4CeeD Backend Services

4CeeD Backend Services

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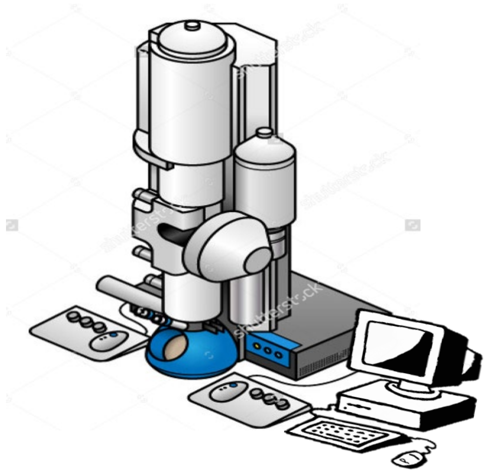
A timely and trusted curator and coordinator of scientific data

Outline

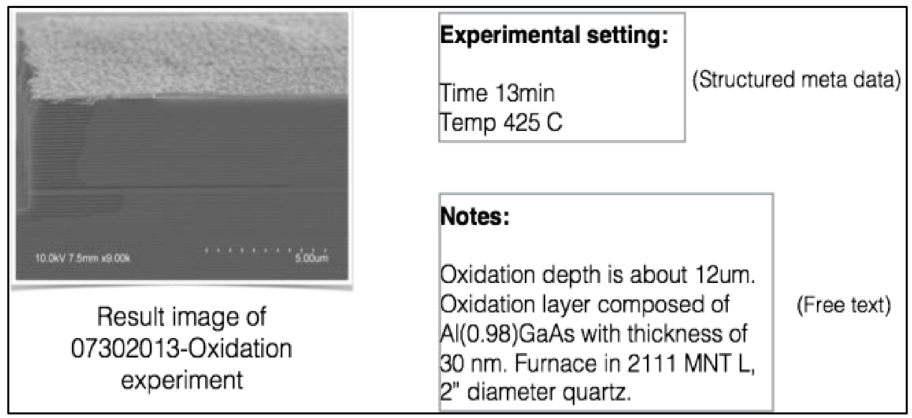
- 4CeeD Distributed Architecture, Backend Cloud Concepts and Services
  - What is 4Ceed and its goals
  - What is behind the 4CeeD Dashboard
  - 4CeeD Cloud Design and Deployment
  - How to deal with Aging Scientific Instrument

