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Dask: From POC to Production

PyData Global 2021

April Rathe

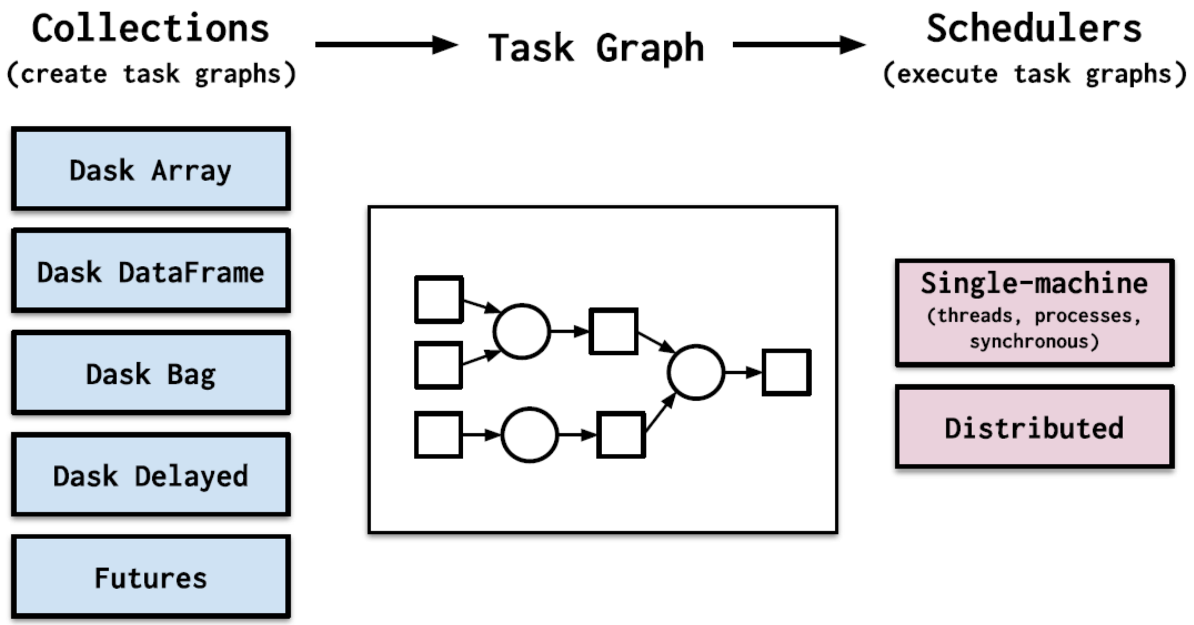
About Me

- > April Rathe (arathe@arrowstreetcapital.com)
  - Head of the Research Data Science Platform
  - Lead a team of Quant Developers
- > Arrowstreet Capital
  - Quantitative investment firm in Boston
  - Aim to generate sustainable alpha for institutional investors
  - Primarily global equity strategies
- > Apply technology to make research innovation cycles faster and easier

What is Dask?

https://docs.dask.org

- **Native**: Enables distributed computing in pure Python with access to the PyData stack.
- **Familiar**: Provides parallelized NumPy array and Pandas DataFrame objects
- **Flexible**: Provides a task scheduling interface for more custom workloads and integration with other projects.
- **Fast**: Operates with low overhead, low latency, and minimal serialization necessary for fast numerical algorithms
- **Scales up**: Runs resiliently on clusters with 1000s of cores
- **Scales down**: Trivial to set up and run on a laptop in a single process
- **Responsive**: Designed with interactive computing in mind, it provides rapid feedback and diagnostics to aid humans



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Context

> Dask was easy to use locally for one-off, individual projects

> How could we expand use to allow all researchers to
  - Seamlessly switch from a local to a remote Dask cluster to expand analysis
  - Create user-dedicated, on-demand Dask clusters from Windows desktops
  - Create job-dedicated, on-demand Dask clusters from scheduled jobs
  - Seamlessly run scripts in different contexts (scheduled vs. ad hoc)

> Challenges
  - How do we create and manage underlying hardware resources and costs?
  - How do we make it easy to use, limiting the stack of technologies to learn?
  - How do we access data (primarily on-prem files, extending to SQL)?
  - Which Dask APIs map best to our use cases?

