

4CeeD: Real-Time Data Acquisition and Analysis Framework for Material-related Cyber-Physical Environments

Phuong Nguyen, Steven Konstanty, Todd Nicholson, Thomas O'brien, Aaron Schwartz-Duval, Timothy Spila, Klara Nahrstedt, Roy H. Campbell, Indranil Gupta, Michael Chan, Kenton McHenry, Normand Paquin

University of Illinois at Urbana-Champaign

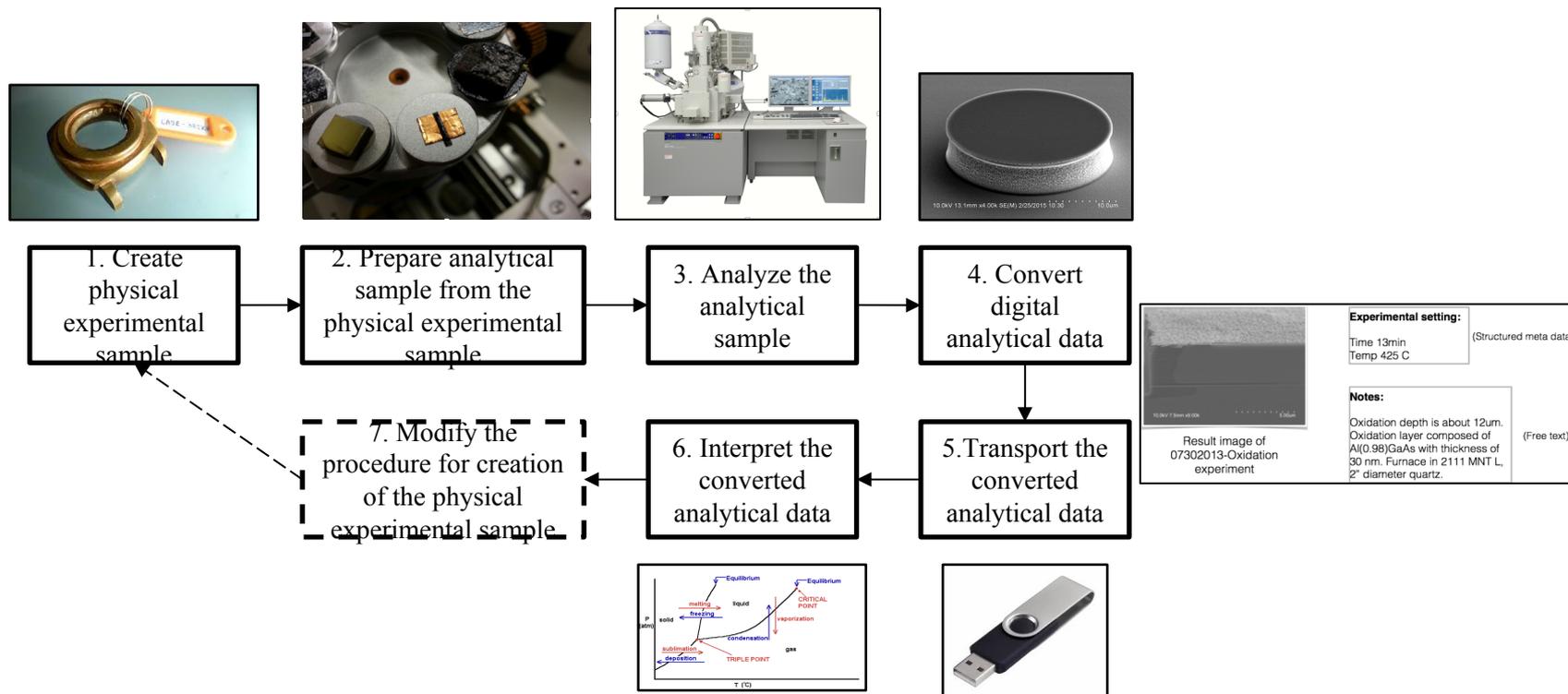


Outline

- **Background & Challenges**
- Our solution: 4CeeD
 - Curation Service
 - Coordination Service
- Evaluation
- Conclusions

Background: Long process from material discovery to device fabrication

- It typically takes 20 years to go from the discovery of new materials to fabrication of new and next-generation devices*



* Holdren, J.P. "Materials genome initiative for global competitiveness". National Science and Technology Council OSTP 2011.

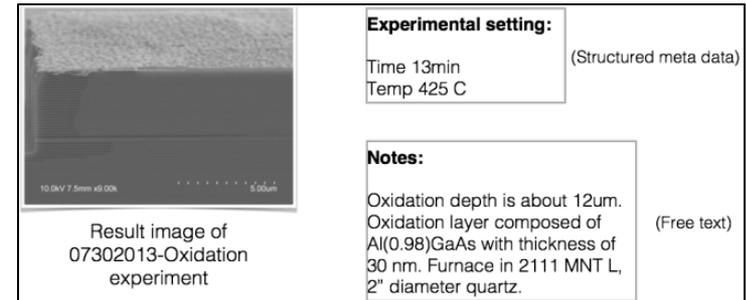
Background: Issues with current experimental cycle

- Data acquisition & transfer
 - “*Sneaker-net*” data transfer
 - No data conversion is available during data acquisition
- Data management & processing
 - Using local file system, or general-purpose cloud storage services (e.g., DropBox, Google Drive, etc.)
- Data access & sharing
 - Materials science & semiconductor fabrication areas have never been digitally connected
 - Only “*best*” results and data are kept for publishing

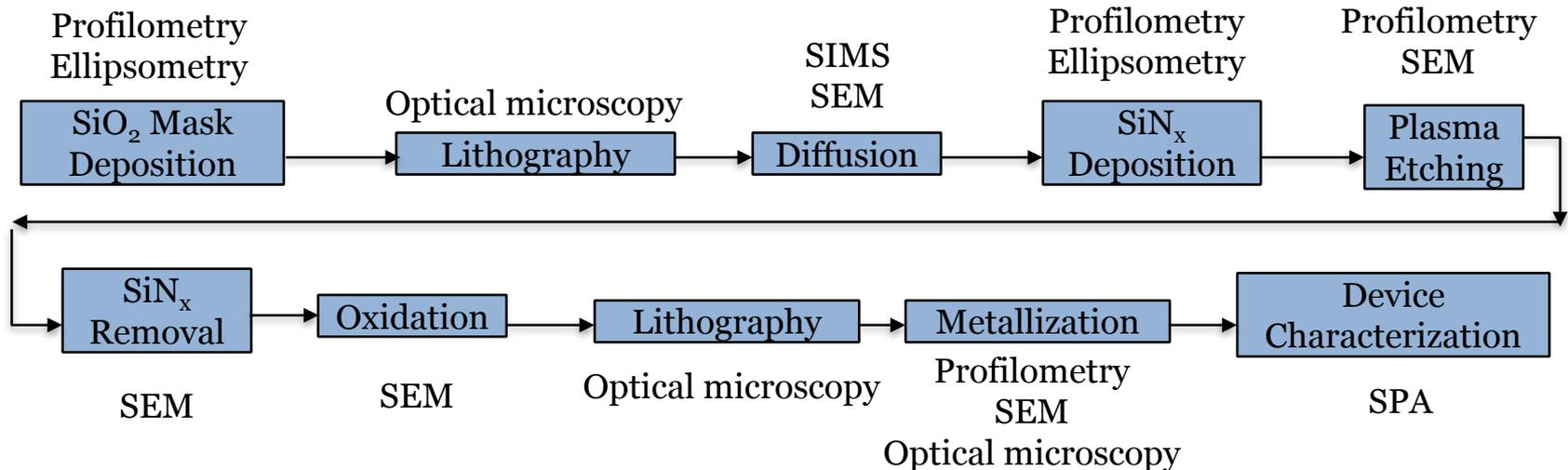


Challenge: Data of multimodality and of heterogeneous types

- Data come of various types and formats
 - Each type requires a different data processing workflow