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

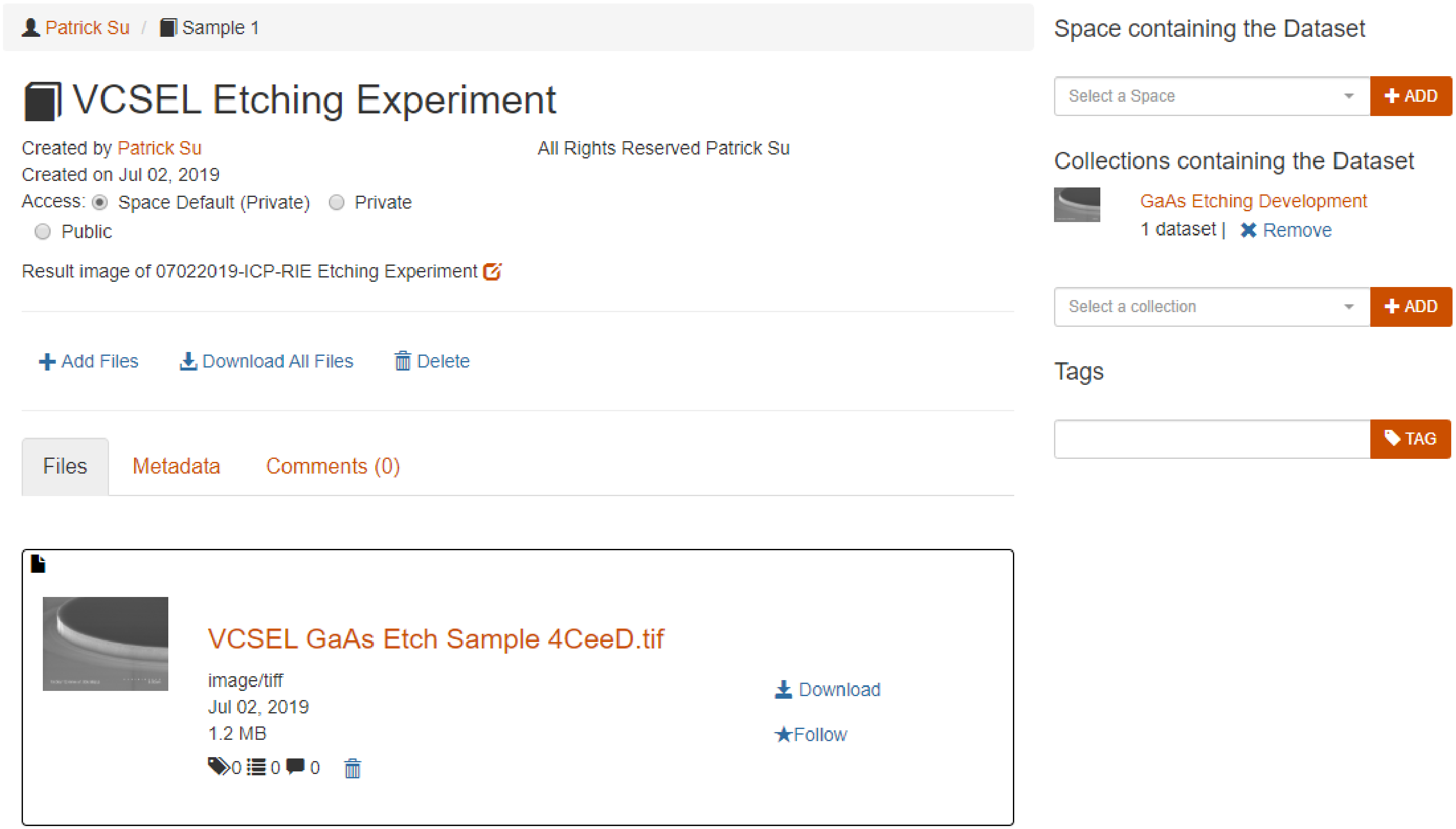


Instrument
(in MRL/HMNTL/BI)



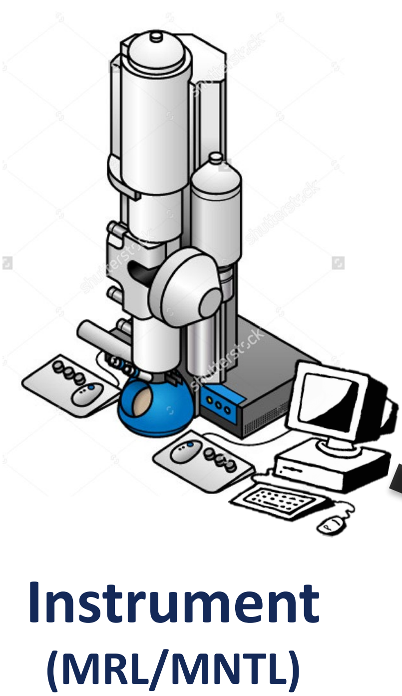
Sample output data from SEM microscopy

How this look from 4CeeD [Datasets]

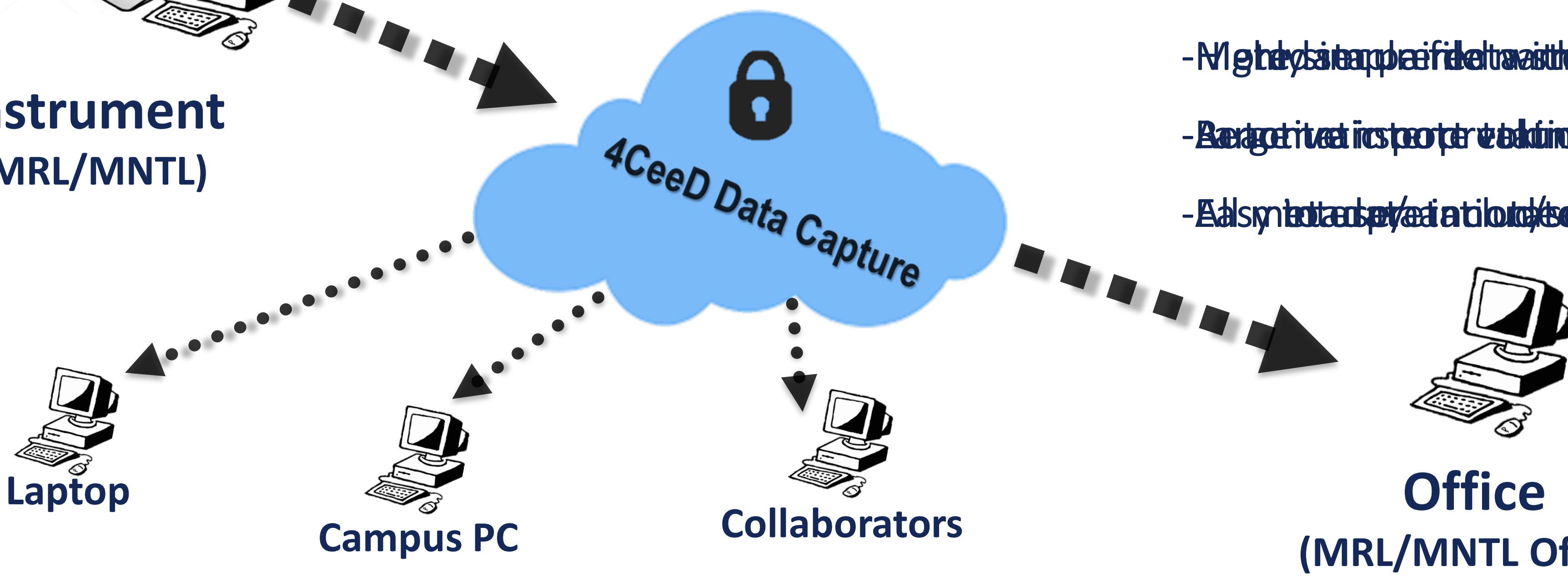


- 4CeeD is designed to present only pertinent information for quick understanding of the experiment