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Dask Integration Roadmap

Use cases
- Usage patterns
- Runtime configurations

Dask cluster infrastructure
- Hardware
- Resource / container management
- Security
- Environment management
- Logs

Dask cluster & client APIs
- Local cluster
- Remote cluster
- Cluster definition templates

Data access
- Client in-memory data
- Files
- Data partitioning strategies

Applying Dask
- Dask APIs
- Initial integrations
- Example results
- Cost transparency

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Stage 1: Our Use Cases

How Can We Use Dask?

> Exploratory research
  - New vendor datasets: panel, unstructured or alternative
  - Initially with smaller subsets, quickly extend to full history
  - Merge analysis results with existing datasets for comparison

> Simulations
  - “What if” analysis

> Historical data processing
  - Backfills
  - Incorporating data restatements

> Computation patterns
  - Embarrassingly parallel (by date)
  - Path dependent
  - Combination

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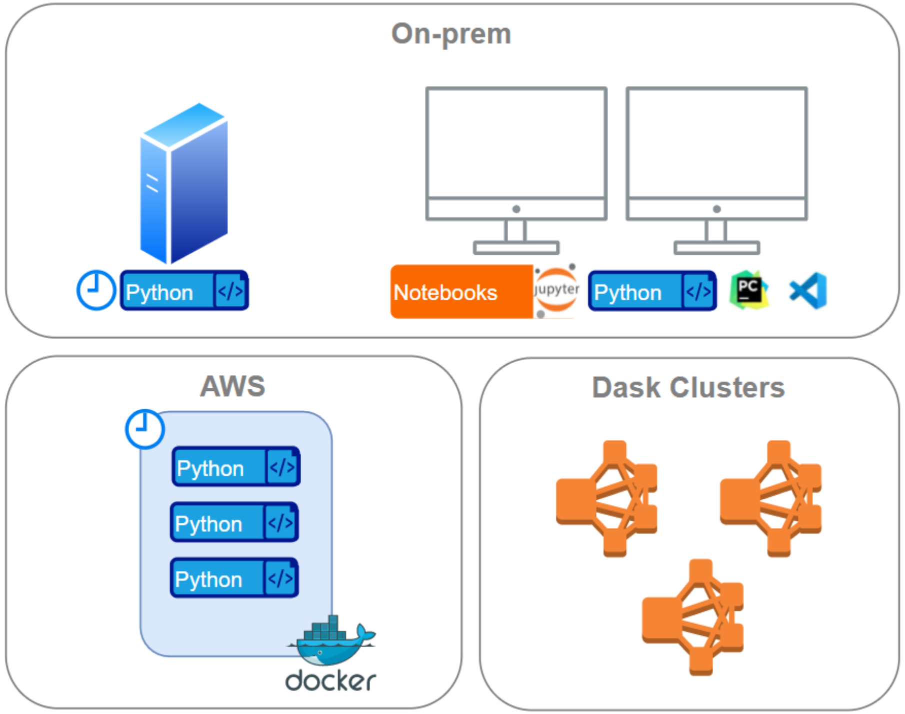
How will we run Dask computations?

> Ad hoc from on-prem Windows or Linux desktops
  - Python scripts (PyCharm, VSCode, command line)
  - Jupyter notebooks

> Scheduled from AWS services

> Scheduled from on-prem servers

> Minimal configuration to change contexts



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Stage 2: Dask Cluster Infrastructure

Challenge

> On-demand, researcher or job-dedicated Dask clusters
  - Ephemeral hardware (as well as Dask Clusters)
  - Burst capacity
  - Minimal startup time (<5 minutes)
  - Ability to apply templated and custom resource specifications (e.g. GPU)
  - Cost transparency and attribution
  - Automatic cleanup of inactive resources

HPC

Collaborative Effort

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Container Service Options

	Cost	Tooling	Flexibility	Complexity
AWS Batch*	EC2 instance cost only	AWS-specific (Console, cli, SDK, CloudWatch, …)	AWS exposed functionality	Low
AWS ECS*	EC2 instance cost only	AWS-specific (Console, cli, SDK, CloudWatch, …)	AWS exposed functionality	Medium
AWS EKS*	EKS cluster cost + EC2 instance cost	Open source (Kubernetes API, kubectl, helm, Kubernetes dashboard, Terraform…)	Most flexibility; any Kubernetes plugin developed by the open source community	High

