

Meteorology and Air Quality Modeling Using the AWS Parallel Cluster Cloud Service

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Why does LADCO need cloud computing?

- Supplement/replace the LADCO local compute cluster
- Access scalable high performance computing (HPC) resources
- Circumvent IT barriers at state air programs
- Enable collaboration in modeling and data analysis across the Consortium





Modeling Platform As a Service (PaaS)

- A PaaS is a pre-configured system with all data, software, and computing capacity needed for an application
- AWS Parallel Cluster provisions computing as needed and to meet demand
- LADCO modeling cluster includes all libraries and modeling software: WRF, SMOKE, CMAQ, CAMx, AMET, NCL, VERDI, R





Why Amazon Web Services Parallel Cluster?

- LADCO developer had familiarity with computing @ AWS
- At the time of development, AWS CfnCluster project was migrating to Pcluster
- How it works?



Design your cluster Based on your application requirements, choose design options in the configuration wizard

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Launch your cluster Once you've configured your cluster, launch it by running the 'create' command



Log in to your cluster Once the cluster reaches the "CREATE COMPLETE" status, connect using your favorite SSH client



Submit job to your scheduler

Image courtesy of AWS

LADCO AWS Modeling Schematic



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LADCO Modeling Statistics @ AWS

Simulation	Simulation Period	EC2 Compute Instance	CPUs/ Run	Total CPUs	Hrs/ Run Day	CPU Costs (\$)	\$/Sim Day
WRF 12/4/1.33/1.33 Annual	15 days + 12 hour spin up	c4.2xlarge	48	1248	8	3,325	8.33
CAMx 12km 2016 and 2028	6 months + 10 day spin up	c4.2xlarge	64	256	1	2,220	2.81
CAMx 12km 2028 PSAT (28 srctags x N+S)	3 months + 10 day spin up	c4.2xlarge	96	384	4	3,830	9.22
CAMx 12km 2028 PSAT (31 src tags x N+S)	3 months + 10 day spin up	r5.2xlarge	96	384	4	3,210	7.74
CAMx 12km 2028 PSAT (24 region+src tags x N+S)	3 months + 10 day spin up	r5.2xlarge	96	288	6	3,860	9.53
CAMx 12km 2028 PSAT (25 region+src tags x N+S)	4 months + 10 day spin up	r5.2xlarge	96	384	5.5	2,420	5.83
CAMx 12km 2028 PSAT (25 region+src tags x Primary)	3 months + 10 day spin up	r4.16xlarge	96	384	6.5	4,825	11.63
CAMx 12km 2016 Annual	3 months + 10 day spin up	r4.16xlarge	64	256	1	1,160	2.80





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Notes on Data Management

- Automate workflows
 - Online EBS volumes are the most expensive storage unit, need to automate moving data between less expensive offline and more expensive online disks
- The AWS Simple Storage Solution (S3) is a relatively cheap place to store data, and it's great for transferring large volumes of data
 - Egress fees ~\$100/Tb to download
 - AWS Command Line Interface (CLI) uses multiple threads to transfer data, up and down from S3; terabyte scale electronic transfers are practical with S3
 - Example: > 4 Tb of WRF data downloaded by IL EPA in ~24 hours @ \$500



Key Outcomes

- All LADCO modeling on AWS is done using Spot Instances
 - Learned to read the AWS Spot Market to find available, lastgeneration instances
- AWS is a practical solution for meteorology and air quality modeling
 - Annual 12km U.S. CAMx simulation costs ~\$2.80/model day
 - Adding nested grids or instrumented models (i.e., PSAT) makes runs more expensive because they require more CPUhours
- Don't be afraid to scale up
 - Larger instances are more expensive per hour, but about the same cost per CPU-hour (the jobs run more quickly)
- LADCO invested ~\$20k over a year to develop modeling capabilities on AWS





Next Steps

• Optimize AWS costs

- Better manage offline and online storage costs
- Shut down our compute servers more often
- Collect more data points on best practices
 - Transfer LADCO capabilities to other interested agencies
 - Learn from others using AWS (or other cloud services)
- Knowledge transfer to others in the community
 - MPI expertise to help determine the best configuration for AWS hardware
- National air quality modeling cloud computing workgroup



LADCO Cloud Computing Development Timeline

Spring 2018: LADCO Business Meeting presented concept of air quality modeling platform as a service (PaaS) on the cloud			February 2020 : Database development system on AWS for MPCA		Sept 202 p: operatio CAMx sin AWS: '08 rs attainme	Sept 2020: First operational 12km CAMx simulations on AWS: '08 O3 NAAQS attainment demo		<u>Jan - Apr 2021</u> : 12km CAMx PSAT simulations on AWS for Regional Haze	
	2018	2018 2019				2020		2021	
Nov/Dec 2018: Contracted Ramboll to review and recommend cloud services for air quality modeling		2019 : LADCO staff developed a WRF modeling system on AWS Parallel Cluster		March operat simulat AWS	<u>2020</u> : First ional WRF tion on <u>Au</u> op sin	gust 2020 : erational V nulation or	IL EPA /RF AWS	Q3-4 2021: 12/4/1.33k modeling a simulations NAAQS atta demos	m CAM nd APC for O3 ainment





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