4CeeD Backend Services

4CeeD Backend Services

Robert Kaufman (rbkaufm2@Illinois.edu), Leah Espenhahn (leahe2@illinois.edu),
Beitong Tian (beitong2@illinois.edu), **Prof. Klara Nahrstedt (klara@illinois.edu)**

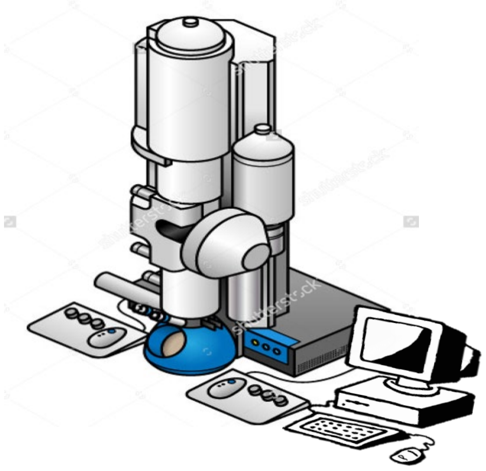
A timely and trusted curator and coordinator of scientific data

Outline

- 4CeeD Distributed Architecture, Backend Cloud Concepts and Services
  - What is 4Ceed and its goals
  - What is behind the 4CeeD Dashboard
  - 4CeeD Cloud Design and Deployment
  - How to deal with Aging Scientific Instrument

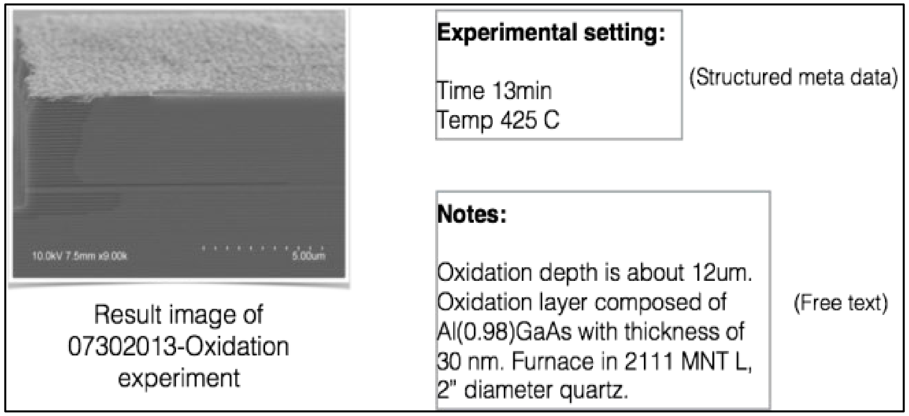
What is 4CeeD and its goals?

- Address Scientific Digital Data Acquisition, Curation and Sharing prior to Scientific Publication of Results via Private Cloud Storage Facility



Instrument

(in MRL/HMNTL/BI)


10.0kV 7.5mm x9.00k
5.00um

Result image of 07302013-Oxidation experiment

Experimental setting:

Time 13min
Temp 425 C

(Structured meta data)

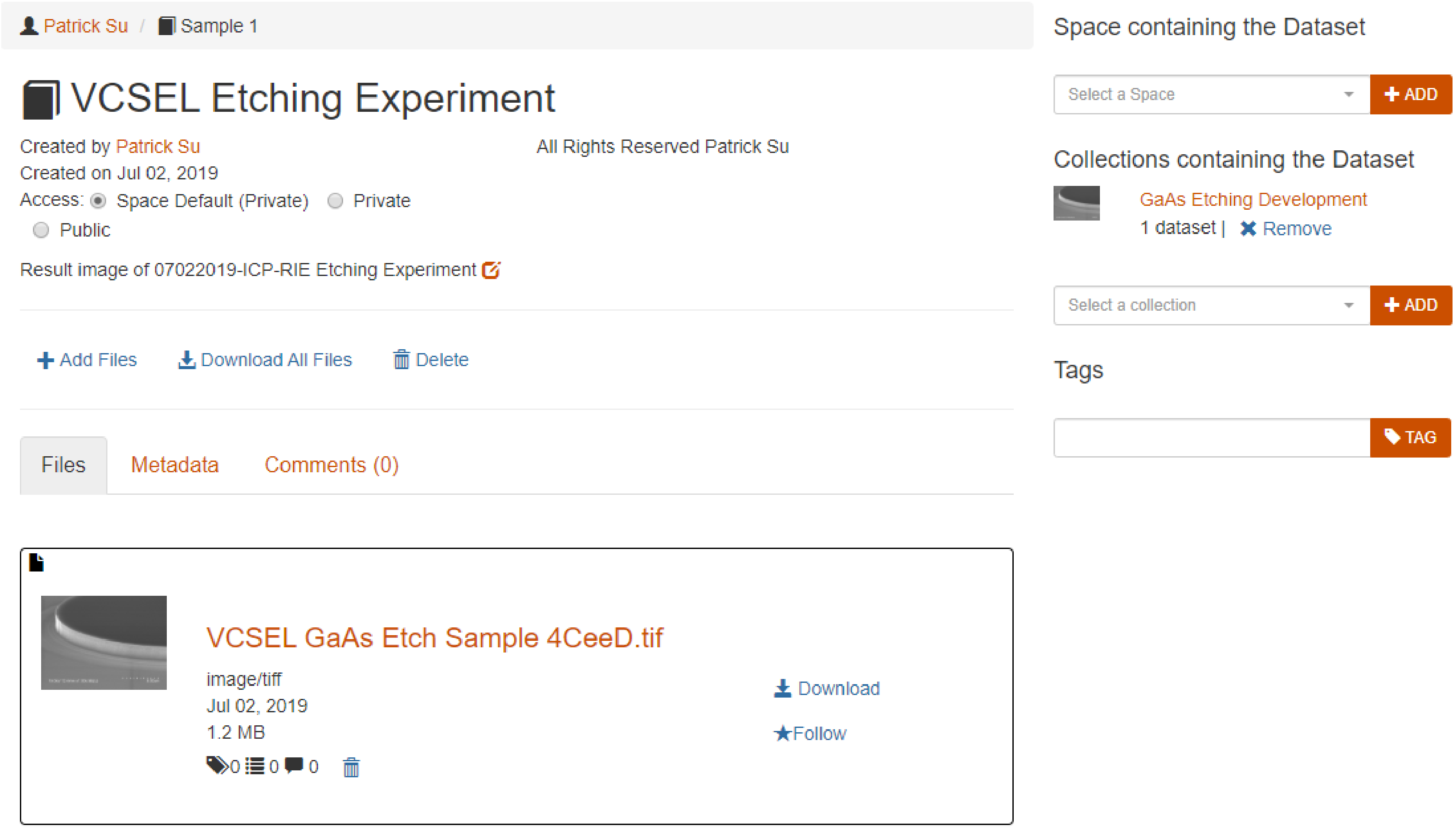
Notes:

Oxidation depth is about 12um. Oxidation layer composed of Al(0.98)GaAs with thickness of 30 nm. Furnace in 2111 MNT L, 2" diameter quartz.

(Free text)

Sample output data from SEM microscopy

How this looks from 4CeeD [Datasets]



Patrick Su / Sample 1

VCSEL Etching Experiment

Created by Patrick Su

Created on Jul 02, 2019

All Rights Reserved Patrick Su

Access: ● Space Default (Private) ○ Private ○ Public

Result image of 07022019-ICP-RIE Etching Experiment

VCSEL GaAs Etch Sample 4CeeD.tif

image/tiff

Jul 02, 2019

1.2 MB

0 0 0

Space containing the Dataset

Collections containing the Dataset

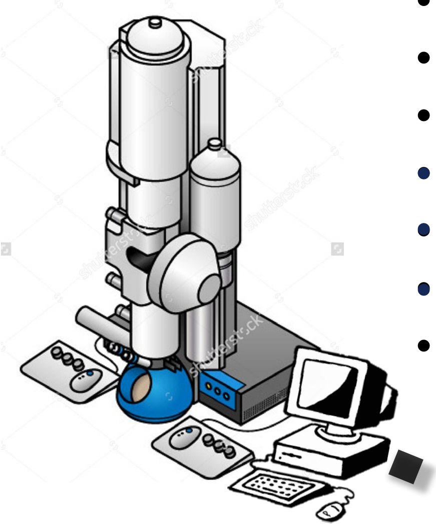
GaAs Etching Development

1 dataset | ✖ Remove

Tags

- 4CeeD is designed to present only pertinent information for quick understanding of the experiment

Scenario with 4CeeD Integration



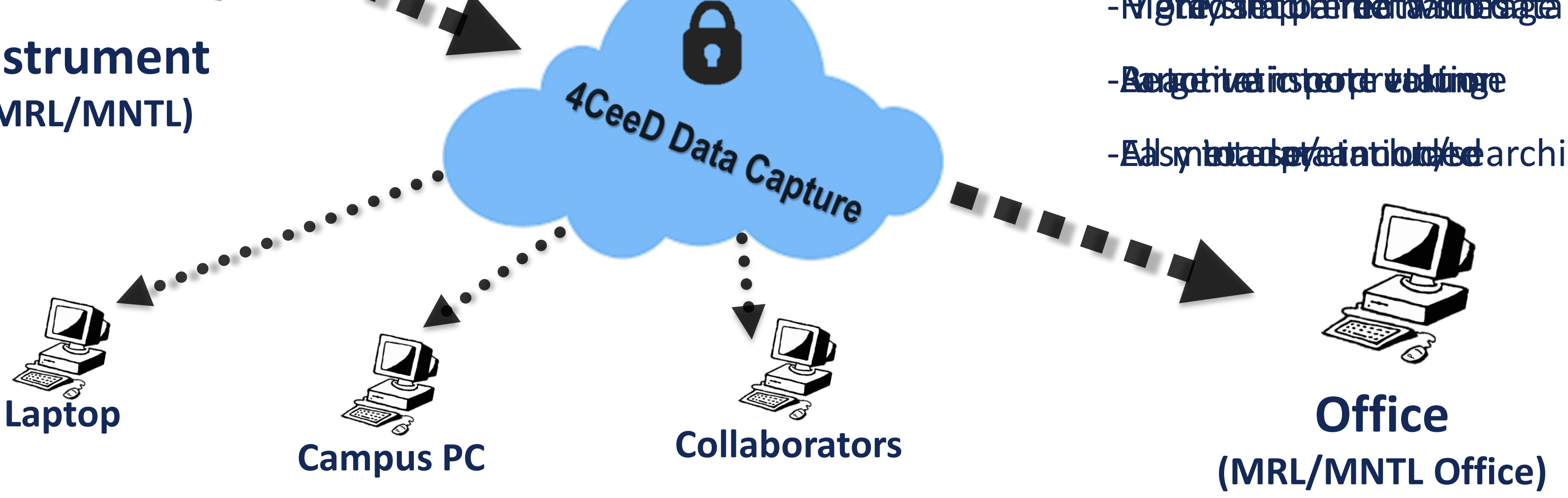
- Fabricate experimental sample
- Prepare analytical sample
- Bring sample to instrument for analysis
- **Extract data (NO FILE CONVERSION)**
- **Transport data to office computer (DIRECT)**
- **Analyze data (REAL TIME)**
- Repeat per iteration

Bendquleteb Dianterface

-Mghdysianpdaifielaoitinedsgta

-Reagcrivetaicsporpe veaktinge

-Ealsymetoatasepytaintioud/searching



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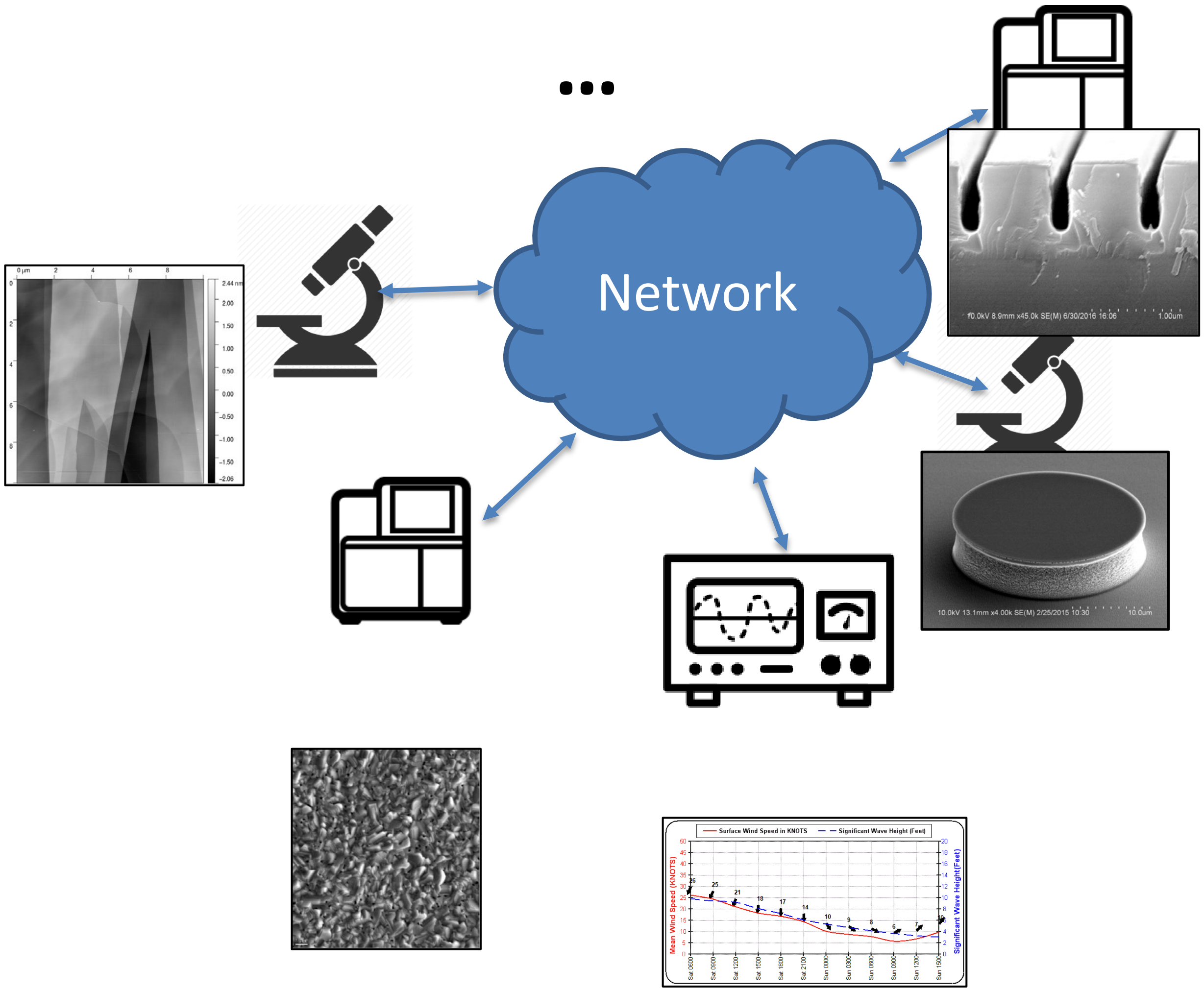
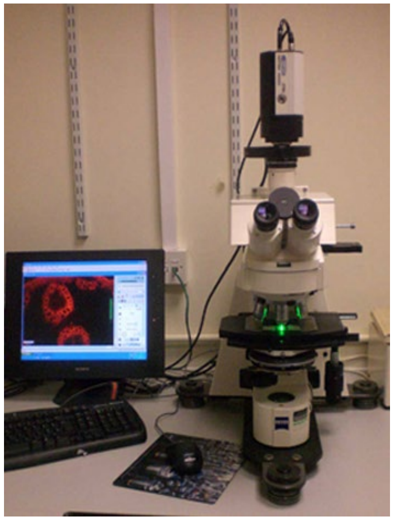
Increasingly data-driven and interdisciplinary scientific research in Physical Sciences and Live Sciences

