0]
0.0	_subset = ds.streamflow.sel(time=time_s).isel(feature_id=ids) ax_val = s_subset.max().compute()
	rint("Maximum value: ",max val.values)

Maximum value: 7701.459827858955 CPU times: user 184 ms, sys: 7.94 ms, total: 192 ms Wall time: 1.68 s

Thanks for your time

For more information please contact:

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