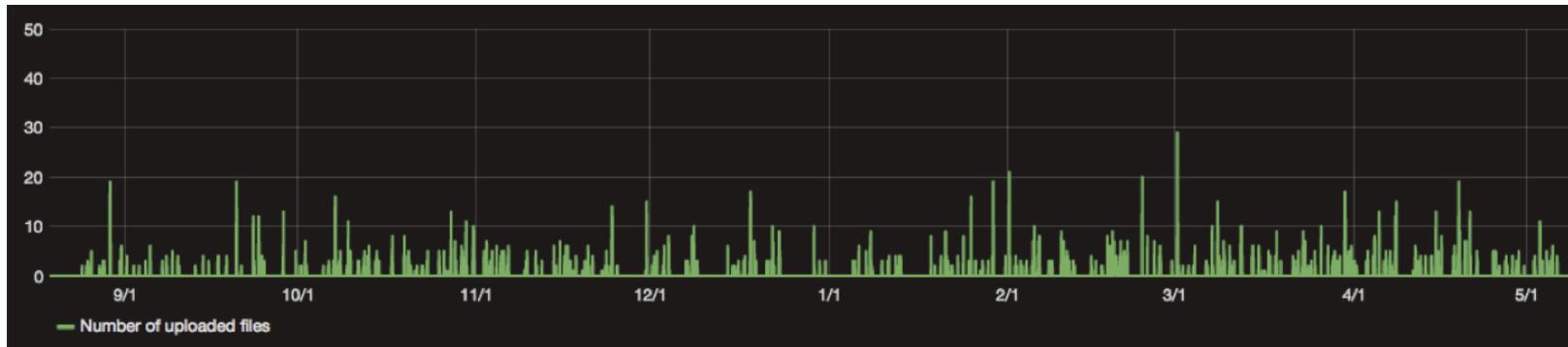
Sample output data from SEM microscopy



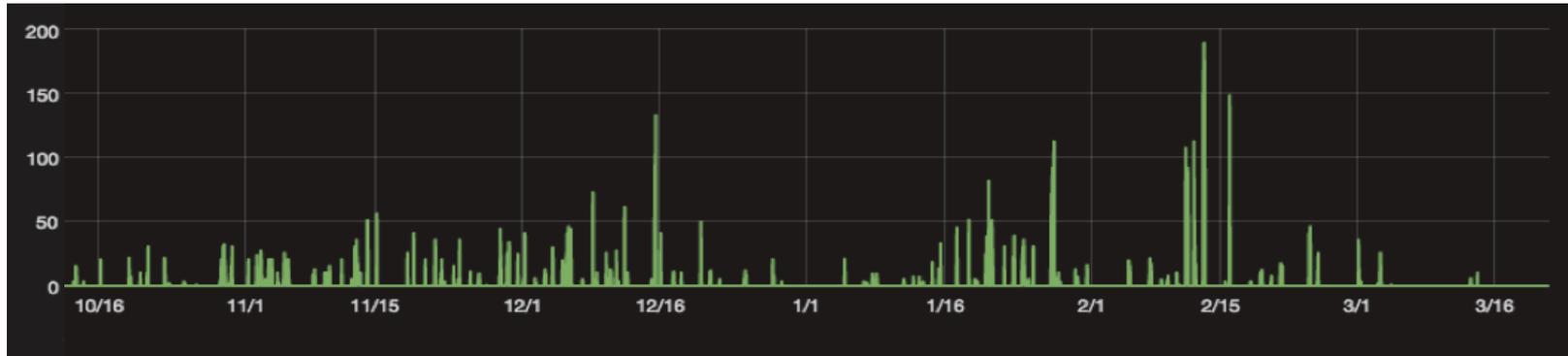
Heterogeneous types of experiments often done on a material sample

Challenge: Shorten time from digital capture to interpretation & insights

- Dynamism of workload: Data generated from scientific instruments are highly variable and often bursty



Number of files generated on a JOEL instrument from Sep 2015 to May 2016



Data (in MB) generated on a HeliosFIB instrument from Oct 2015 to March 2016

Outline

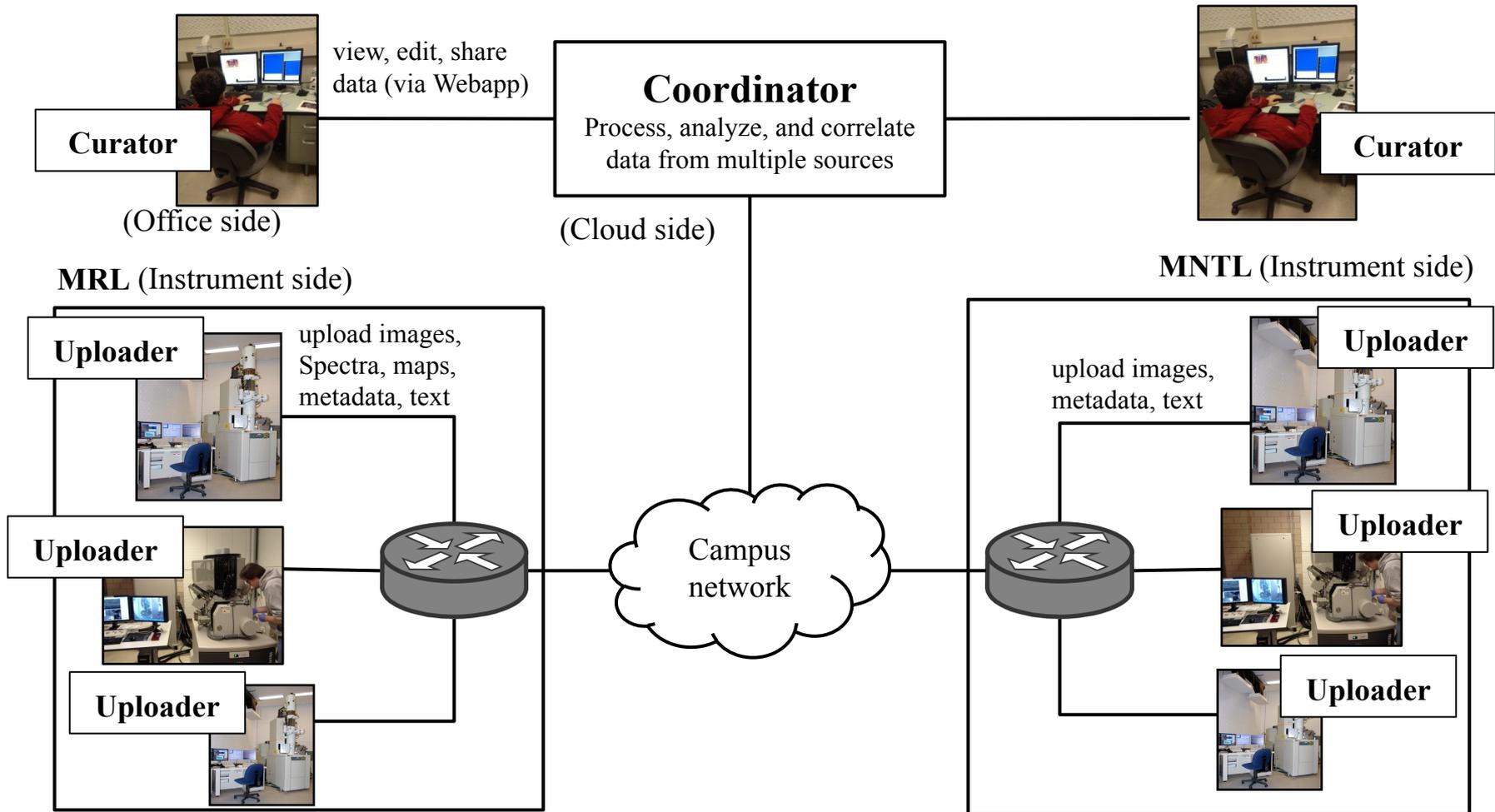
- Background & Challenges
- **Our solution: 4CeeD**
 - Curation Service
 - Coordination Service
- Evaluation
- Conclusions