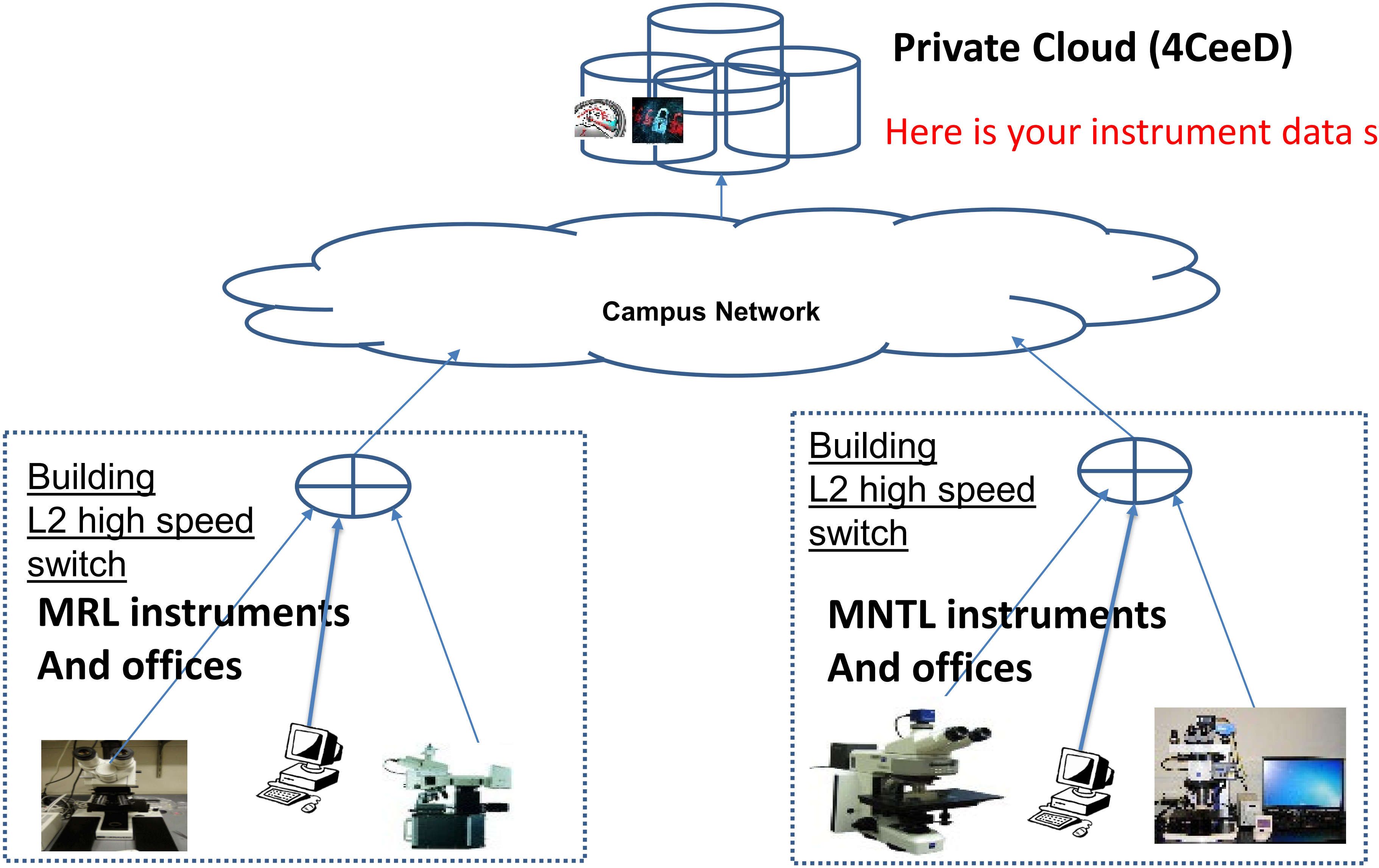
- *Key enabling factor*: Network connected scientific instruments capable of real-time data capture


…
Network
10.0kV 8.9mm x45.0k SE(M) 6/30/2016 16:06
1.00um
10.0kV 13.1mm x4.00k SE(M) 2/25/2015 10:30
10.0um
Surface Wind Speed in KNOTS
Significant Wave Height (Feet)
Mean Wind Speed (KNOTS)
Significant Wave Height(Feet)



Digital microscope

4CeeD Design Considerations - Distributed View



Private Cloud (4CeeD)

Here is your instrument data stored

Campus Network

Building L2 high speed switch

MRL instruments

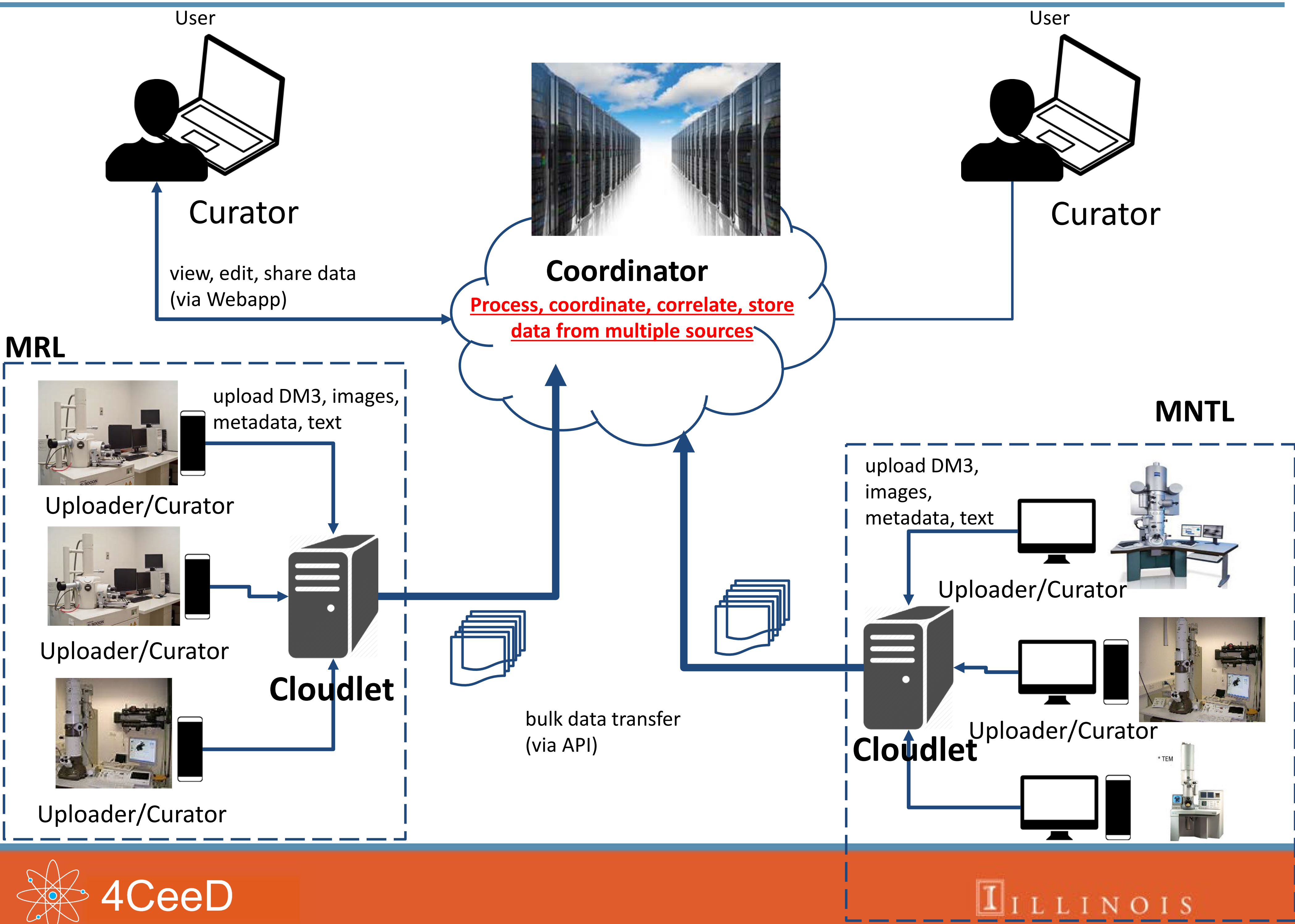
And offices

Building L2 high speed switch

MNTL instruments

And offices

4Ceed Design Considerations – Component View



User

Curator

view, edit, share data (via Webapp)

Coordinator

Process, coordinate, correlate, store data from multiple sources

User

Curator

MRL

upload DM3, images, metadata, text

Uploader/Curator

Uploader/Curator

Uploader/Curator

Cloudlet

bulk data transfer (via API)

MNTL

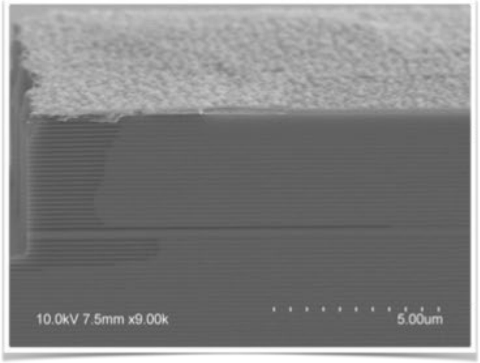
upload DM3, images, metadata, text

Uploader/Curator

Uploader/Curator

Cloudlet

4CeeD Design Considerations - Multimodal data format View



Result image of 07302013-Oxidation experiment

Experimental setting:

Time 13min
Temp 425 C

(Structured meta data)

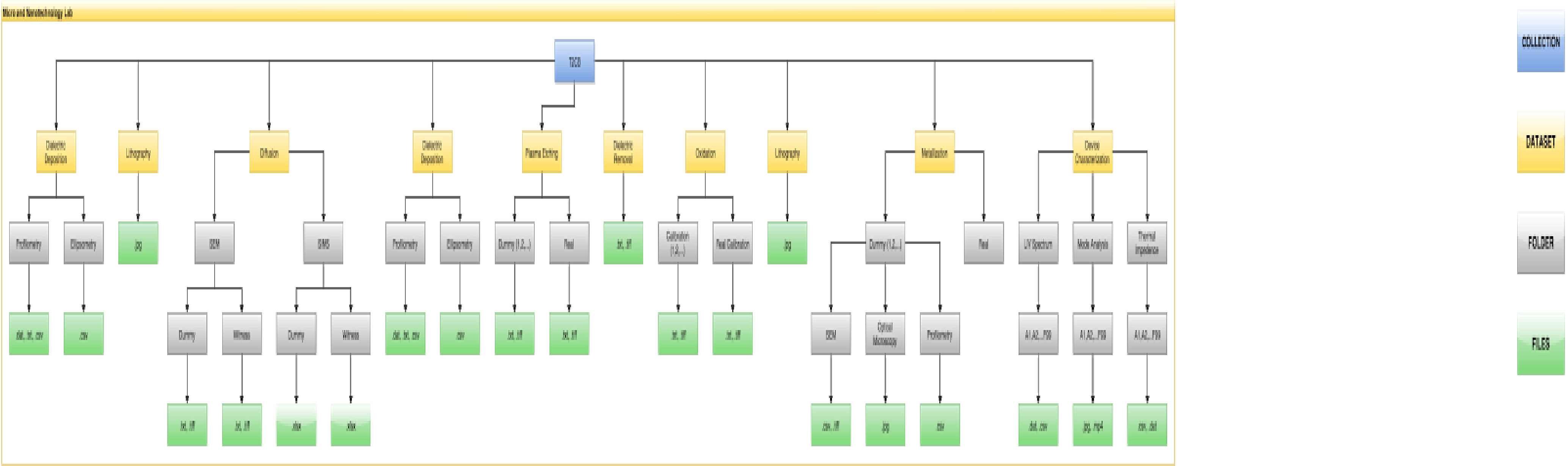
Notes:

Oxidation depth is about 12um. Oxidation layer composed of Al(0.98)GaAs with thickness of 30 nm. Furnace in 2111 MNT L, 2" diameter quartz.