* Running on EC2 or Fargate

References
https://blog.dask.org/2020/07/23/current-state-of-distributed-dask-clusters
https://docs.dask.org/en/latest/setup.html
https://www.youtube.com/watch?v=deX0GlW4uew (PyCon 2020: Deploying Dask at Scale)

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Compute Layer Options

	Startup Time	Capacity Limits per AWS Account	Resource Flexibility (e.g. GPU)
AWS Fargate	30-90 seconds	Pod limits / account (can be raised) Scaling limits, e.g. # tasks / second	Limited to • <= 4 vCPUs • <=30 GiB of memory
AWS EC2	1-5 minutes	vCPU limits / account (can be raised)	All EC2 instance types, with options of • GPU • ARM-based AWS Graviton CPU • custom AMI

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EKS on EC2

> AWS accounts for ad hoc vs. scheduled (production) use

> Namespaces for user and job isolation (multiple per user)

> AWS autoscaling groups (per EC2 instance type)

Cluster	Name	Min	Desired	Max	Pending	InService	Terminating
pdeks001	arathe-c5-xlarge-nodegroup	0	8	30	0	8	0
pdeks001	arathe-t3-xlarge-nodegroup	0	0	30	0	0	0

> Tagging for cost visibility (username, namespace, and job)

> CLIs for investigations (e.g. kubectl)

> ELK for logging (logs persist across clusters)

> S3 for data

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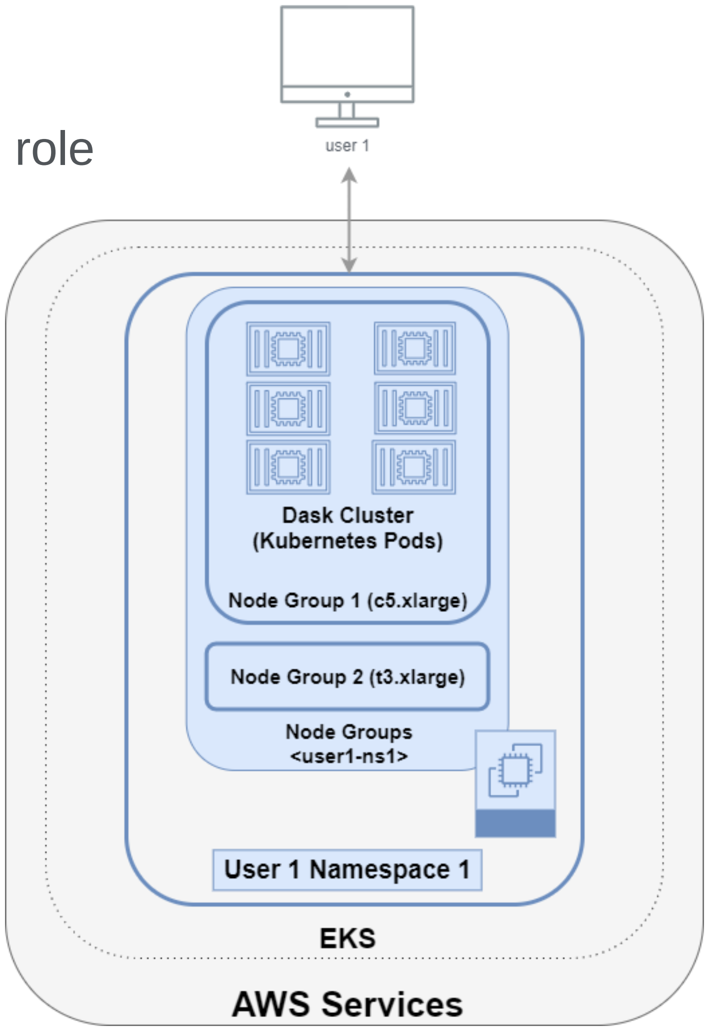
Cluster Lifecycle