Our approach

- Existing systems focusing on:
 - Making *existing datasets* more accessible & sharable (e.g.: DataUp, SkyServer)
 - *Long-term preservation* of data (e.g., SEAD)
 - *Easy access* to grid/cloud infrastructure & collaboration (e.g.: HubZero, NanoHub, BrownDog, Data Conservancy Instance)

Our approach is to provide an expedient mean to capture, transfer, and process the digital data in real-time and in trusted manner **before** archiving, further analysis, visualization and sharing of the experimental results

4CeeD: Real-time data acquisition and analysis framework for material-related environment



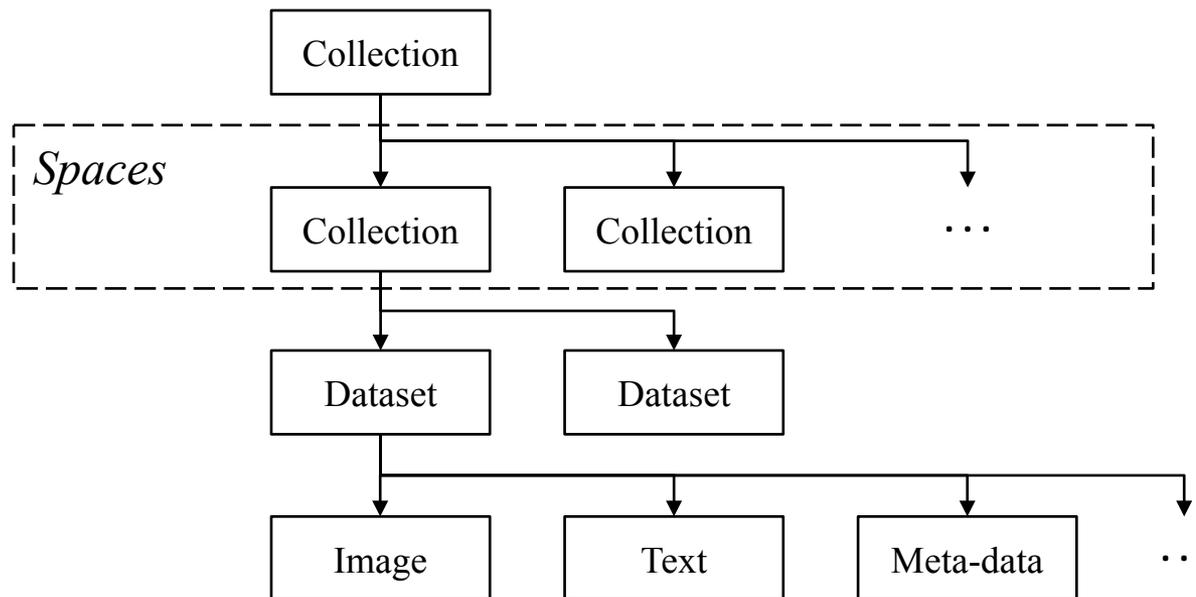
* 4CeeD stands for Capture, Curate, Coordinate, Correlate, and Distribute material-related experimental data.

Outline

- Background & Challenges
- Our solution: 4CeeD
 - **Curation Service**
 - Coordination Service
- Evaluation
- Conclusions

4CeeD's curation service: Data model

- Extendable data model
 - **Vertical** organization: Using concepts of *collections*, *datasets*, and *files* to provide flexible data organization
 - **Horizontal** organization: Using *spaces* to support sharing of data



4CeeD's curation service: Data uploader

- Uploader offers a simple 3-step interface, following the data model

01 Choose a collection... what's this?

Existing collections

Search your collections

Right click a collection to create a sub-collection.

- 123
- Au-shelled micelles
- Gd filled micelle project
- In vitro growth
- Au-Brij-M
- Au-PEG-M
- polyvilli

New Root Collection

Create collection

02 Choose a dataset... what's this?

Existing Datasets

New Dataset

Basic Load Template Create Template Load Previous

My Templates: Global Templates: Template Tag Search:

Choose a name for your dataset:

Dataset Description:

Add New Field Clear Template

Name:	Unit Type:	Data Type:	Default Value:	
Brij mass (mg)		String		Remove
What's internalized		String		Remove
mass of internalized molecules (mg)		String		Remove
What outer shell aminated polymer w		String		Remove

Create dataset &
associated meta-data

03 Click browse or drag and drop files..

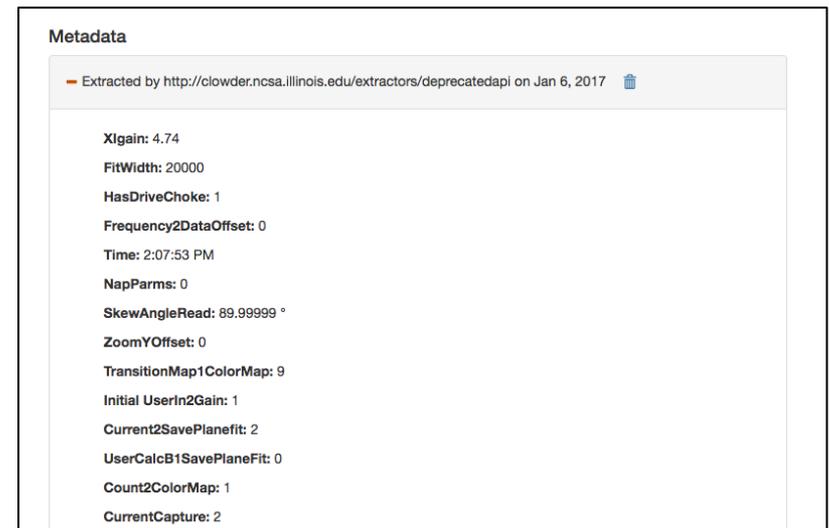
Browse Drag & Drop Files

Submit

Select raw data files
to upload

4CeeD's curation service: Data curator

- Uploaded raw data is processed and available for curation (tagging, annotation) and sharing
- Processed data is indexed and available for search