(Free text)

A lot of useful information is hidden in unstructured text

Example of multimodal experimental d

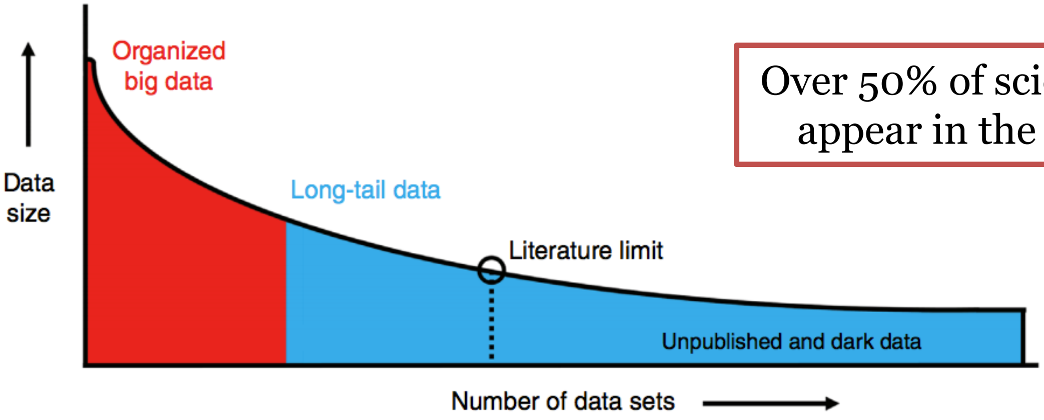


Heterogeneity of experimental data (Spaces, Collections Datasets)

4CeeD Design Considerations - long-tail scientific data

- Related efforts mainly focus on ***homogenous, well-organized data*** in an offline or batch manner

- Much less effort has been on ***long-tail scientific data***:
  - Small/medium sized data sets collected during day-to-day research
  - "Dark data", e.g., unpublished data of failed experiments



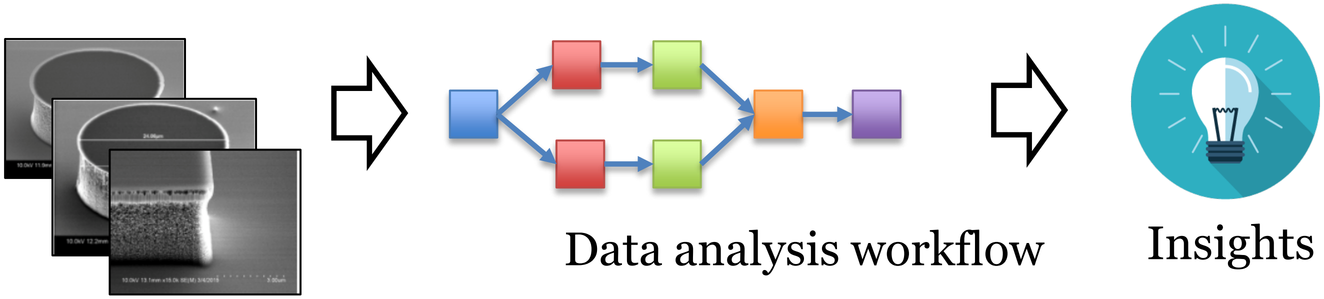
Over 50% of scientific findings do not appear in the published literature

Long-tail scientific data

Source: Ferguson et al. *Nature neuroscience* 17.11 (2014)

4CeeD Design Considerations - Long-tail scientific data processing challenges

- ***Challenges***: Support execution of heterogeneous types of data processing & analysis workflows

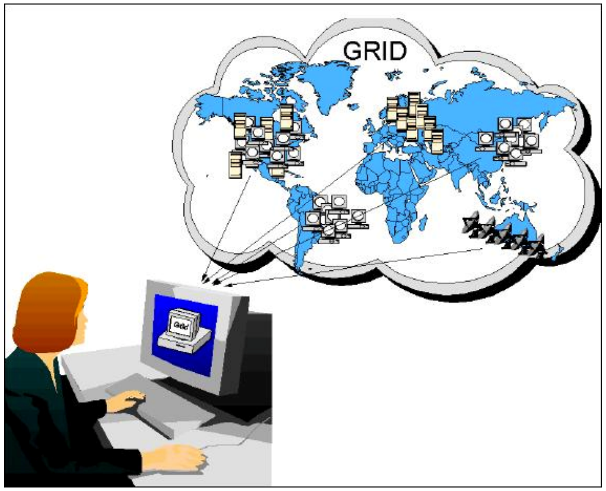


Raw data

Data analysis workflow

Insights

- Previous work often employs a monolithic approach in workflow implementation and execution
  - E.g.: Pegasus, Taverna, Kepler, etc.
  - Run on large-scale & homogeneous datasets

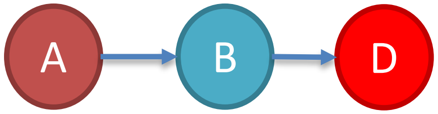


Executing workflows on grid infrastructure

4CeeD Design Considerations – Task Workflows

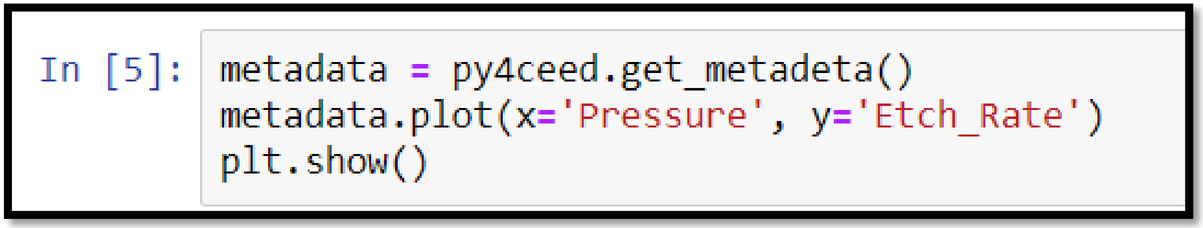
- Application is a Computational Workflow

- Workflow is Set of Tasks (e.g., A, B, C, D) executing over materials data



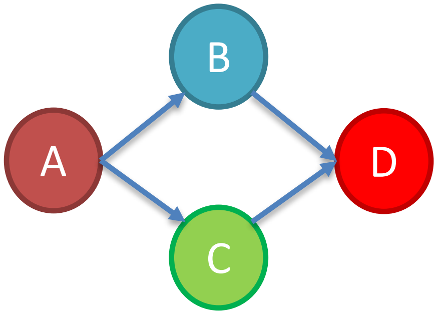
Workflow type 1

1. Example of a Task C: “Plotting a graph”



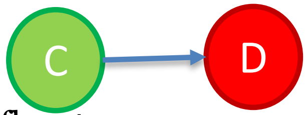
```
In [5]: metadata = py4ceed.get_metadeta()
        metadata.plot(x='Pressure', y='Etch_Rate')
        plt.show()
```

2. Example of a Task D: “Filter Data”



Workflow type 2

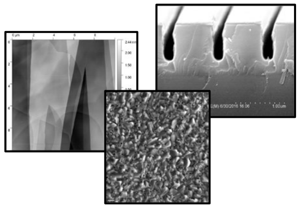
In [6]: metadata[metadata [‘Pressure’] >=7]



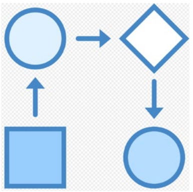
Workflow type 3

- Other examples of tasks: Extraction of features from an image, compression of image, …

Summary of 4CeeD Design Challenges



- ➢ Heterogeneous scientific data management and processing



- ➢ Support ad hoc and complex data analysis workflows

- ➢ Shorten time from digital capture to interpretation & insights

- ➢ Real-time data capture and acquisition

- ➢ Analytics support to gain insights from data

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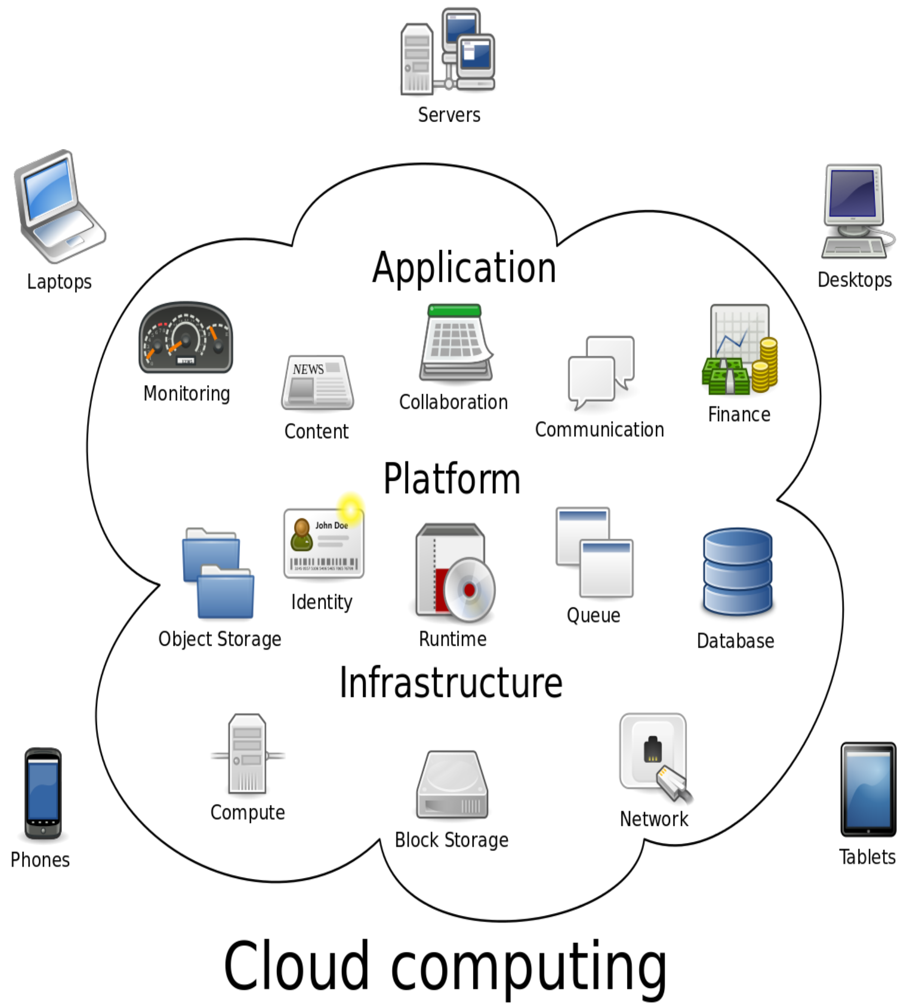
4CeeD Cloud Design

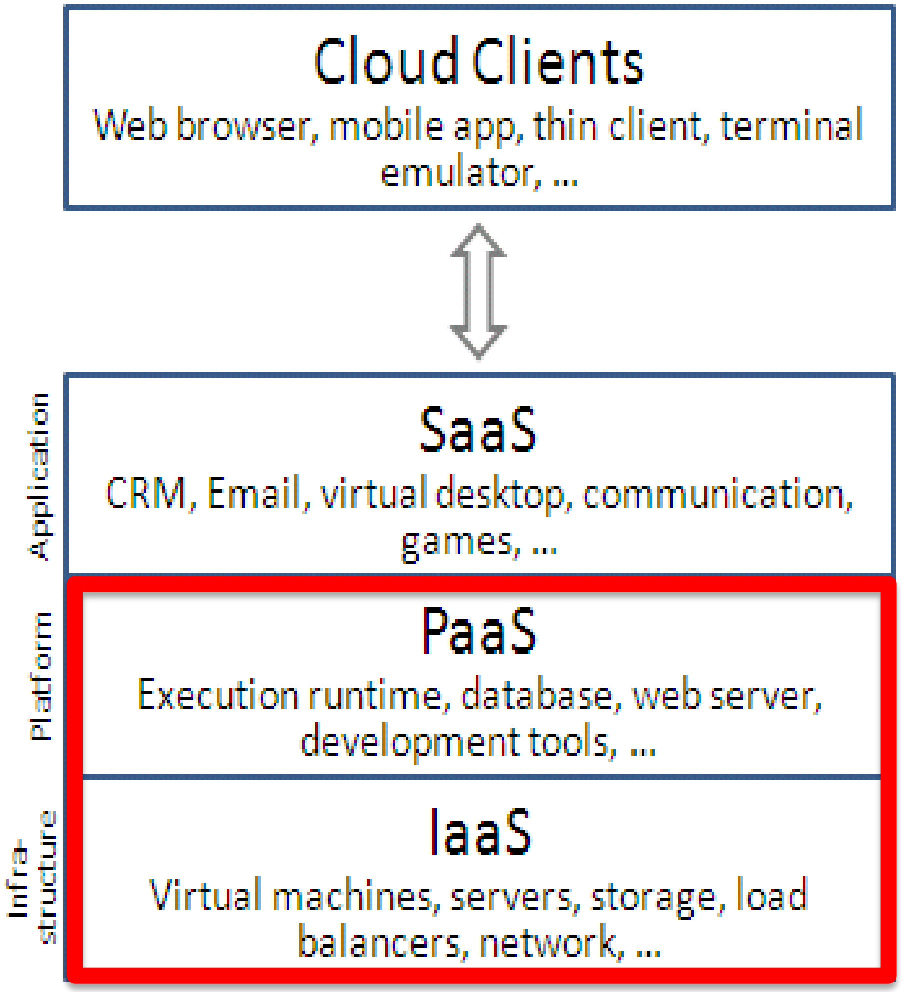
✓ Cloud Concept

✓ Micro-service execution environment

✓ Data Management

Cloud Computing Concept





Cloud Clients

Web browser, mobile app, thin client, terminal emulator, ...

SaaS

CRM, Email, virtual desktop, communication, games, ...

PaaS

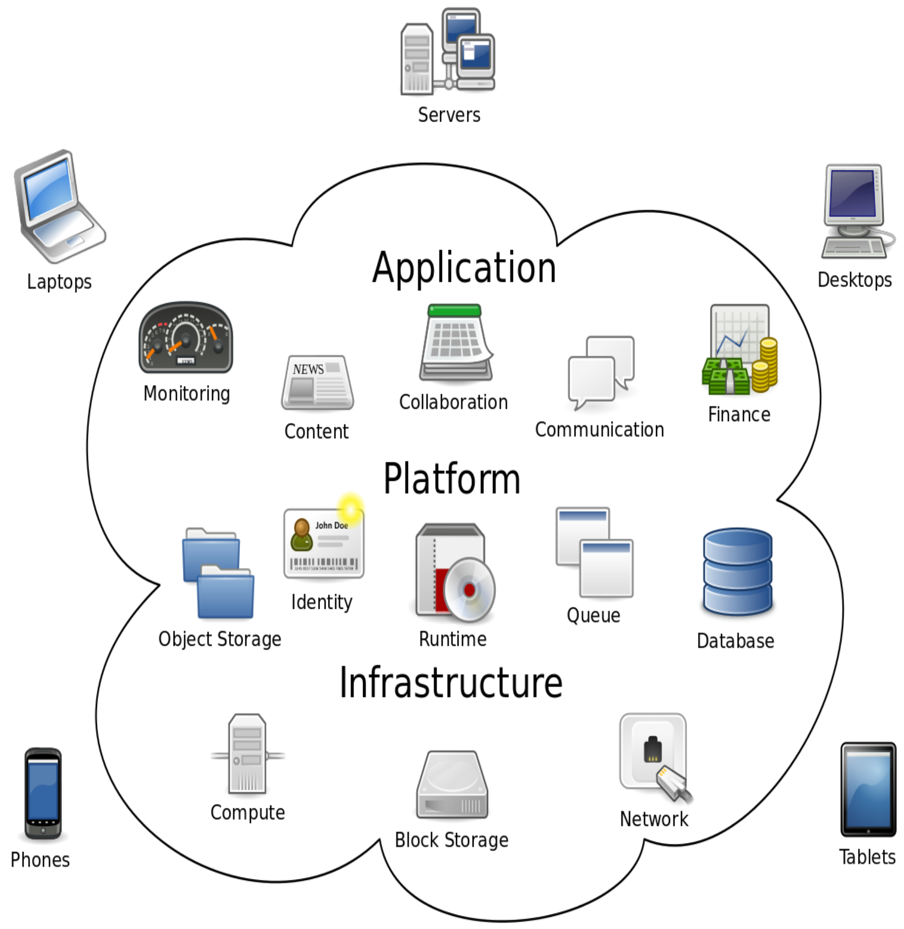
Execution runtime, database, web server, development tools, ...