Cluster creation

1. Map AD user to IAM role to Kubernetes role
2. Create namespace (EKS)
   - Configure security
   - Configure networking
3. Create AWS autoscaling groups
   - Create nodes (group target)
   - Nodes join cluster
4. Create Kubernetes deployment
   - Dask scheduler pod
   - Dask worker pods
   - Ingress services
   - Certificates



Cluster deletion

1. Client closes cluster or Harvester terminates the cluster
2. Delete Kubernetes deployment
3. Scale groups to 0
4. Delete namespace

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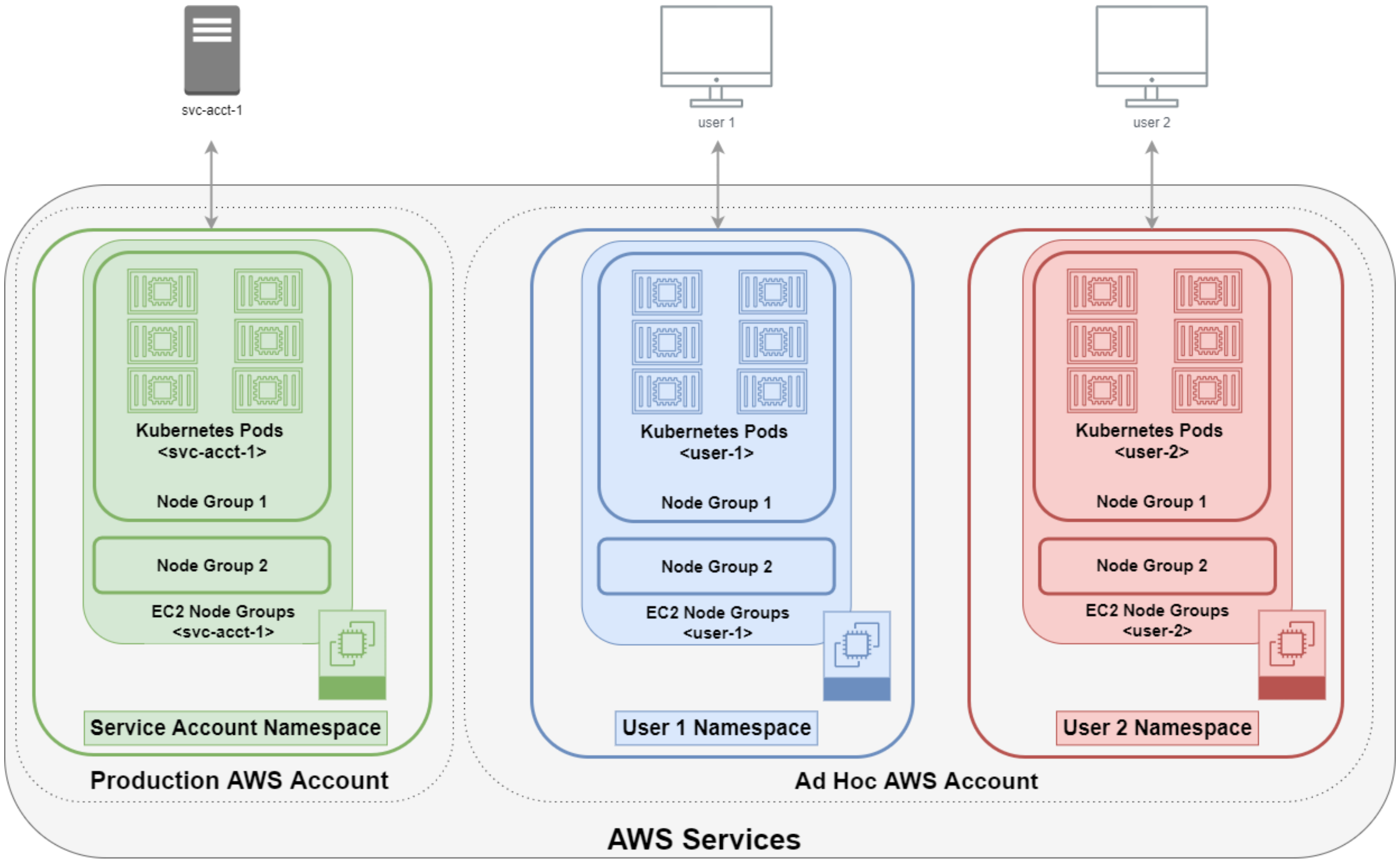
Multi-user Example