Example of processed AFM experiment data with gray-shade preview & meta-data

Outline

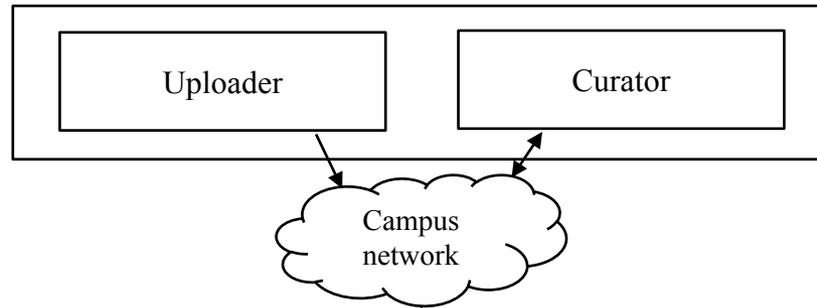
- Background & Challenges
- Related work
- Our solution: 4CeeD
 - Curation Service
 - **Coordination Service**
- Evaluation
- Conclusions

4CeeD's coordination service design methodology

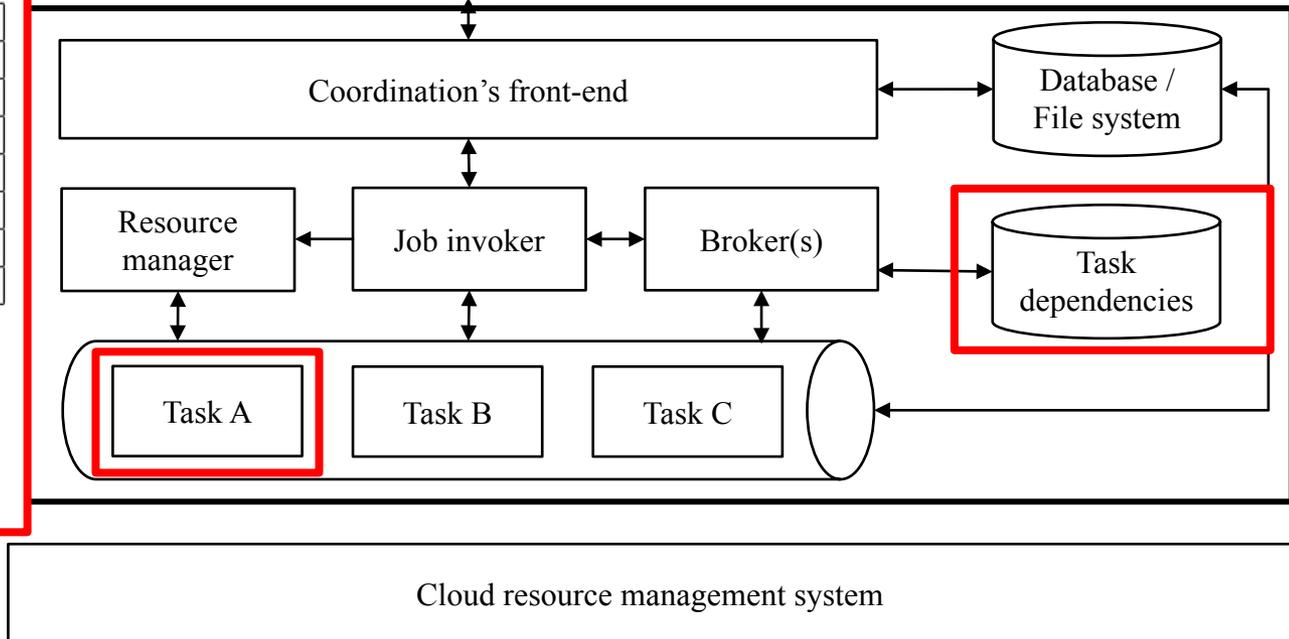
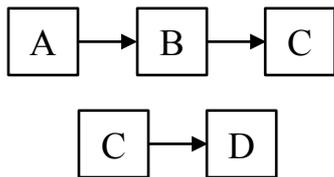
- Challenges/requirements (revisited)
 - Support heterogeneous data processing workflows
 - Handle variable & bursty workload
- Our approach:
 - Leverage resource abstraction provided by cloud resource management system (e.g., Kubernetes, YARN, Mesos)
 - Micro-service execution model:
 - Separate task dependencies from task implementation & deployment
 - Dynamic resource scheduling using system's performance model

4CeeD's coordination service's architecture

Curation services



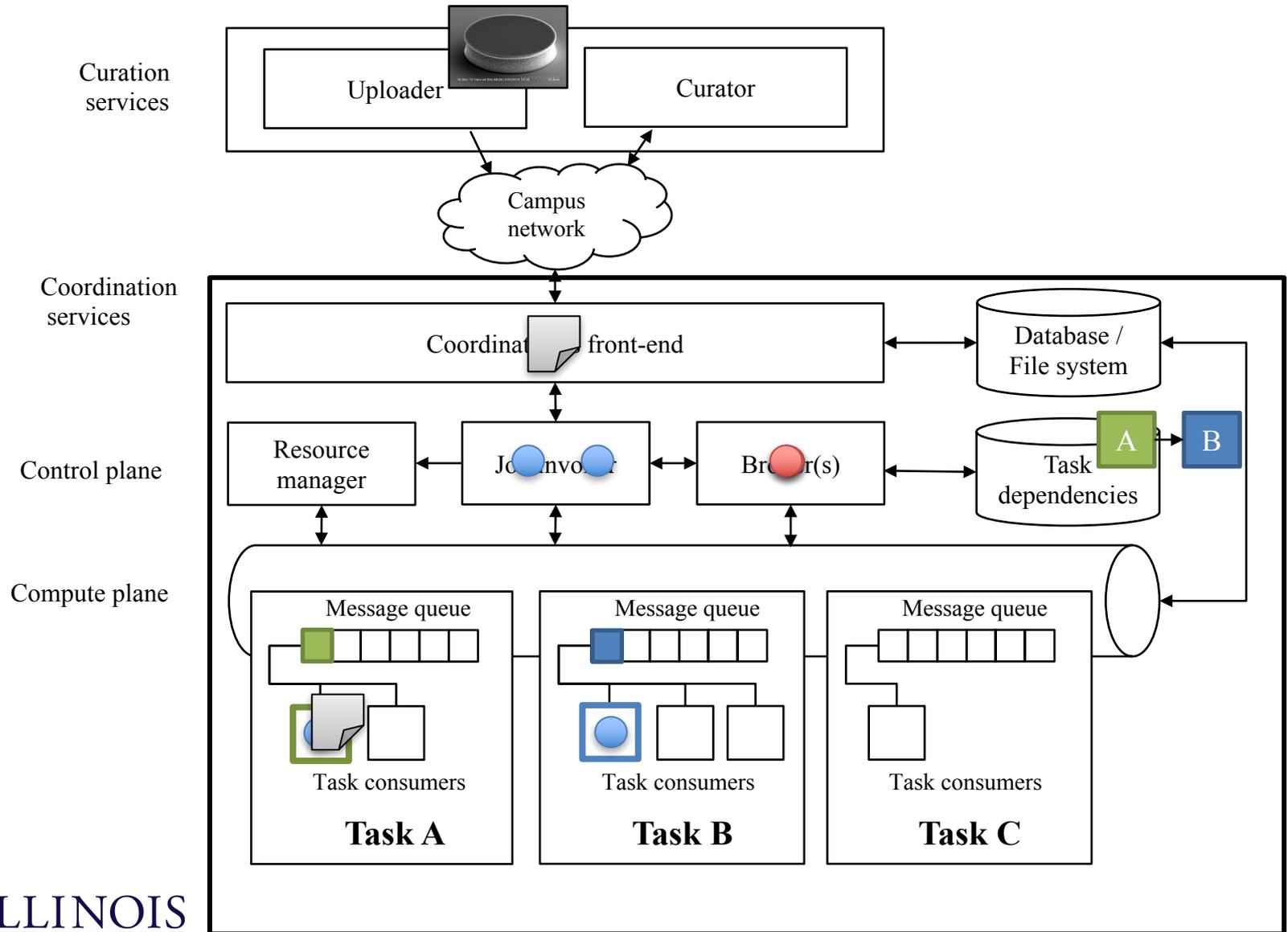
Job type	From	To
1	A	B
1	B	C
1	Start	A
1	C	End
3	Start	C
3	D	End
...