IaaS

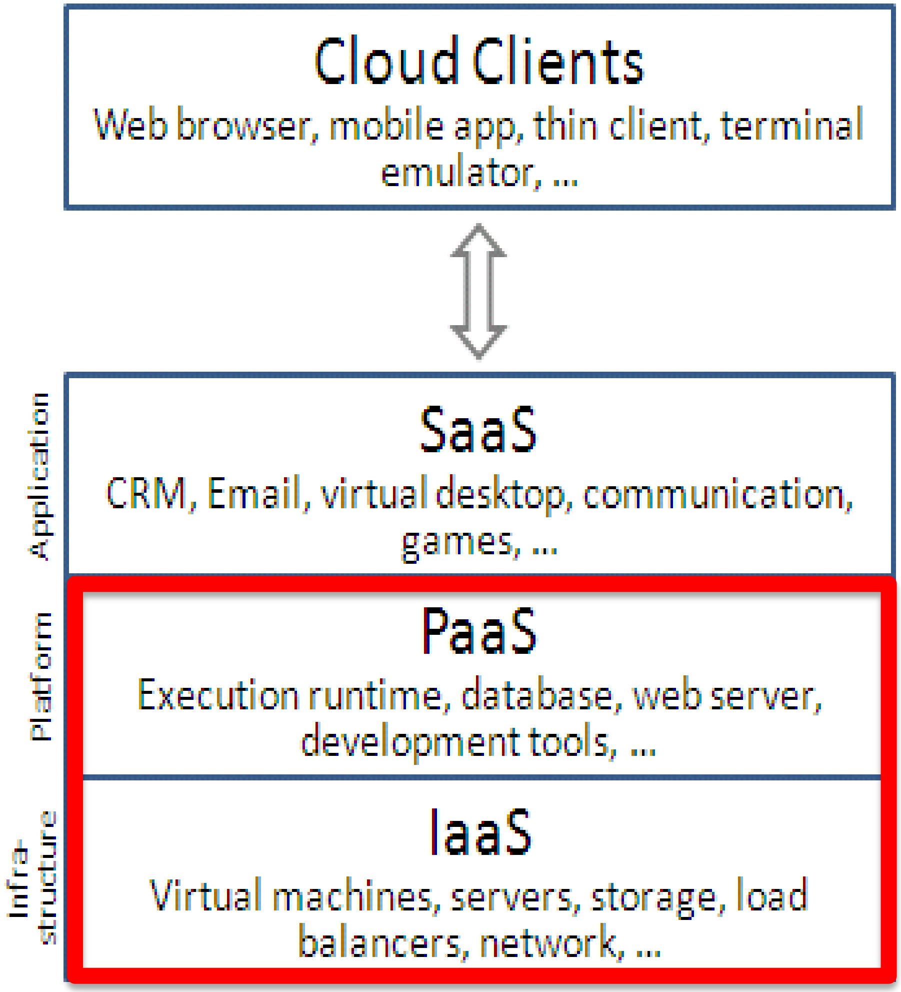
Virtual machines, servers, storage, load balancers, network, ...

Figure Source: Wikipedia

Cloud Computing Concept



Cloud computing



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IaaS

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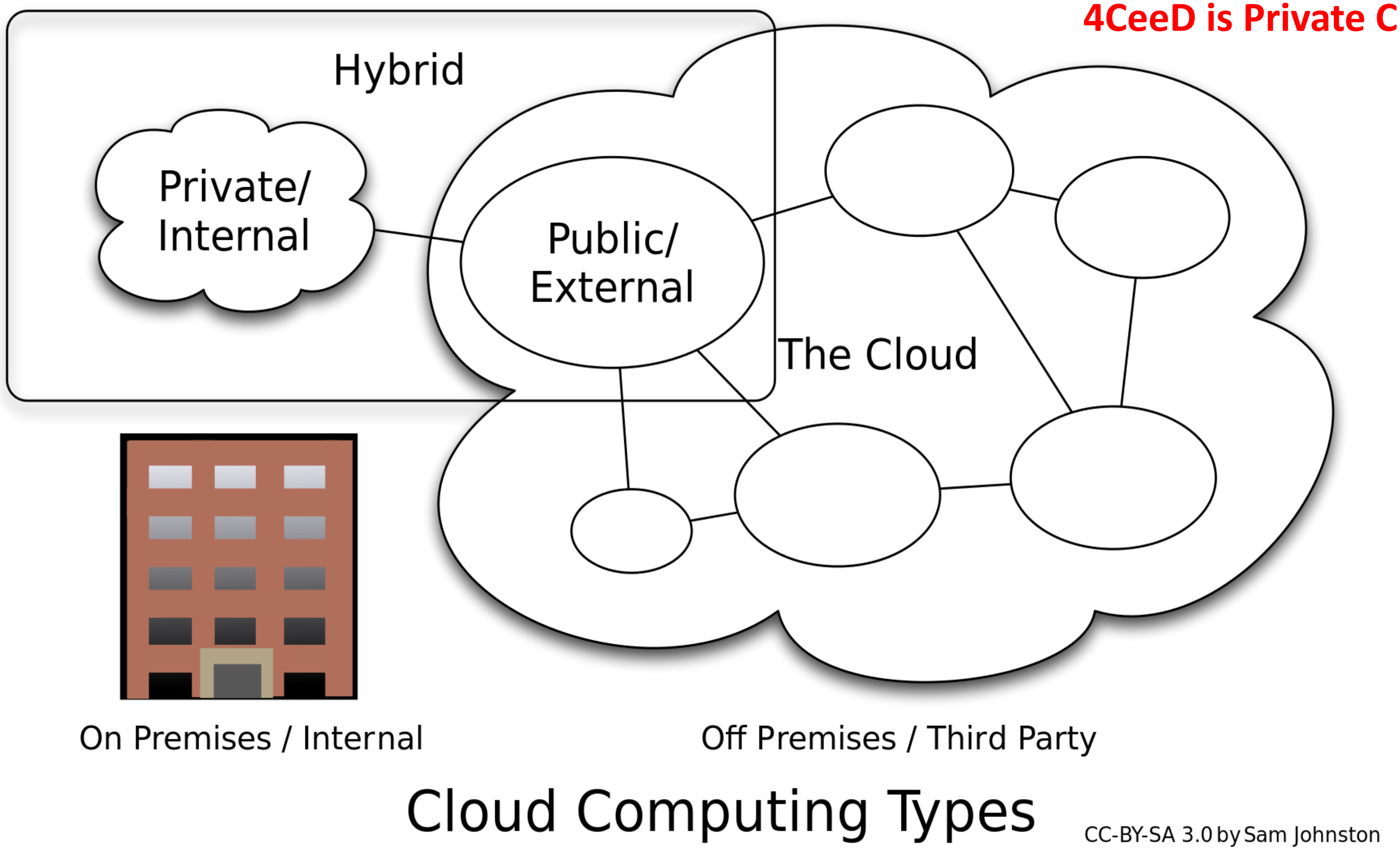
4CeeD Cloud

Private and Public Clouds

4CeeD is Private Cloud



CC-BY-SA 3.0 by Sam Johnston

Figure Source: Wikipedia

Example of Cloud Components

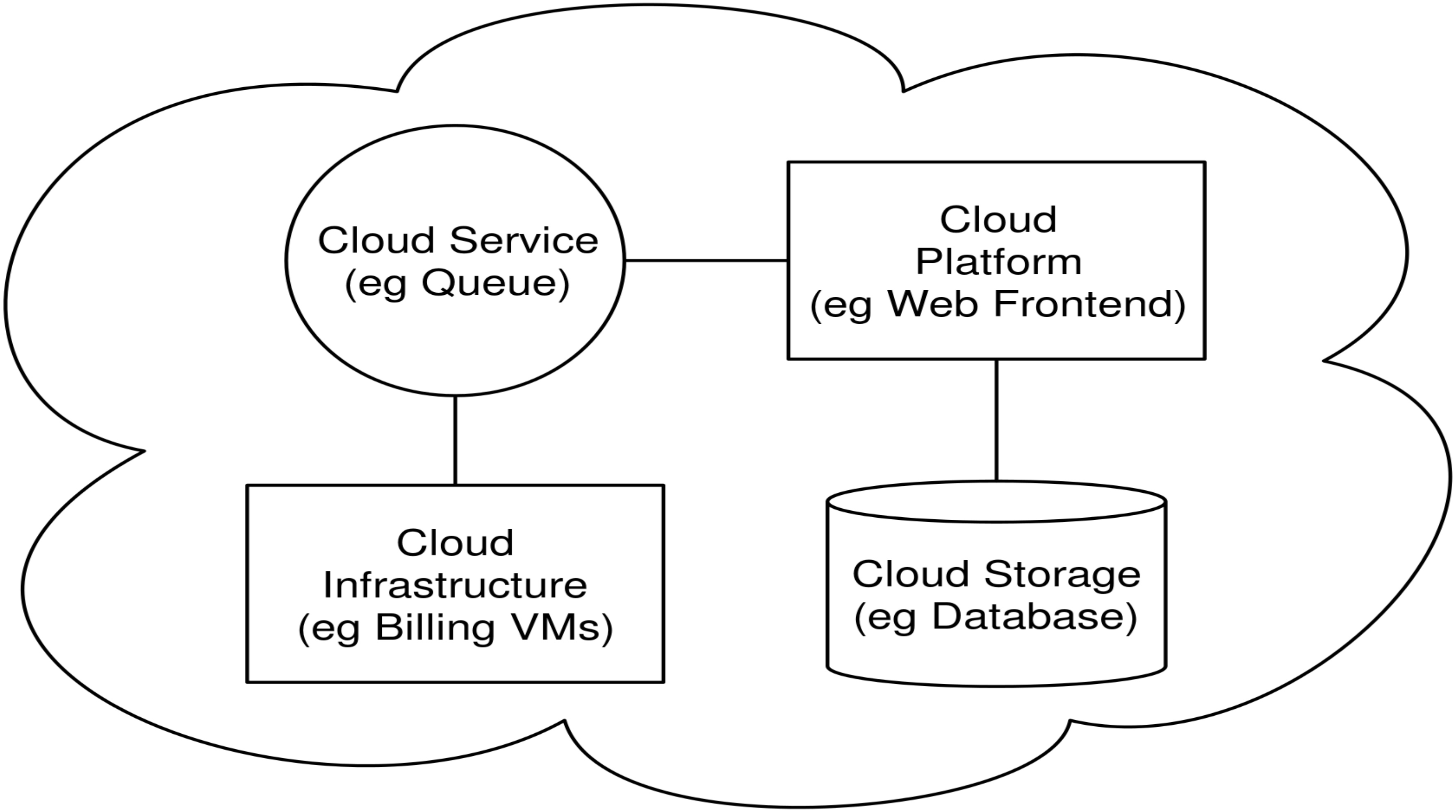
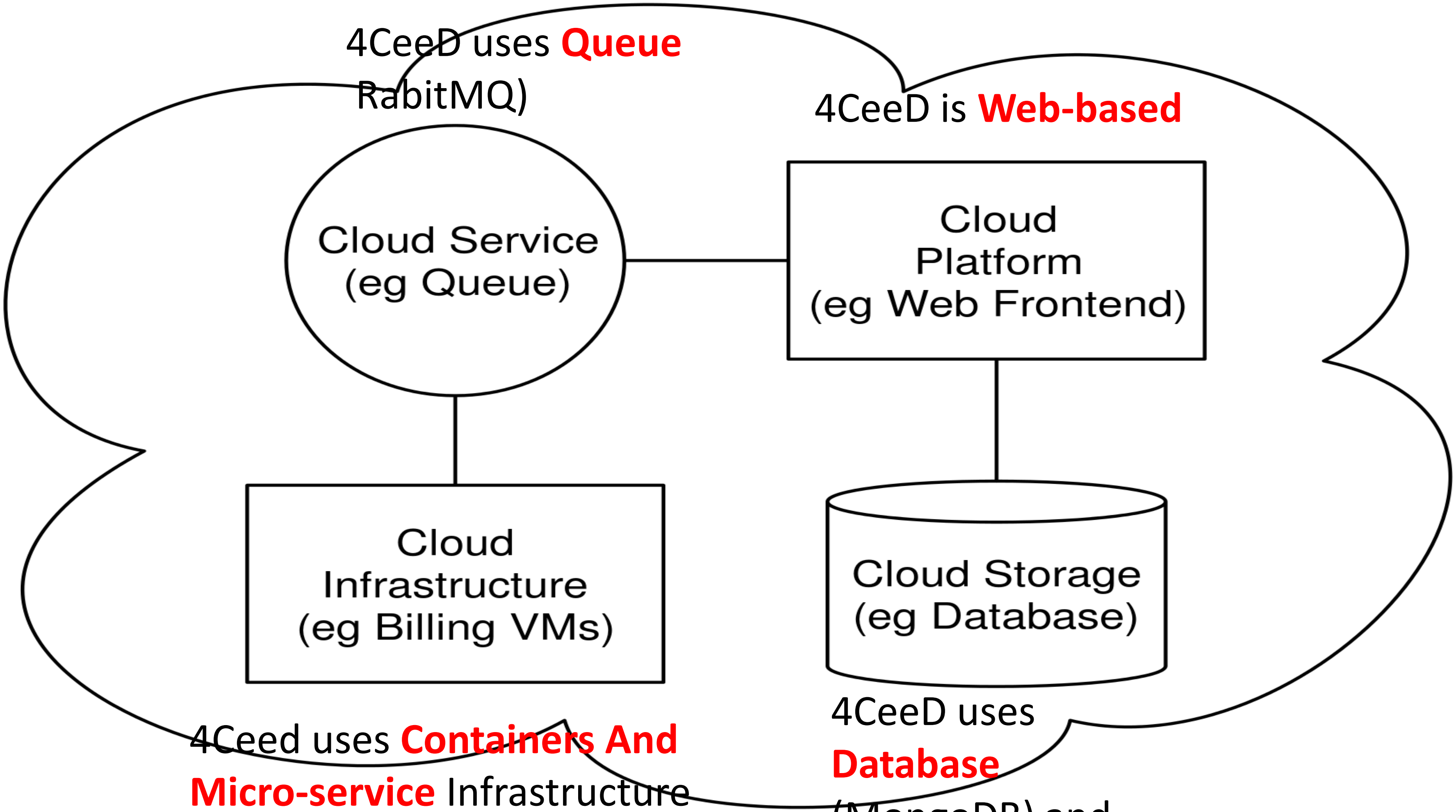


Figure Source: Wikipedia

4CeeD Cloud Components



4CeeD uses **Queue** RabitMQ)