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Stage 3: Dask Client & Cluster Interfaces

Challenge

> Create researcher Dask cluster interfaces that…

- Lower the barrier for use
- Minimize the need to learn all underlying technologies (Docker, Kubernetes, kubectl, helm…)
- Allow for expert user customization
- Integrate with EKS and AWS to create and delete clusters
- Connect securely to Dask Cluster from all Dask Clients
- Easily transition between local and remote clusters

Options Considered

> dask-kubernetes
  - Cluster manager for creating Dask Clusters on externally managed Kubernetes clusters
  - Did it fit our use case?
    - No. We wanted ephemeral infrastructure that exists only for the life of the Dask Cluster. It also requires the Client and Cluster to be in the same network space.

> dask-gateway
  - Central, coordinating service for creating Dask clusters in a shared, centrally managed cluster environment (Kubernetes, Yarn, HPC)
  - Did it fit our use case?
    - No. We are using ephemeral infrastructure that exists only for the life of the Dask Cluster.

> dask-cloudprovider
  - Cluster managers integrated with cloud APIs, including AWS ECS (EC2 and Fargate)
  - Did it fit our use case?
    - No. We wanted to use EKS. It also requires the Client and Cluster to be in the same network space to connect securely.

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Research Elastic Compute Cluster (RECC)

> Built a custom Python module and CLI to manage EKS Node Groups and Nodes
> Uses boto3 for AWS service interactions
> Uses Kubernetes API for interacting with EKS
> Automatically applies security, namespaces and tagging to clusters
> Harvests inactive clusters for cost control (after an inactive period)
> Applies parameterized, Kubernetes yaml files to create Dask Clusters

Research Elastic Compute Cluster (RECC) Dask Cluster

> Extends dask.distributed.Cluster

> Applies default, templated or custom ClusterSpecs

- EC2 instance type (node group and nodes)
- Number of Dask workers
- Dask worker memory and CPU
- Dask scheduler memory and CPU
- Custom resource tags, e.g. GPU

> Calculates the number of EC2 instances required

> Applies environment customization

- Docker image name
- Sets select source code paths from EFS (published git branches)
- Sets standard environment variables

RECC Dask Client

> Extends dask.distributed.Client
  - Sets security context (AWS services, desktop or on-prem servers)
  - Registers default worker plugins

> Examples

```
In [ ]: from rshcore.rshdask RECCCluster, RSHClient, get_template_path
```

```
In [ ]: # Create a RECCCluster with default parameters (c5.xlarge, 20 workers, 1.5BGiB memory, 1 CPU)
        cluster = RECCCluster()

        # Create a RECCCluster with parameter from a specific template file (stardardized templates or custom)
        cluster = RECCCluster(get_template_path("some_template"))

        # Create a RECCCluster from the default template with params overridden
        cluster = RECCCluster(n_workers=100, scheduler_memory_GiB=4)

        # Get a RECCCluster using a feature branch
        cluster = RECCCluster(source_git_branch="RSH=XXXX-git-branch-name")

        # Get a RECC Client or RECCCluster for an EC2 instance type
        cluster = RECCCluster(instance_type="p3.8xlarge")
```

```
In [ ]: # Use Client connected to a RECCCluster
        with RECCCluster() as cluster:
            with RSHClient(cluster) as client:
                result = client.map(lambda x: x ** 2), range(10).result()
```

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Stage 4: Data Access

Challenge

> Apply Dask to datasets in existing storage formats
  - Primarily files on NFS, on-prem
  - Single interface for data access, both for on-prem and AWS access
  - Single interface for Dask running locally or remotely

> Different data partitioning strategies (stacked or by date)

> Data interfaces
  - Intra-process data exchange (in-memory, intermediate files)
  - Inter-process data exchange (scheduled within a wider processing flow)

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S3, Datastore and IO Modules