4CeeD's coordination protocol

- Coordination front-end:
 - Receives data, stores it in database, and create a job request to process the data.
 - Forwards the request to Job invoker
- Job invoker:
 - Notifies Resource manager about the new arrival request
 - Asks Brokers about the **first** task micro-service to handle the request
 - Forwards the request to the corresponding first task micro-service
- Task micro-service:
 - Pick-ups new request from its request queue & process the request
 - Asks Brokers about the **next** task micro-service(s) to handle the request
 - Forwards the request to the corresponding next task micro-service(s)

4CeeD's coordination service's architecture



Coordination service's resource scheduling

- Objective:
 - To decide how many consumers should be allocated to each task's micro-service to optimize the performance, subjected to resource constraint
- We use *work-in-progress* as system performance metric:
 - $WIP = \sum_j WIP_j$ (WIP is proportional to response time, via Little's law)
 - Leverage our previous work* on performance model of elastic pub/sub system to represent WIP_j as a function of number of consumers of task j -th: $WIP_j(m_j)$

$$\operatorname{argmin}_{\{m_j\}} \sum_j WIP_j(m_j)$$
$$\sum_j m_j \leq C$$

* Nguyen, P. and Nahrstedt, K., "Resource Management for Elastic Publish Subscribe Systems: A Performance Modeling-based Approach", IEEE CLOUD 2016

Dynamic resource scheduling algorithm (GRESMAN)

- Greedily allocate additional consumer (one for each iteration) to the task that maximize the benefit of reducing system's WIP , until the performance threshold (\mathcal{T}) or resource constraint (\mathcal{C}) is met.

Algorithm 1 Dynamic Greedy Elastic Scaling Algorithm (GRESMAN)

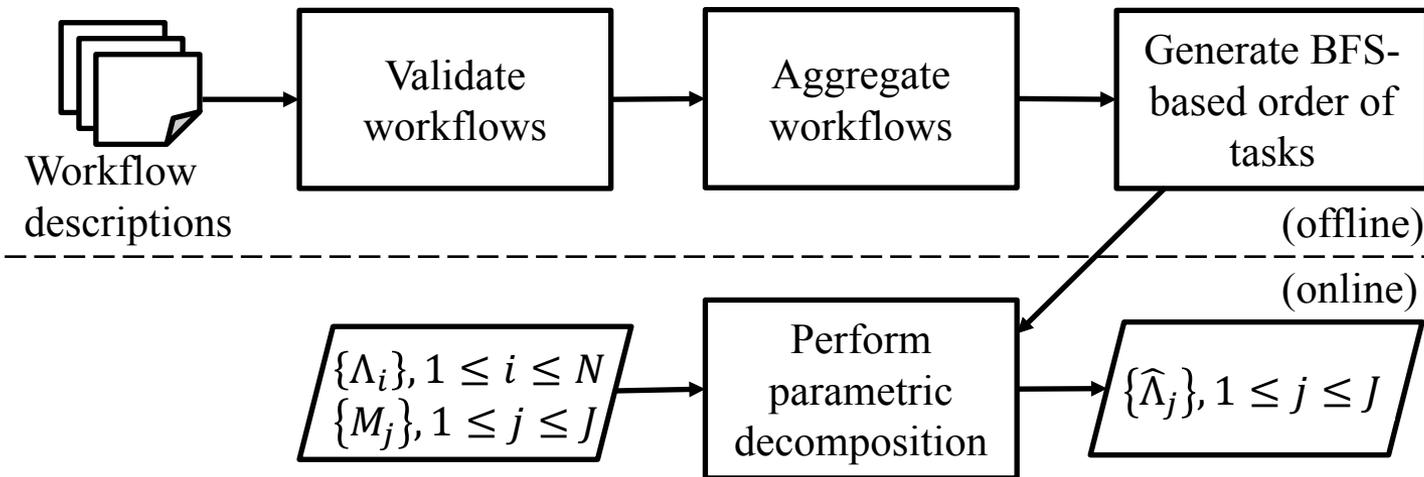
```

1: procedure GRESMAN
2:   Define  $\mathbf{m}^0$  as the current configuration of consumers
3:   Initialize allocation plan  $\mathcal{A} = []$ 
4:   Initialize iteration count  $i = 1$ 
5:    $\{\hat{\Lambda}_j\} = \text{DECOMPOSE}(\{\Lambda_j\}, \{M_j\}, \mathbf{m}^0)$   $\triangleright$  Initial decomposition
6:   while  $WIP(\mathbf{m}^0) > \mathcal{T}$  and  $F(\mathbf{m}) < \mathcal{C}$  do
7:      $\hat{j} = \text{argmax}_{1 \leq j \leq J} \Delta(m_j^i, m_j^i + 1)$   $\triangleright$  Find the most
       beneficial PC
8:      $m_j^i = m_j^i + 1$   $\triangleright$  Add one consumer to that PC
9:      $\mathcal{A}.\text{append}(\hat{j})$   $\triangleright$  Update allocation plan
10:     $\{\hat{\Lambda}_j\} = \text{DECOMPOSE}(\{\Lambda_j\}, \{M_j\}, \mathbf{m}^i)$   $\triangleright$  Update  $\{\hat{\Lambda}_j\}$ 
11:     $i = i + 1$   $\triangleright$  Update iteration count
12:   Return  $\mathcal{A}, \mathbf{m}^i$ 

```

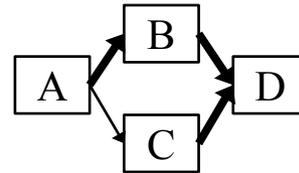
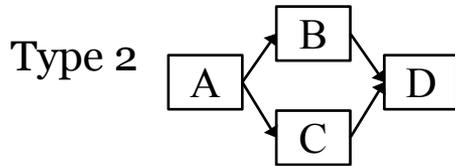
Coordination service's resource scheduling

- Under micro-service execution model, calculating $WIP_j(m_j)$ requires **decomposition** of system-specific workload into task-specific's workloads
 - From $\{\Lambda_i\}, 1 \leq i \leq N$ (and known $\{M_j\}, 1 \leq j \leq J$) to $\{\hat{\Lambda}_j\}, 1 \leq j \leq J$