4CeeD is **Web-based**

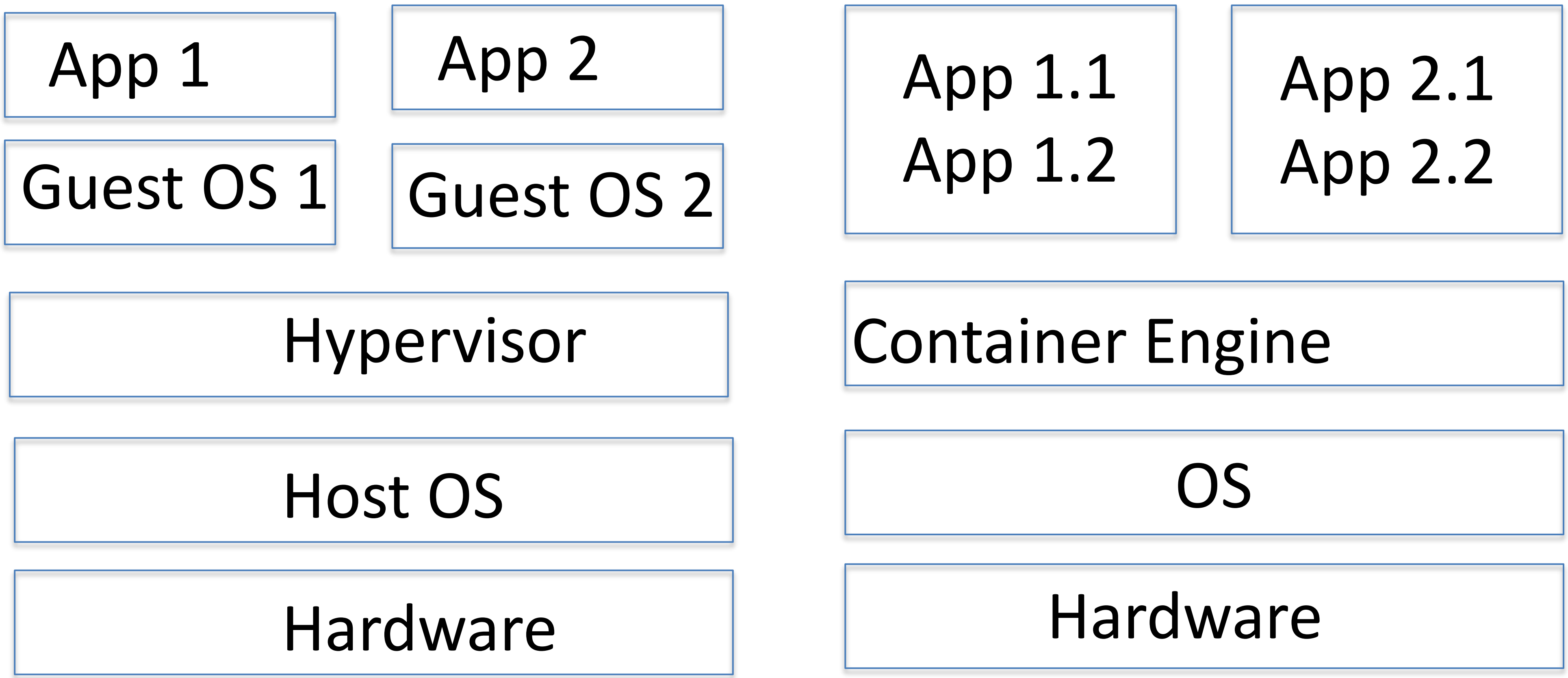
4Ceed uses **Containers And Micro-service** Infrastructure (Docker and Kubernates/Docker Compose)

4CeeD uses **Database** (MongoDB) and Filesystem (HFS)

Figure Source: Wikipedia

Hardware Virtualization

- Two types of hardware virtualization
  - Emulation-based virtualization
  - Container-based virtualization



App 1

Guest OS 1

App 2

Guest OS 2

Hypervisor

Host OS

Hardware

App 1.1
App 1.2

App 2.1
App 2.2

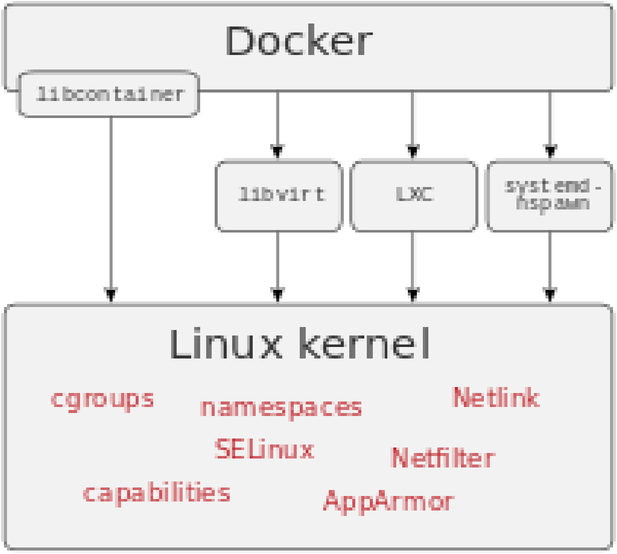
Container Engine

OS

Hardware

Container

- Container – Software Unit that bundles its own software, libraries and configuration files
  - Containers are isolated from one another and can communicate with each other through well-defined channels.
  - All containers are run by a single operating system kernel and therefore use fewer resources than virtual machines.
  - Virtual Container, called Docker, is professional software package developed by *Docker Inc*. as part of PaaS.

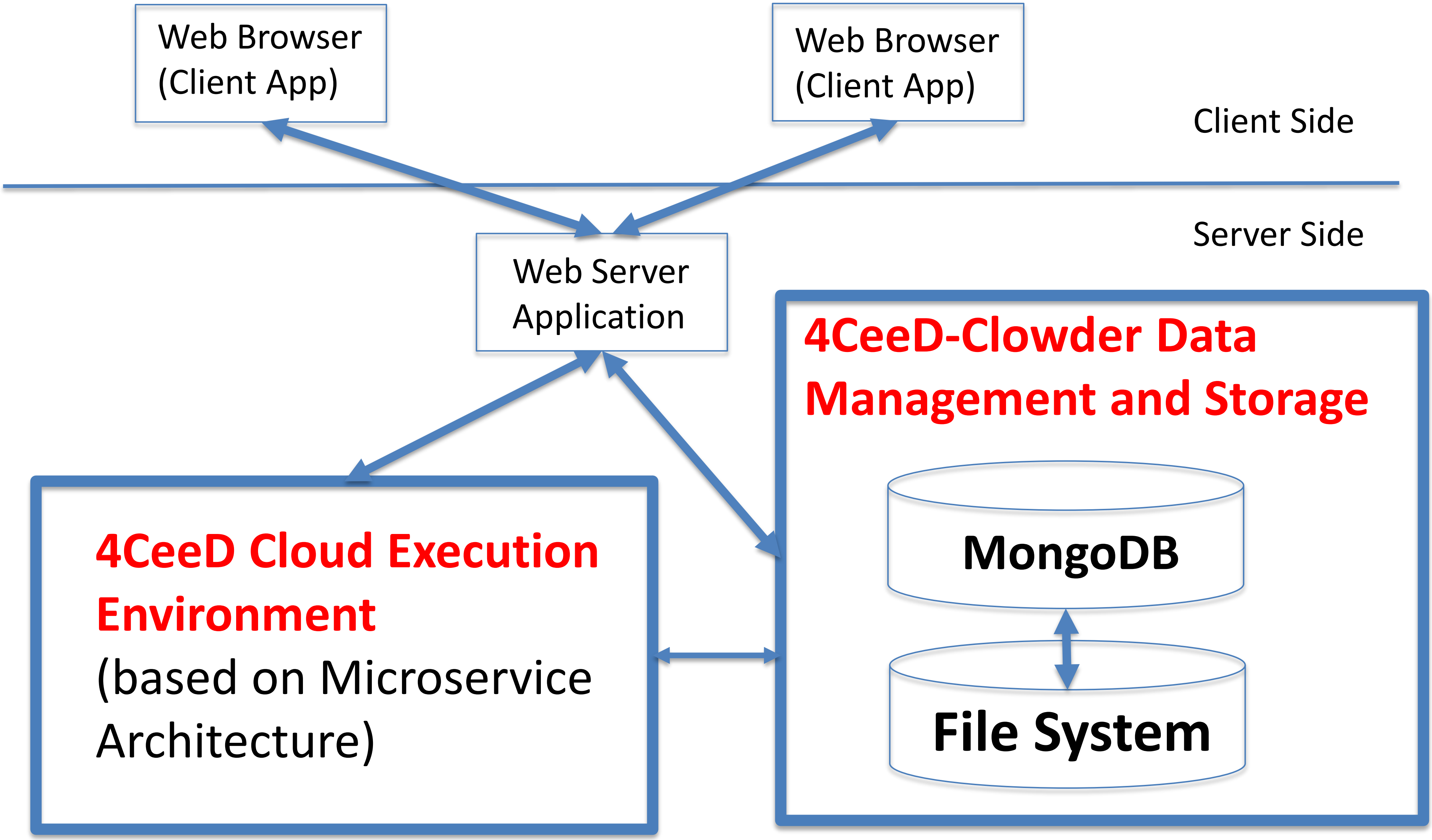


Source: Wikipedia

Micro-Service

- Microservice
  - a software development technique (a variant of the service-oriented architecture (SOA) structural style)
  - an application is arranged via microservices as a collection of loosely coupled services.
- In a microservices architecture, services are *fine-grained* and the protocols are *lightweight*.

4CeeD Cloud Architecture Components – Putting it Together


Web Browser (Client App)

Web Browser (Client App)

Client Side

Server Side

Web Server Application

4CeeD-Clowder Data Management and Storage

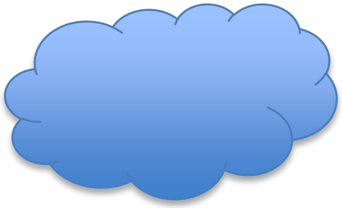
MongoDB

File System

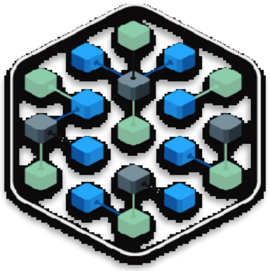
4CeeD Cloud Execution Environment

(based on Microservice Architecture)

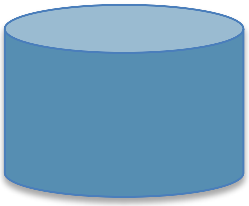
4CeeD Cloud Design



✓ Cloud Concept



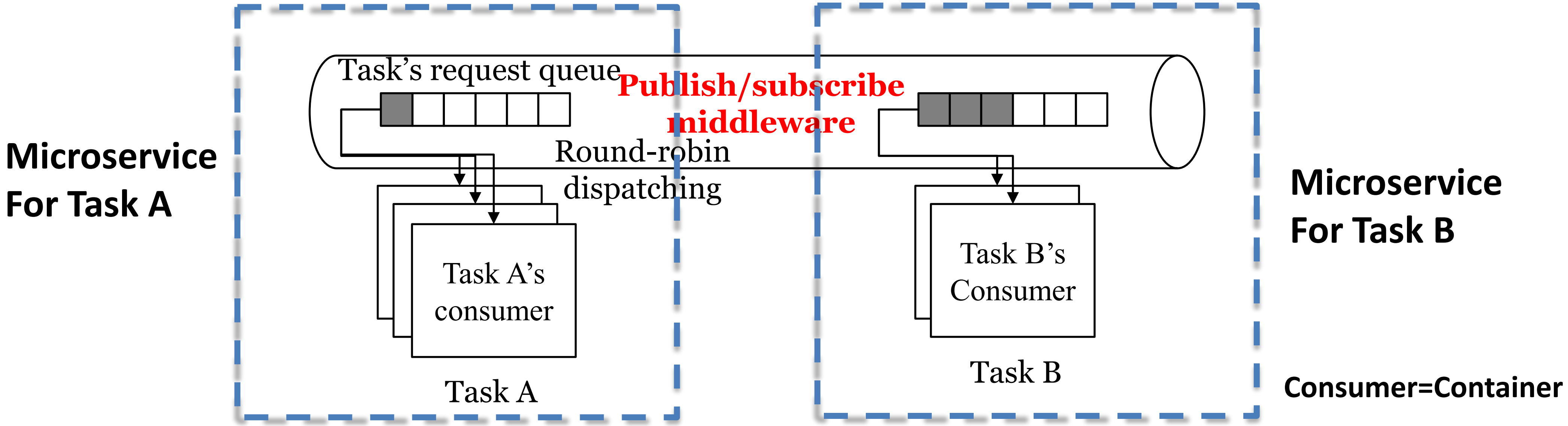
✓ Micro-service execution environment



✓ Data Management

In Cloud - Micro-service execution environment

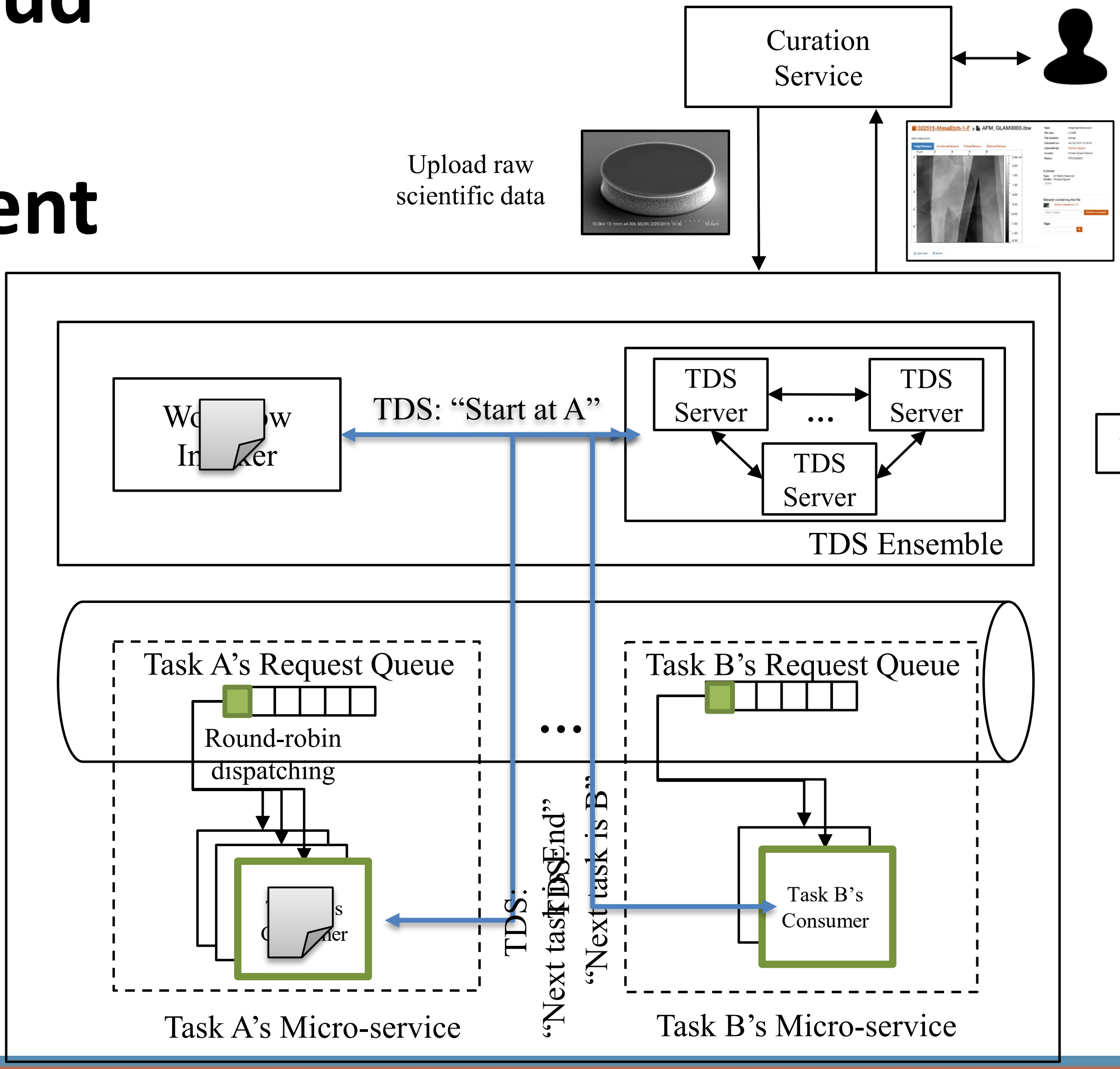
- ***Micro-services over monoliths***: Each task is modeled as a micro-service
  - Use publish-subscribe middleware to connect between micro-services