- Synchronize between local and S3 (s3fs, boto3)
- Seamlessly switch between S3 and local datastores
- Automatically configured based on environment variables
- Ability to override and select specific datastores
- Read precedence fall-through for datastores

```
In [1]: import numpy as np
        import pandas as pd
        import rshcore.pandasextensions.io as pdx
        from rshcore.datastore import get_read_datastore_names, get_write_datastore_names

In [2]: get_read_datastore_names()
Out[2]: ['LOCAL', 'FP_LOCAL', 'S3', 'FP_S3']

In [3]: get_write_datastore_names()
Out[3]: ['LOCAL']

In [4]: df = pd.DataFrame(np.array([[1, 2, 3], [4, 5, 6], [7, 8, 9]]), columns=['a', 'b', 'c'])
        pdx.write_df(df, "demo/example.csv")

In [5]: df_local = pdx.read_df("demo/example.csv")
        df_local.head()

        Loading from LOCAL
Out[5]:
```

	a	b	c
0	1	2	3
1	4	5	6
2	7	8	9

```
In [6]: pdx.write_df(df, "demo/example.csv", datastores="S3")

In [7]: df_s3 = pdx.read_df("demo/example.csv", datastores="S3")
        df_s3.head()

        Loading from S3
Out[7]:
```

	a	b	c
0	1	2	3
1	4	5	6
2	7	8	9

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Stage 5: Applying Dask

Applying Dask APIs

> Selected processes on two dimensions

- Runtime: three longest running historical processes (on the critical path)
- Dask integration patterns: three different approaches

> Example 1: Embarrassingly parallel

- Larger-than-memory dataset
- Files partitioned and processed by date
- Switch from LocalCluster to RECCCluster
- dask.delayed

Dask Task Graph


```
In [ ]: from rshcore.rshdask RECCCluster, RSHClient
```

```
In [ ]: # Before: Using Local Cluster
        with RSHClient(n_workers=n_workers, threads_per_worker=threads_per_worker, processes=processes) as client:
            _parallel_process(client, args, BATCH_SIZE)
```

```
In [ ]: # After: Using RECC Cluster
        with RECCCluster("large-cluster-large-workers", n_workers=N_WORKERS) as client:
            with RSHClient(cluster) as client:
                _parallel_process(client, args, BATCH_SIZE)
```

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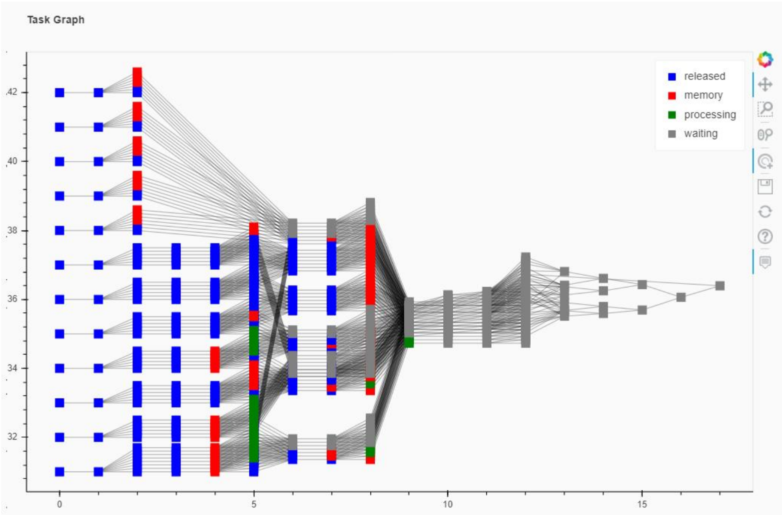
Applying Dask APIs cont.