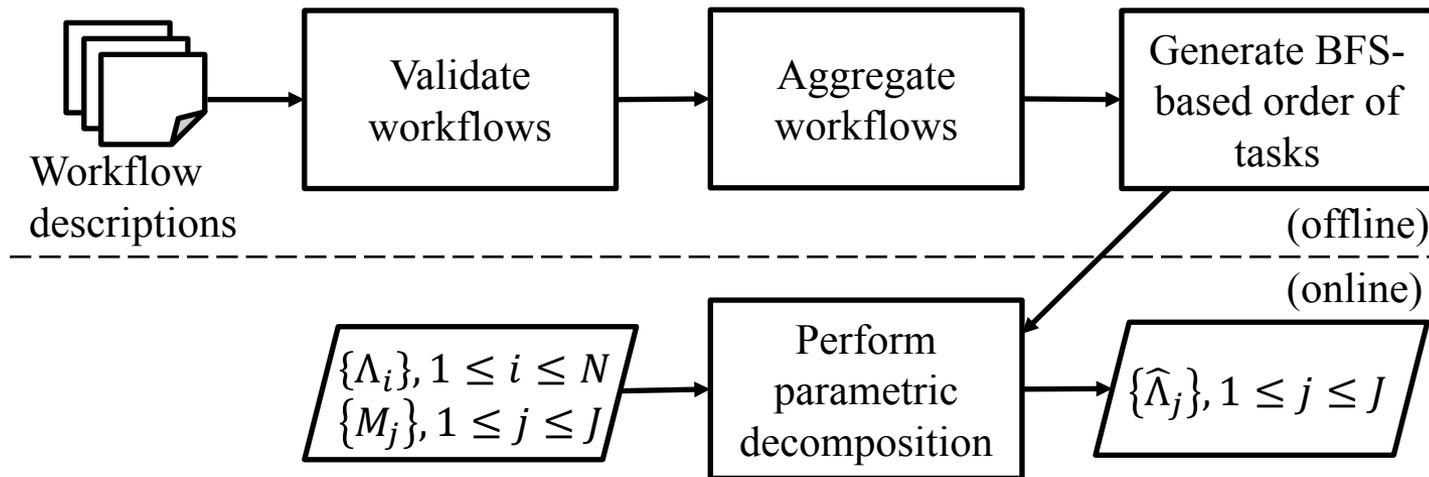


Workload parameters decomposition procedure

Coordination service's resource scheduling



{A, B, C, D}

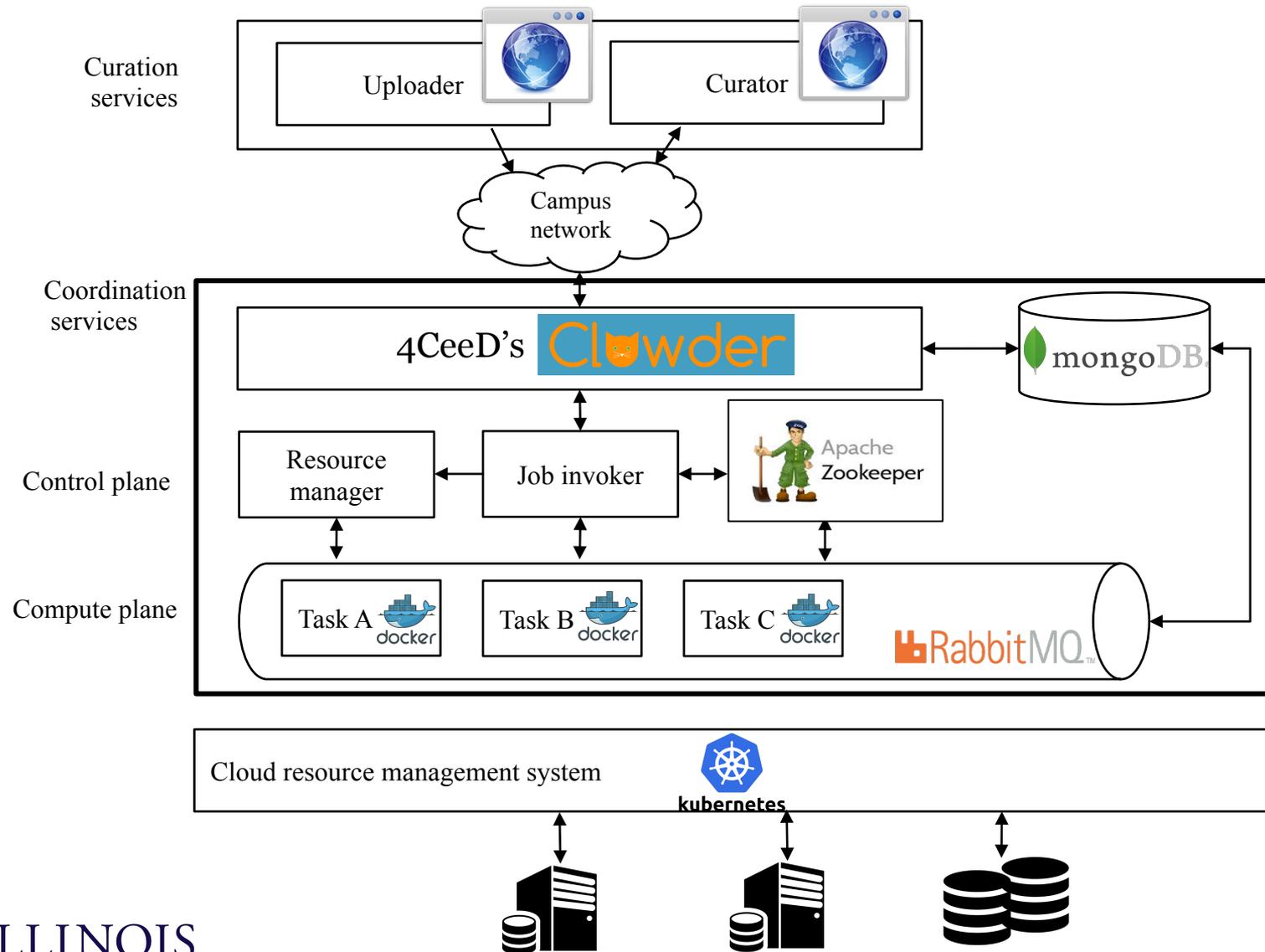


E.g.: Type 1 & type 2 workloads merge at A, and then split to B & C

Outline

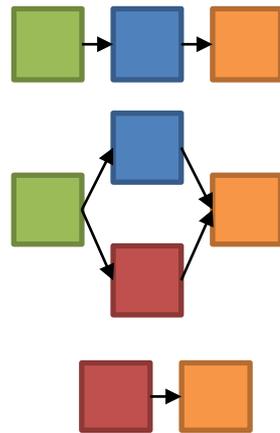
- Background & Challenges
- Our solution: 4CeeD
 - Curation Service
 - Coordination Service
- **Evaluation**
- Conclusions