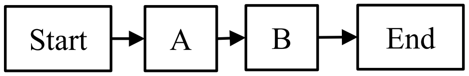
- **Separate task dependencies** from task implementation & deployment
  - Enable flexible workflow composition
  - Task-level resource provisioning

4CeeD Executing scientific data processing workflow

4CeeD Cloud Execution Environment



Task Graph



TDS – Task Dependency Service

Task A: Example - Color Extraction from TEM Image

Task B: Example - Detect Edge in TEM Image

4CeeD Cloud Design

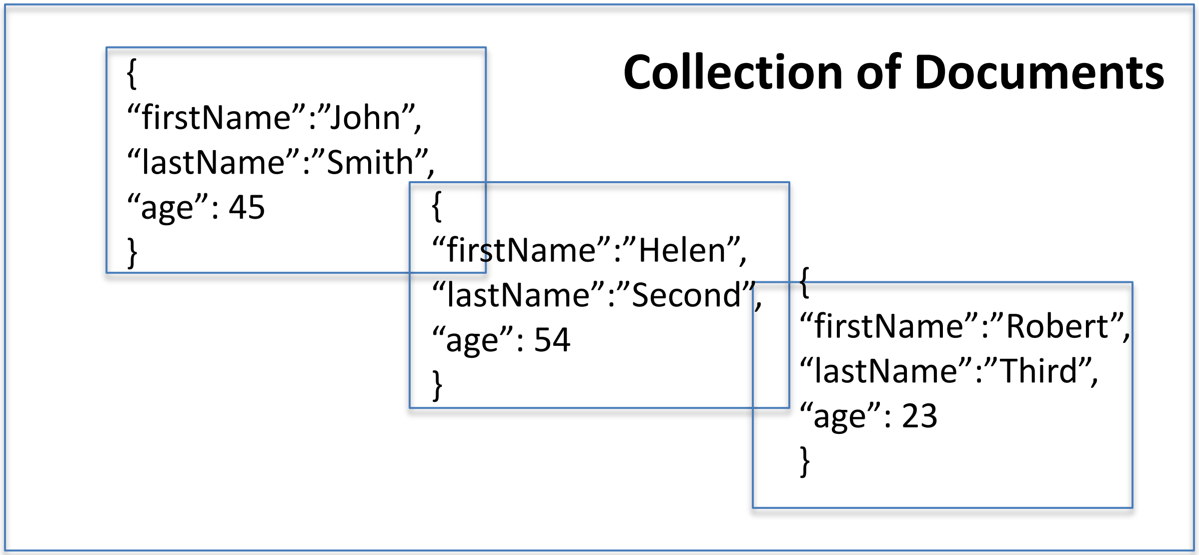
- ✓ Cloud Concept
- ✓ Micro-service execution environment
- ✓ Data Management

4CeeD Data Management and Storage

- 4CeeD uses NoSQL database to store spaces, collection and dataset metadata and some data
- MongoDB is open-source NoSQL database
  - Non-relational database (NoSQL), i.e., data storage and retrieval are not organized in tabular relations
  - Developed due to the limits of relational databases and their scalability to very large datasets (scale was limited because of the requirement for consistency in relational databases)
  - 4 models of NoSQL
    - key-value stores,
    - graph stores,
    - column stores,
    - document stores

4CeeD-Clowder Data Management and Storage (2)

- Document Store Model
  - Store data in semi-structured form, called documents
  - Documents encoded in standardized format such as
    - XML format
    - Javascript Object Notation (JSON)
- Example of Document store database



Collection of Documents

```
{
"firstName":"John",
"lastName":"Smith",
"age": 45
}
```

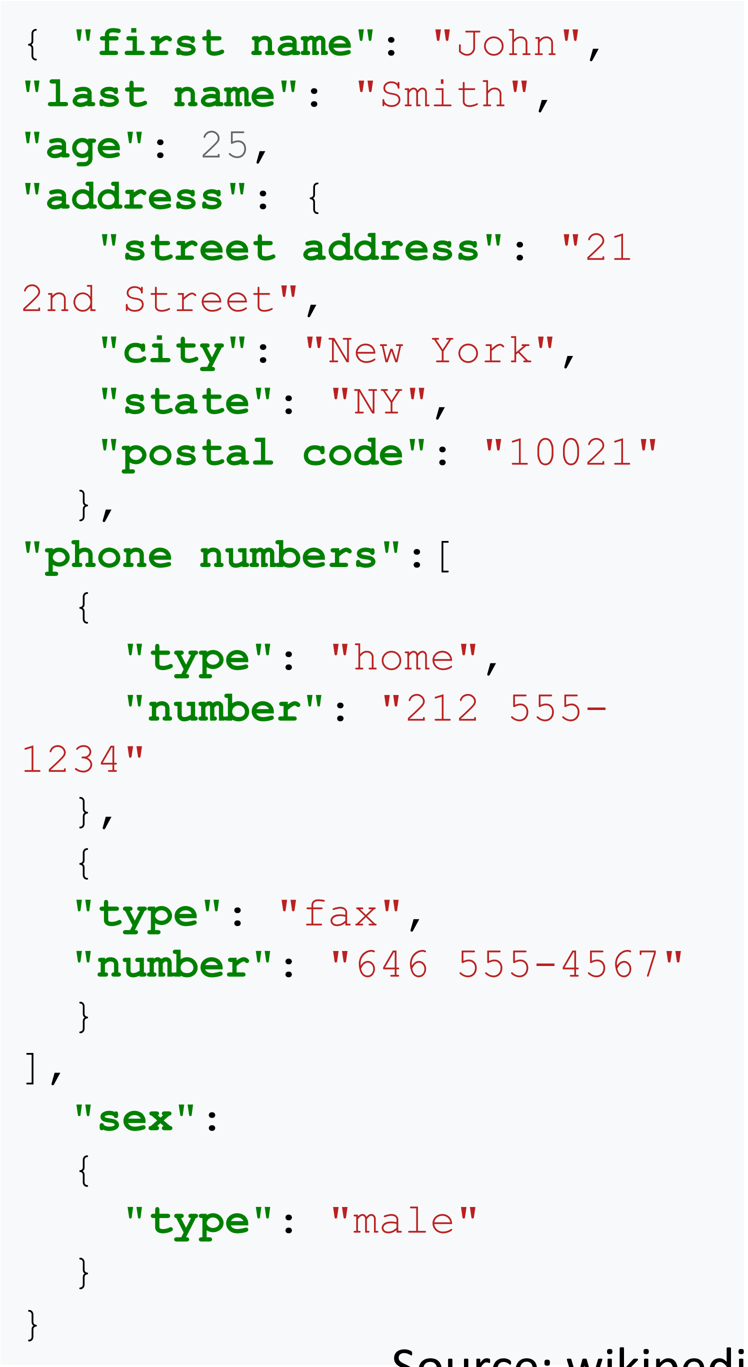
```
{
"firstName":"Helen",
"lastName":"Second",
"age": 54
}
```

```
{
"firstName":"Robert",
"lastName":"Third",
"age": 23
}
```

Source: P. Bajcsy et al. “Web Microanalysis
Of Big Image Data”, Spring, 2018

4CeeD Data Management and Storage (3)

- 4CeeD uses MongoDB
- In MongoDB
  - Documents are stored in a JSON-like format
- Example of JSON-like Format
- 4CeeD Data Model organizes projects into collections, datasets, and files.
- These can then be shared in spaces. 4CeeD utilizes and modifies NCSA Clowder data management system.

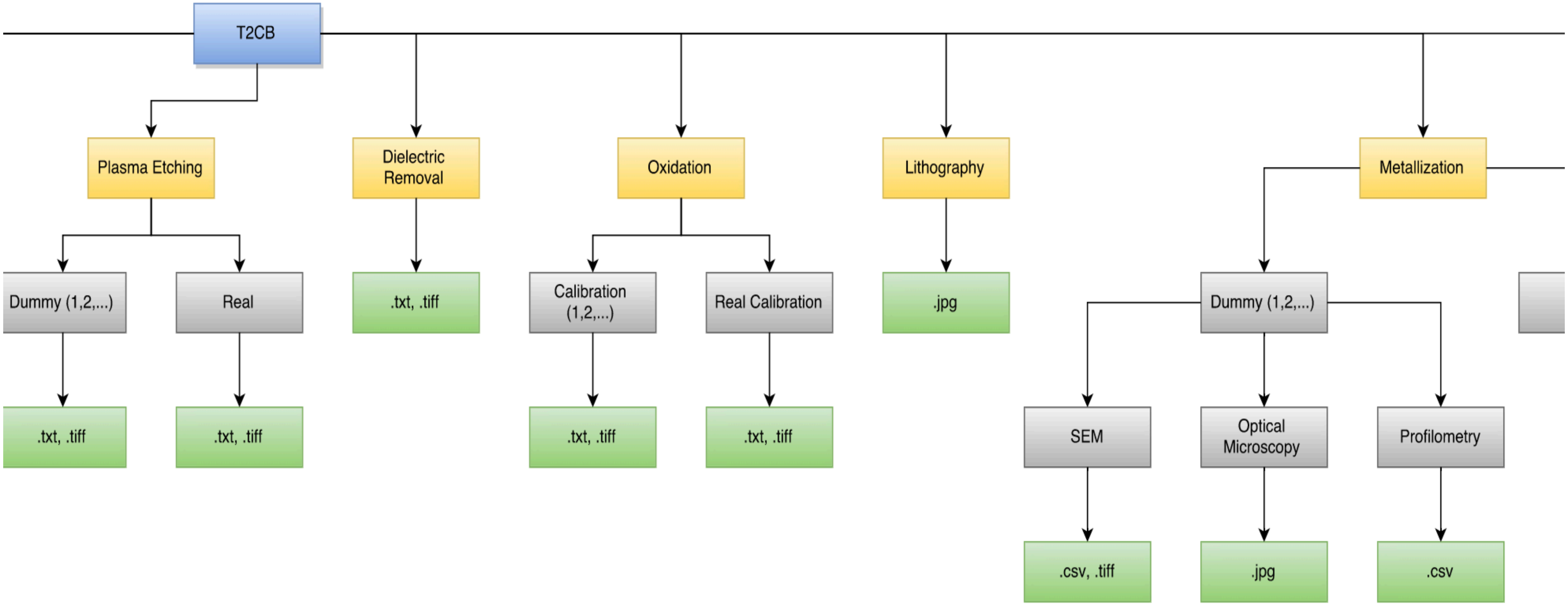


```
{ "first name": "John",
"last name": "Smith",
"age": 25,
"address": {
   "street address": "21
2nd Street",
   "city": "New York",
   "state": "NY",
   "postal code": "10021"
  },
"phone numbers":[
  {
    "type": "home",
    "number": "212 555-
1234"
  },
  {
  "type": "fax",
  "number": "646 555-4567"
  }
],
  "sex":
  {
    "type": "male"
  }
}
```

Source: wikipedia

4CeeD Smart Data Management

Collection: T2CB; **Datasets**: PlasmaEtching, …., Metalization
Folders: Calibration, SEM, Optical Microscopy…, **Files**: txt files, tiff files, …



4CeeD Deployment – Cloud Production System

Goals:

- Redundancy
- Availability
- Scalability

Storage Layer:

- **40 TB (20 TB per investor)**
- Replicated for redundancy

Compute Layer:

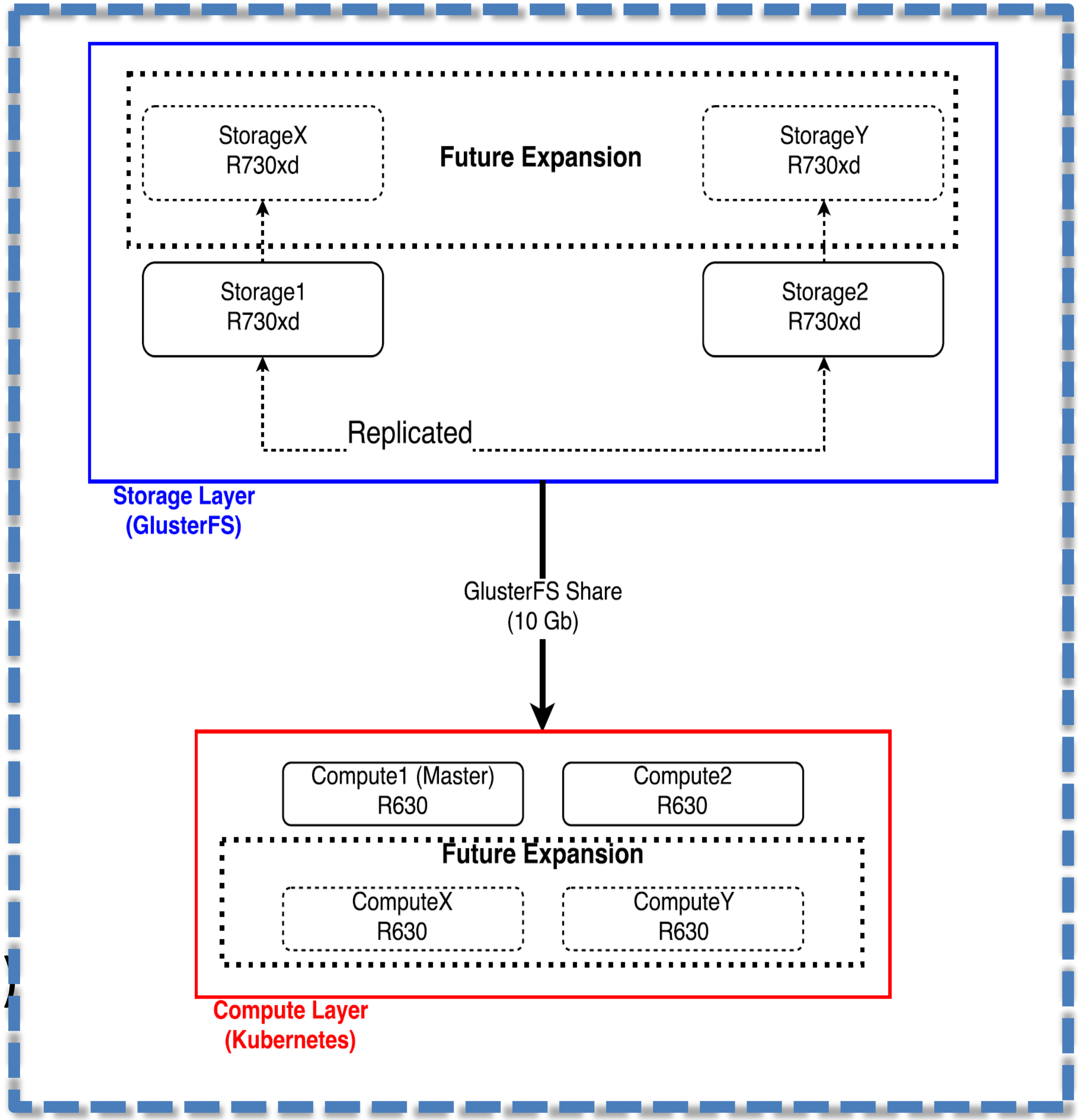
- Docker container

orchestration (Kubernetes)