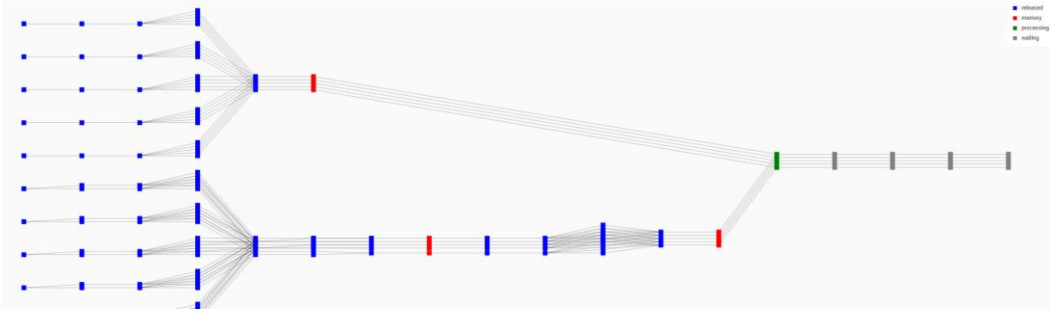
> Example 2: Dataframe parallelization

- Long-running computations
- Repartioning due to custom functions (groupby / apply)
- Major structural rewrite
- dask.dataframe (map_partitions and set_index)



> Example 3: Combined serial and parallel processing

- Larger-than-memory dataset
- Major structural rewrite
- Multi-stage processing: local, Dask, and joining
- dask.delayed



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Dask Results

Processing Type	Dask APIs	Data Interfaces	EC2 Instance Types	EC2 Instances	Dask Workers	Estimated Cost	Speedup
Embarrassingly parallel (by date)	dask.delayed	Date partitioned files on S3	m5.4xlarge	26	300	$50	9.1x
Dataframe parallelization	dask.dataframe	Client-side dataset sent with tasks	r5.12xlarge	16	300	$62	34x
Combined serial and parallel processing	dask.delayed	Client-side data sent with tasks; date partitioned files	r5.4xlarge	5	50	$130	3.3x

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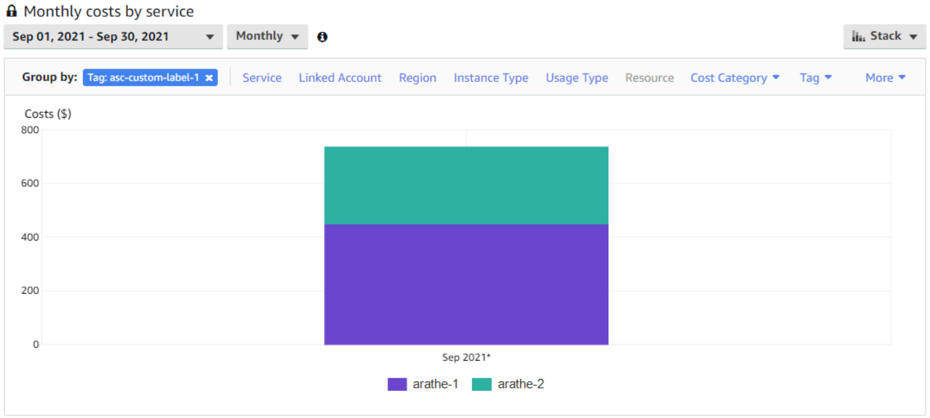
Cost Transparency

> RECCCluster reports estimated EKS cost / hour when created (using EC2 prices)

> AWS Budget Reports by user, namespace and job

> Email alerts per user and namespace based on thresholds



To see usage data, filter by "Usage Type" or "Usage Type Group" filters with matching units (e.g., hours).

Download CSV

asc-custom-label-1	Sep 2021*	asc-custom-label-1 Total
Total cost ($)	736.05	736.05
arathe-1 ($)	449.13	449.13
arathe-2 ($)	286.92	286.92

To April Rathe

AWS Budget Notification September 29, 2021
AWS Account XXXXXXXXXXX

Dear AWS Customer,

You requested that we alert you when the FORECASTED Cost associated with your Ad Hoc budget is greater than $1,000.00 for the current month. The FORECASTED Cost associated with this budget is $1,024.08. You can find additional details below and by accessing the AWS Budgets dashboard [1].

Budget Name: Ad Hoc
Budget Type: Cost
Budgeted Amount: $2,000.00
Alert Type: FORECASTED
Alert Threshold: > $1,000.00
FORECASTED Amount: $1,024.08

[1] https://console.aws.amazon.com/billing/home#/budgets

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We’re hiring!

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Website: https://www.arrowstreetcapital.com

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