System implementation

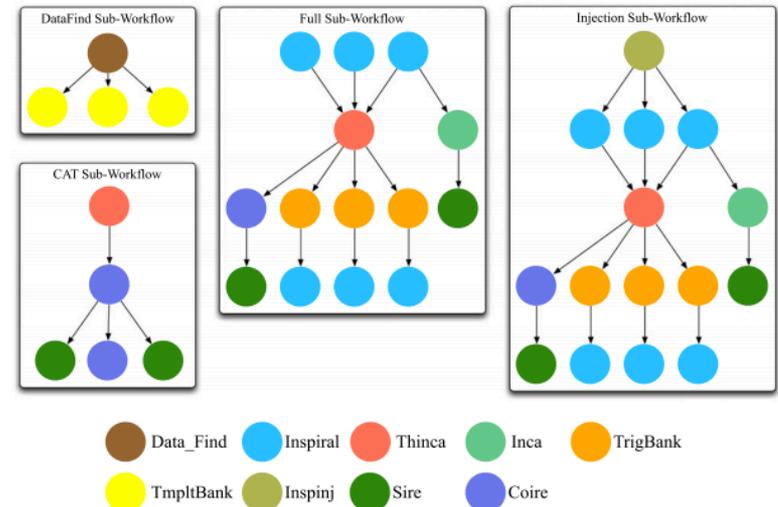


Evaluation settings

- Data processing workflows:
 - MDP: material data processing workflows (to process DM3, AFM, etc.)
 - LIGO: analyze data to study stars and black holes



MDP workflows

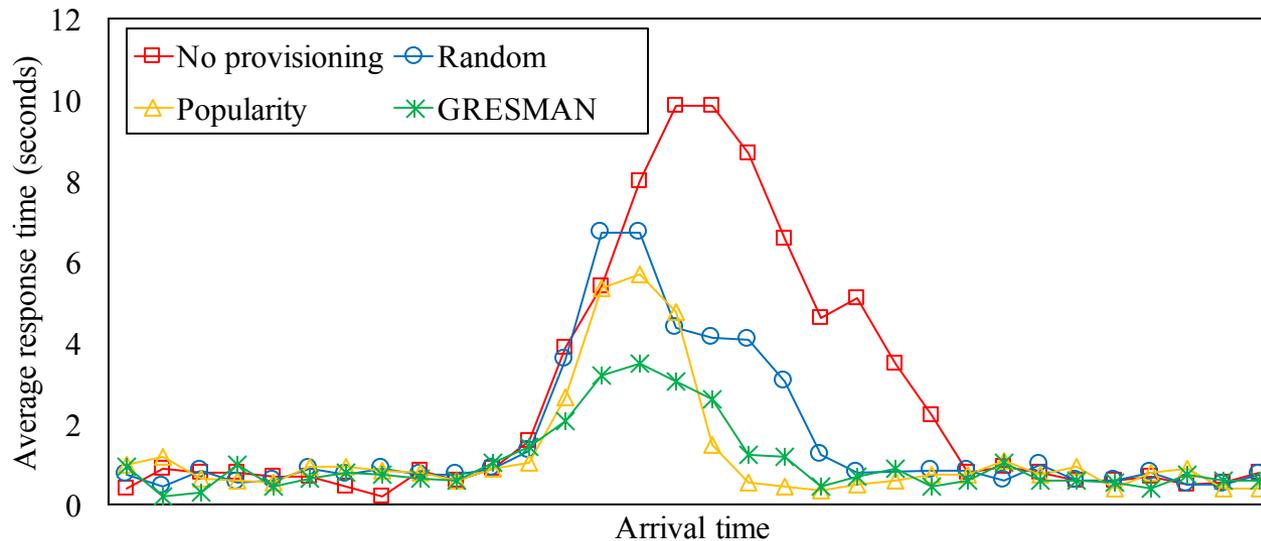


LIGO workflows

Evaluation settings (cont.)

- Emulate the bursty workload situation by abnormally increasing the arrival rates of requests to up to **10x higher** on MDP and LIGO workflows
- Performance threshold (\mathcal{T}): Absolute delay guarantee on average processing time
 - Set to 2s for the MDP and 10s for LIGO workflows
- Resource constraint (\mathcal{C}): Maximum number of (homogeneous) consumers that can be allocated by the system
 - Set to 10 and 60 consumers for the MDP and LIGO workflows respectively
- 4CeeD coordination service is deployed on a cluster of three nodes, each node is equipped with an Intel Xeon quad core processor (1.2Ghz for each) and 16GB of RAM.

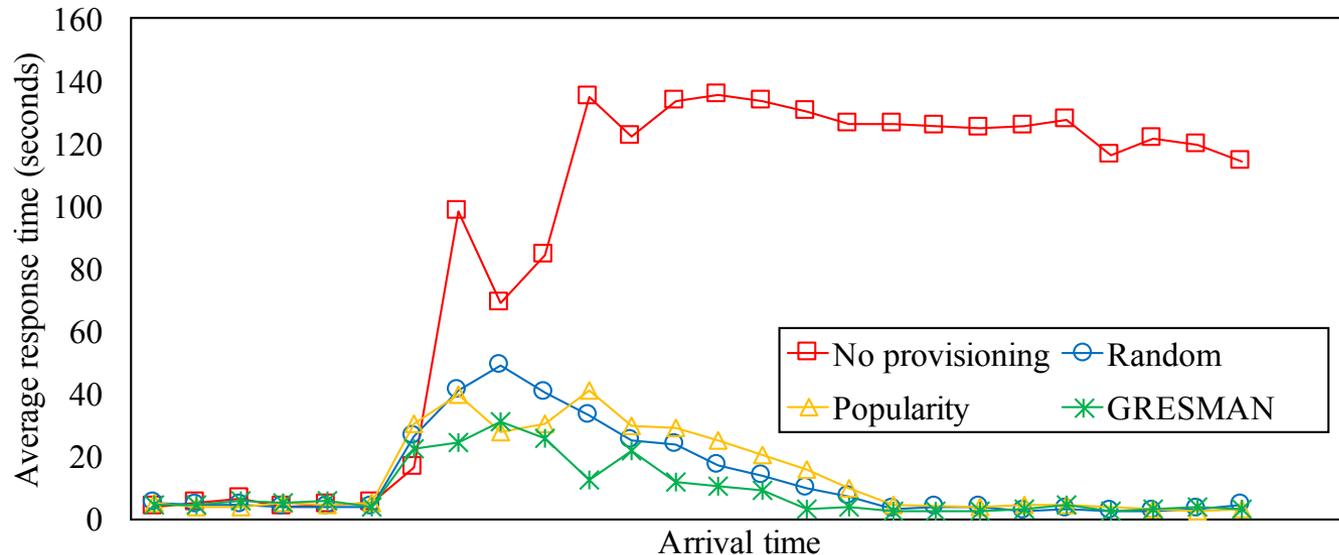
Effectiveness of coordination service in handling bursty workload



MDP workflows

Our resource scheduling strategy (GRESMAN) demonstrates effectiveness in bursty workload situation.