- Single master

(High Available masters in future)

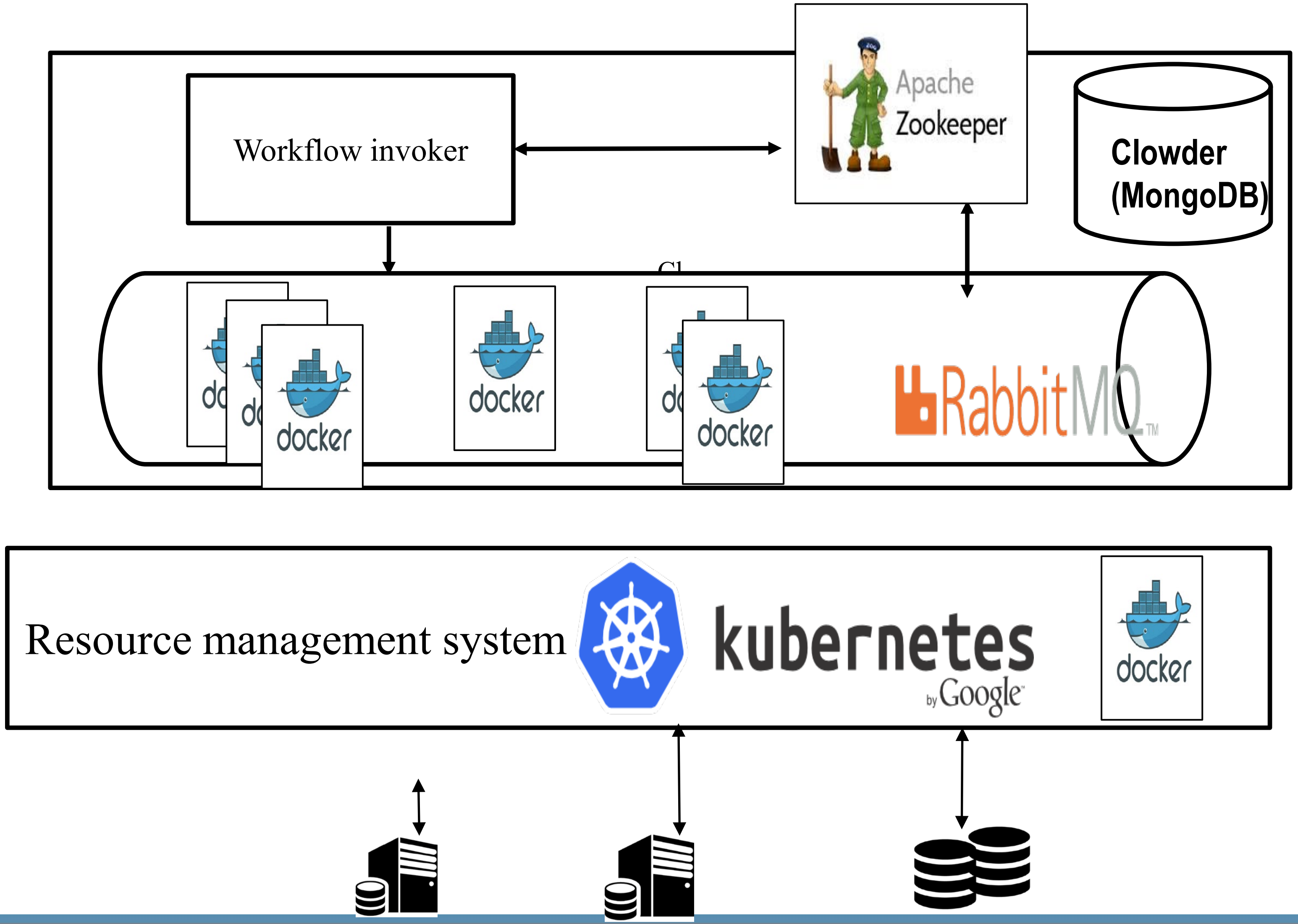
4CeeD Cloud



4CeeD Micro-service implementation system (in Compute Layer)

Micro-service execution layer

Infrastructure layer



Workflow invoker

Clowder (MongoDB)

Resource management system

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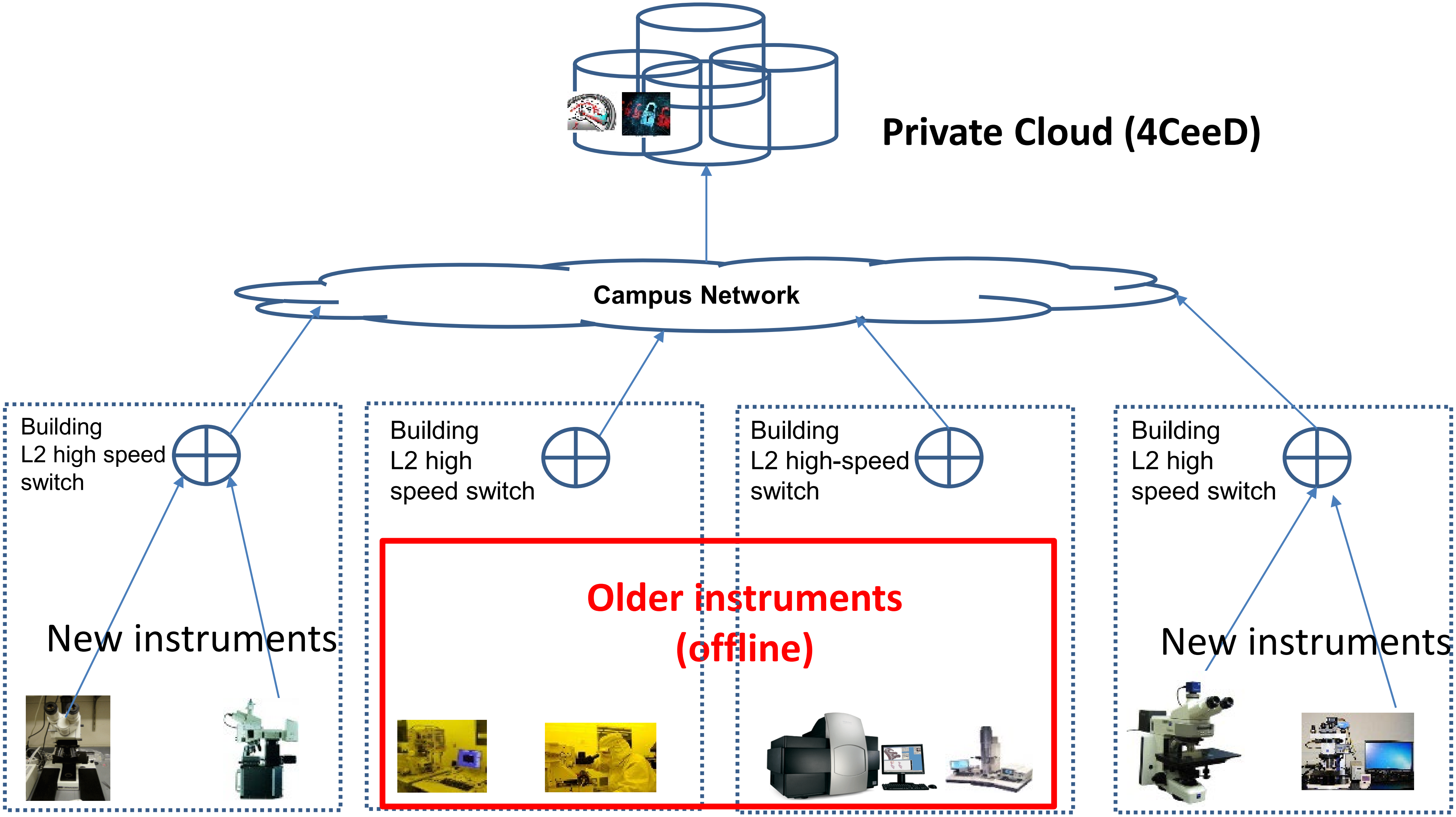
Current situation in campus cyberinfrastructure



Private Cloud (4CeeD)

Campus Network

Building L2 high speed switch

Building L2 high speed switch

Building L2 high-speed switch

Building L2 high speed switch

New instruments

Older instruments (offline)

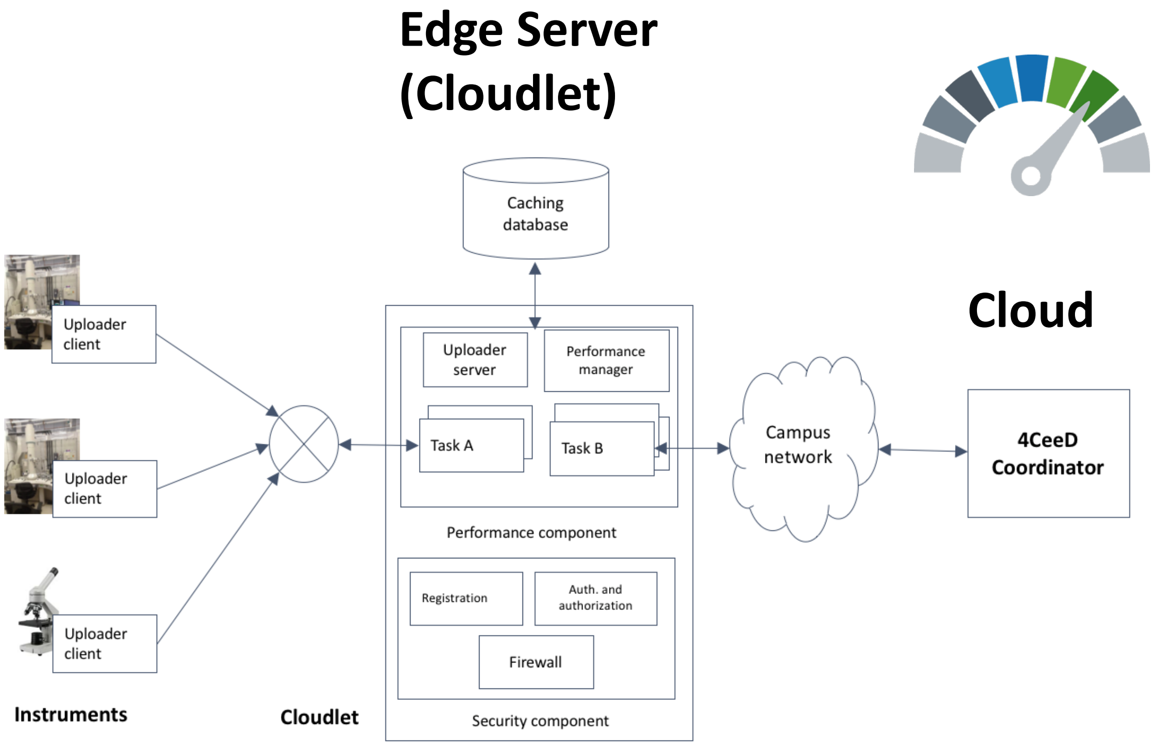
New instruments

Challenges of connecting offline older instruments

- **Performance mismatch**: Older instruments' Windows NT or XP runs network protocols at lower bandwidth speeds (10Mbps or 100Mbps)

- **Obsolete security**: Older devices and their OS systems cannot be patched, hence being vulnerable & taken offline

BRACELET: Putting edge device between older instruments and private cloud



BRACELET in 3-tier architecture

Performance:

- Have two network interfaces configured at different speeds
- Traffic shaping & offloading between edges & cloud

Security:

- User & instrument registration
- Data encryption during upload
- Firewall to protect against external threats

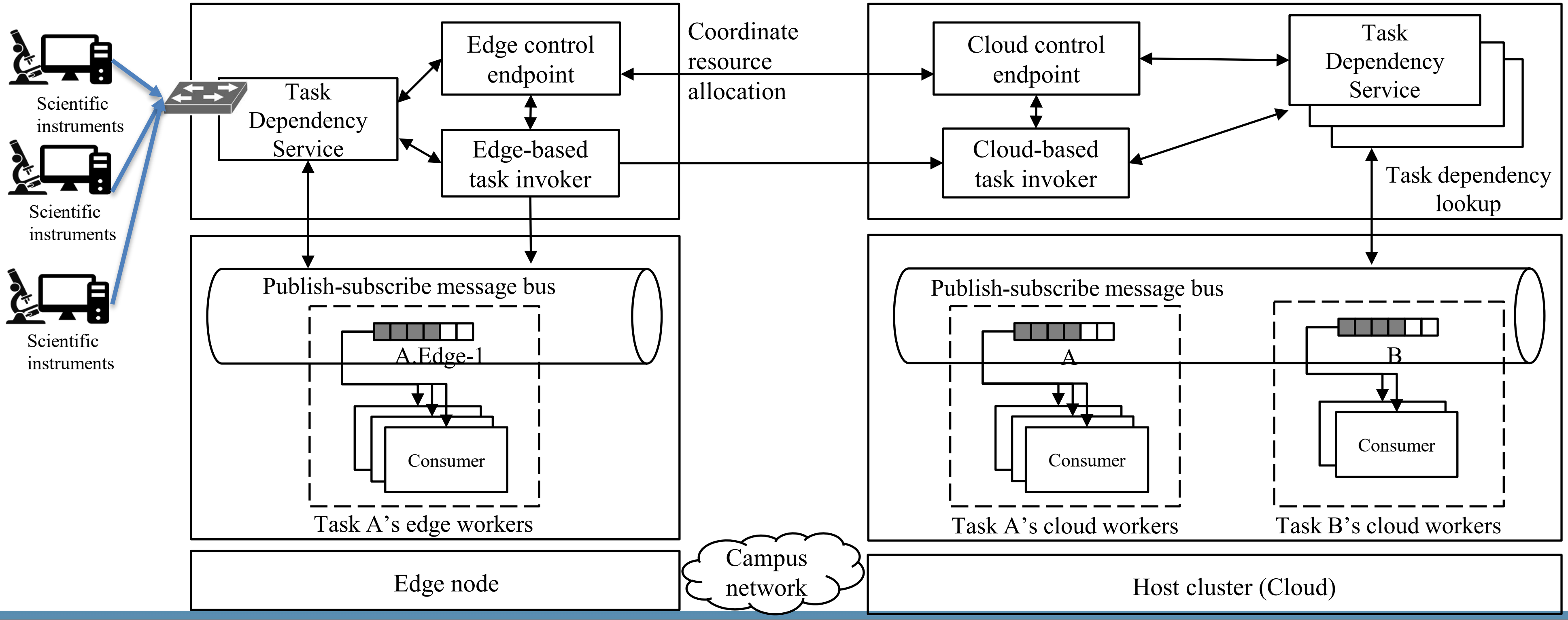
BRACELET Design

Edge Server

- Security service
  - Check equipment address
  - Authenticate user and his reservation
- Compute/Transport service
  - Forward and upload data