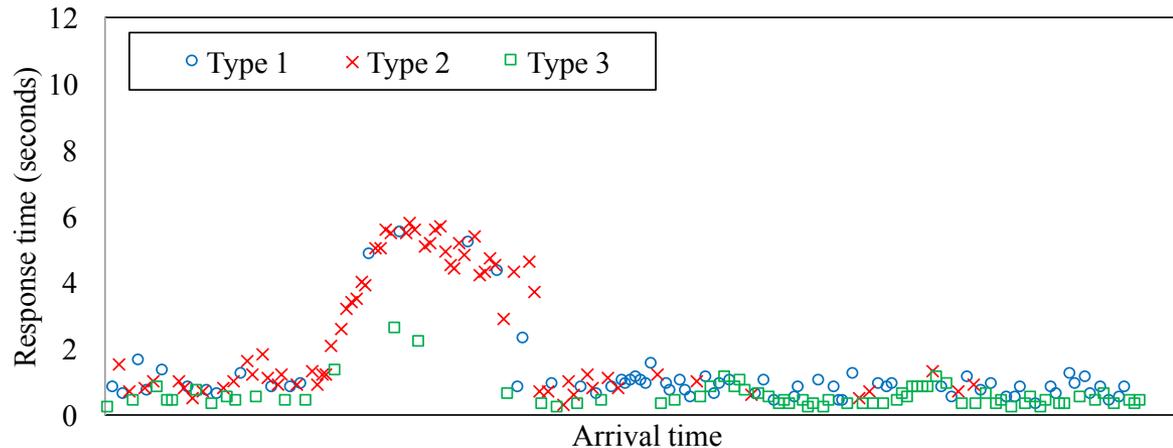
Effectiveness of coordination service in handling bursty workload



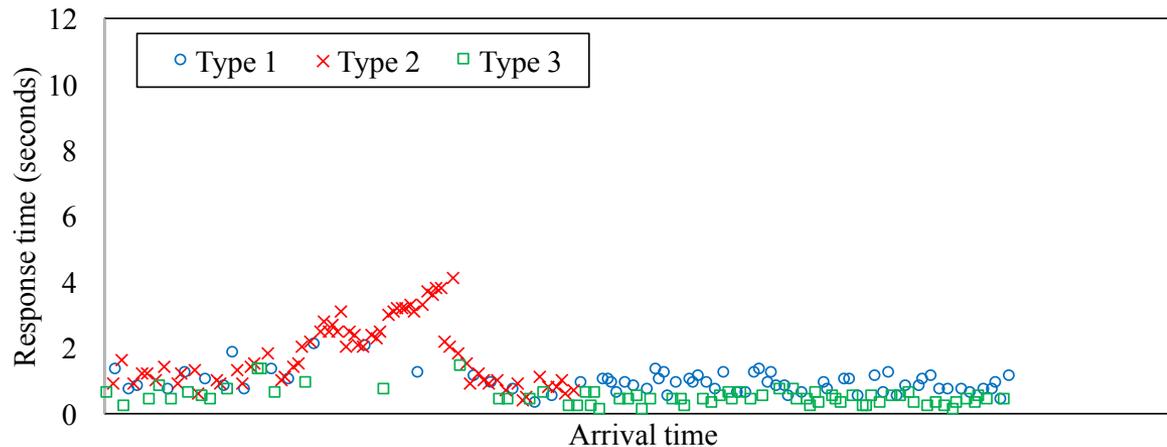
MDP workflows

Our resource scheduling strategy (GRESMAN) demonstrates effectiveness in bursty workload situation.

Impact of order of scheduled resource in handling bursty workload with MDP workflows

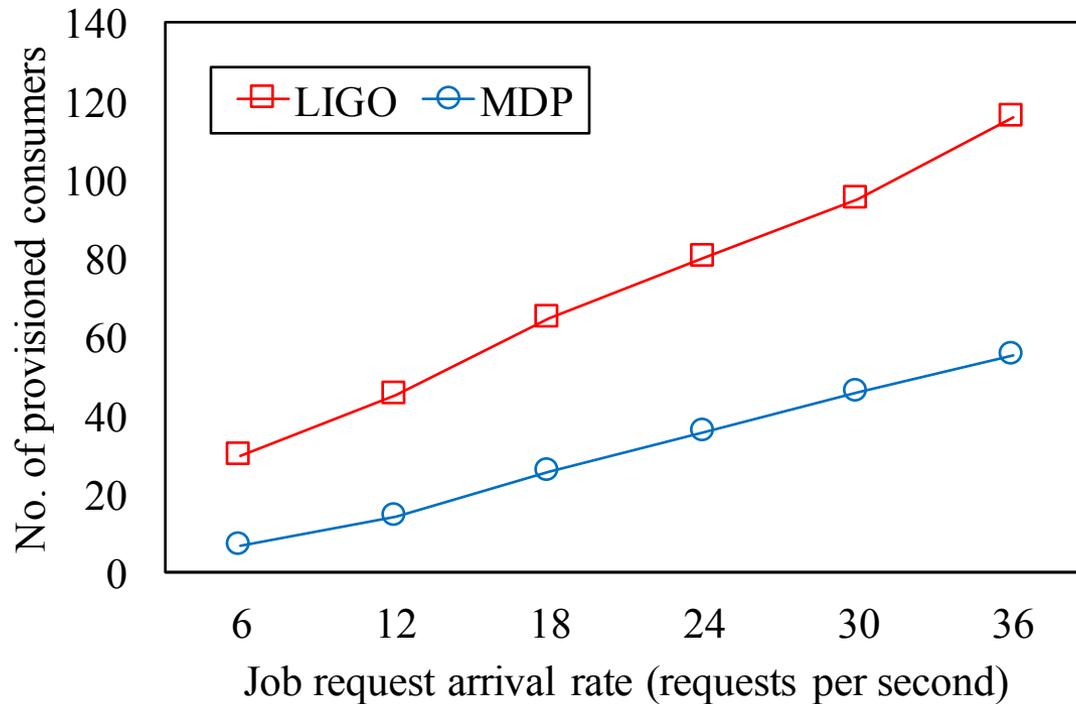


Non-optimal order



Optimal order

Scalability of coordination service



Our resource scheduling strategy (GRESMAN) demonstrates linear scalability in terms of required number of consumers to meet performance constraint

Outline

- Background & Challenges
- Our solution: 4CeeD
 - Curation Service
 - Coordination Service
- Evaluation
- **Conclusions**

Conclusions

- We present the *first* real-time data acquisition and analysis framework for materials-related and semiconductor fabrication areas
 - Novel curation service for nimble, comprehensive data collection and management
 - Novel scalable cloud-based system architecture for processing of heterogeneous multi-modal material-related data.

4CeeD's research impacts

- Implemented and deployed the 4CeeD system at the University of Illinois at Urbana-Champaign (UIUC)
 - ~30 test users from Micro and Nano Technology Lab (MNTL) and Material Research Lab (MRL)
- 4CeeD is open-sourced and is being evaluated at NIST
 - <https://4ceed.github.io/>
- Feedbacks for users:
 - Using 4CeeD achieves about **30% time saving** during experimental sessions (e.g., file transfer, save metadata, export previews, etc.)
 - This time saving translates into saving \$25 to \$30 each hour of lab session cost
 - Shorten time from digital capture to curation, interpretation & insights
 - Traditionally takes hours
 - Other benefits include better data preservation, exploration, and security

Thank you!

Back-up slides

Related work

- Systems focusing on making *existing datasets* more accessible & sharable
 - E.g.: DataUp, SkyServer
- Systems focusing on *long-term preservation* of data
 - E.g.: SEAD
- Systems providing *easy access* to grid/cloud infrastructure & focus on collaboration
 - E.g.: HubZero, NanoHub (for nanotechnology simulation); BrownDog, Data Conservancy Instance (for cloud-based data curation)

Compute layer implementation