Cloud

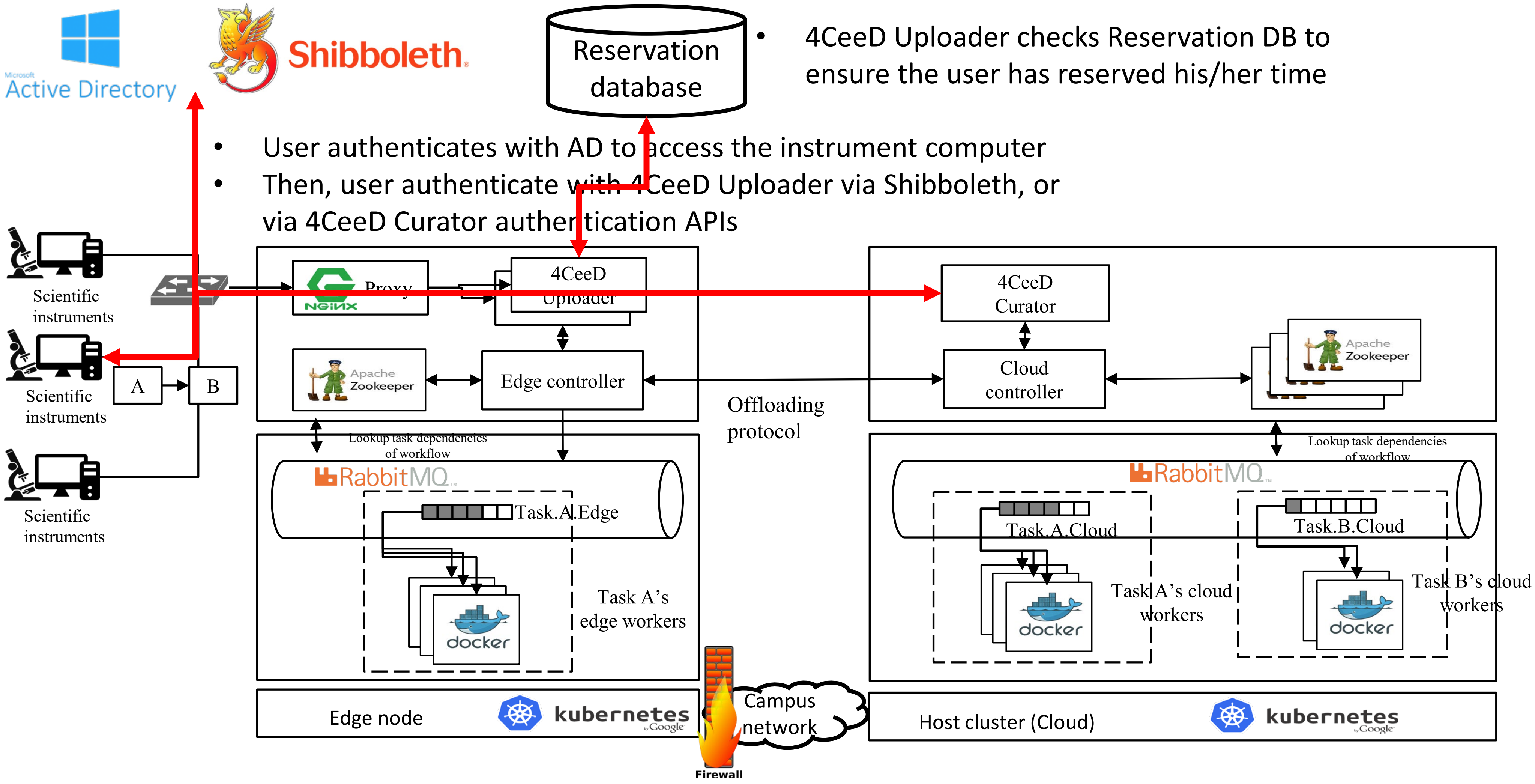
- Compute/Data service
  - Compute tasks/workload
  - Store/Retrieve metadata, data
- Security service
  - Authenticate user, access control



User authentication from instruments via BRACELET

Bracelet Edge Server

4CeeD Cloud



- 4CeeD Uploader checks Reservation DB to ensure the user has reserved his/her time

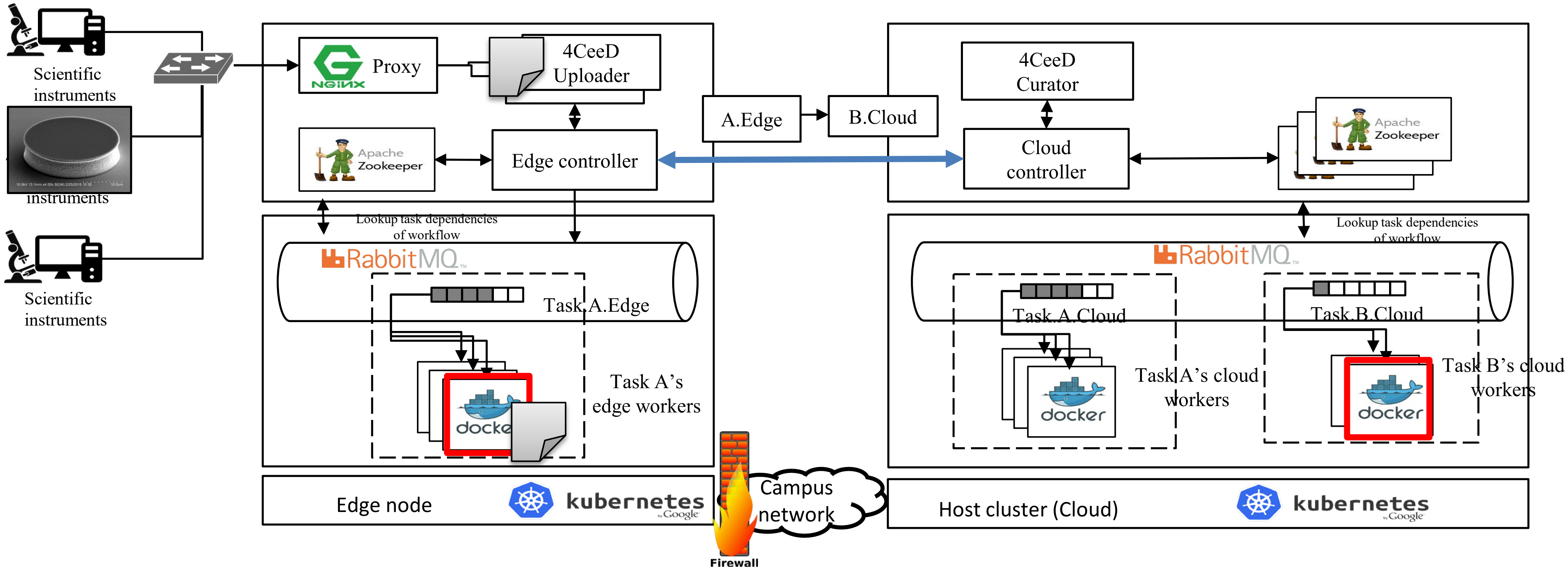
- User authenticates with AD to access the instrument computer
- Then, user authenticate with 4CeeD Uploader via Shibboleth, or via 4CeeD Curator authentication APIs

Transport service between edge & cloud

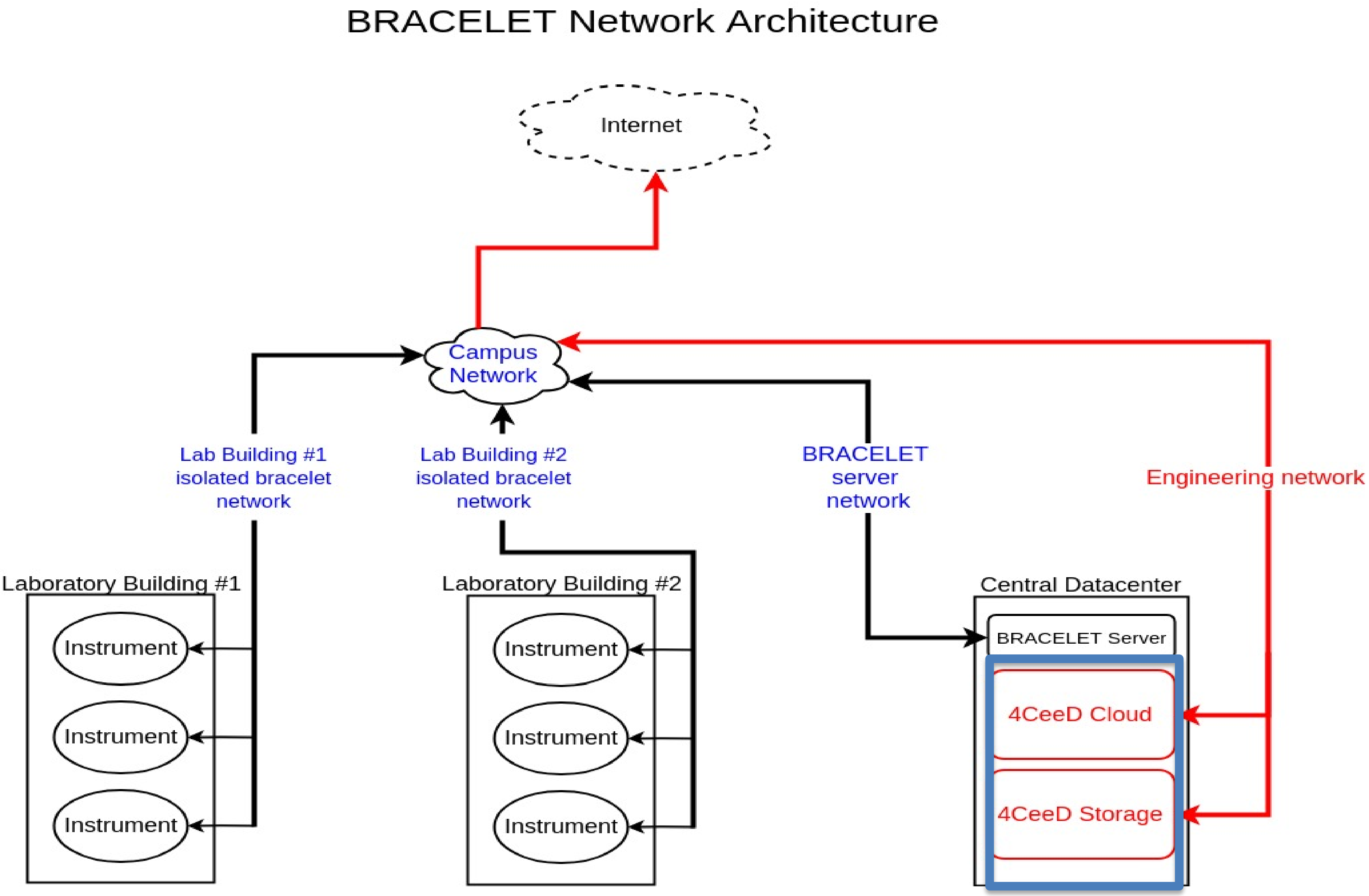
- After processing request, the task consumer forwards request to the next task (following current placement)

- After learning about the placement, data processing request is sent to the first task

- 4CeeD Uploader communicates with local Edge controller to learn about where to send request to
- Edge controller periodically communicates with cloud controller to update task placements



BRACELET Deployment



4CeeD Summary

- Lightweight microservice cloud architecture for materials genomic challenge
- Real-time cloud service for
  - Curation Service
  - Data Analysis (Jupyter Notebook)
- Smart data management system for materials data

- Novel usage of edge computing for aging IoT devices to enable security
- Sources (code and project description):
- https://4ceed.github.io/
- http://t2c2.csl.illinois.edu/

Publications

- Phuong Nguyen, Steven Konstanty, Todd Nicholson, Thomas O'Brien, Aaron Schwartz-Duval, Timothy Spila, Klara Nahrstedt, Roy Campbell, Indranil Gupta, Michael Chan, Kenton McHenry and Normand Paquin, "4CeeD: Real-Time Data Acquisition and Analysis Framework for Material-related Cyber-Physical Environments", IEEE/ACM 17th **IEEE/ACM International Symposium on Cluster, Cloud and Grid Computing**. Madrid, Spain, May 14-17, 2017– **Best Paper Award**
- Phuong Nguyen, Klara Nahrstedt, "MONAD: Self-adaptive Micro-service Infrastructure for Heterogeneous Scientific Workflows", **14th IEEE International Conference on Autonomous Computing (ICAC 2017**), July 17-21, 2017, Columbus, Ohio
- Zhe Yang, Phuong Nguyen, Haiming Jin, Klara Nahrstedt, "MIRAS: Model-based Reinforcement Learning for Microservice Resource Allocation over Scientific Workflows", **IEEE International Conference on Distributed Computing Systems (ICDCS 2019)**, July 2019, Dallas, TX; DOI: 10.1109/ICDCS.2019.00021
- Phuong Nguyen, Tarek Elgamal, Steve Konstanty, Todd Nicholson, Stuart Turner, Patrick Su, Michael Chan, Klara Nahrstedt, Tim Spila, Kenton McHenry, John Dallesasse, Roy Campbell, "Bracelet: Edge-Cloud Microservice Infrastructure for Aging Scientific Instruments", **IEEE International Conference on Computing, Networking, and Communications (ICNC)** 2019, Hawaii, February 2019.