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



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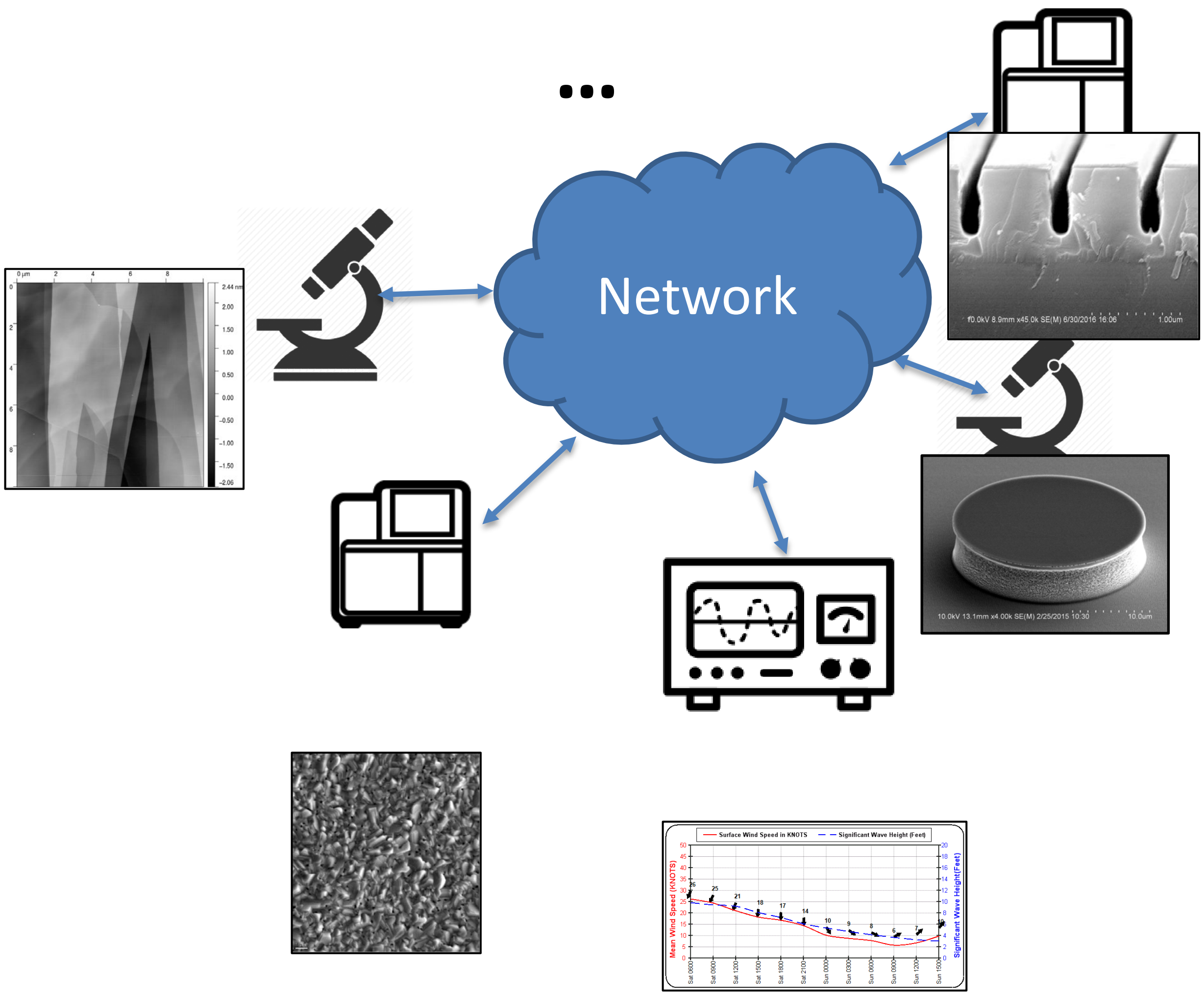
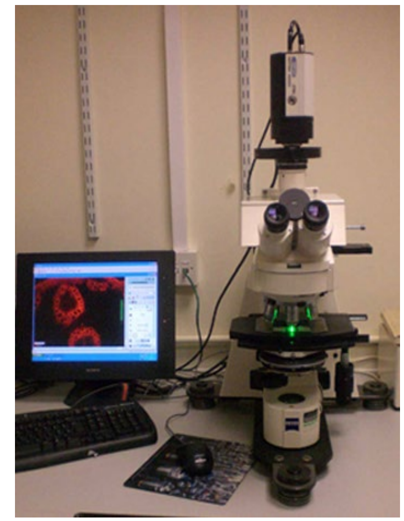
Increasingly data-driven and interdisciplinary scientific research in Physical Sciences and Live Sciences

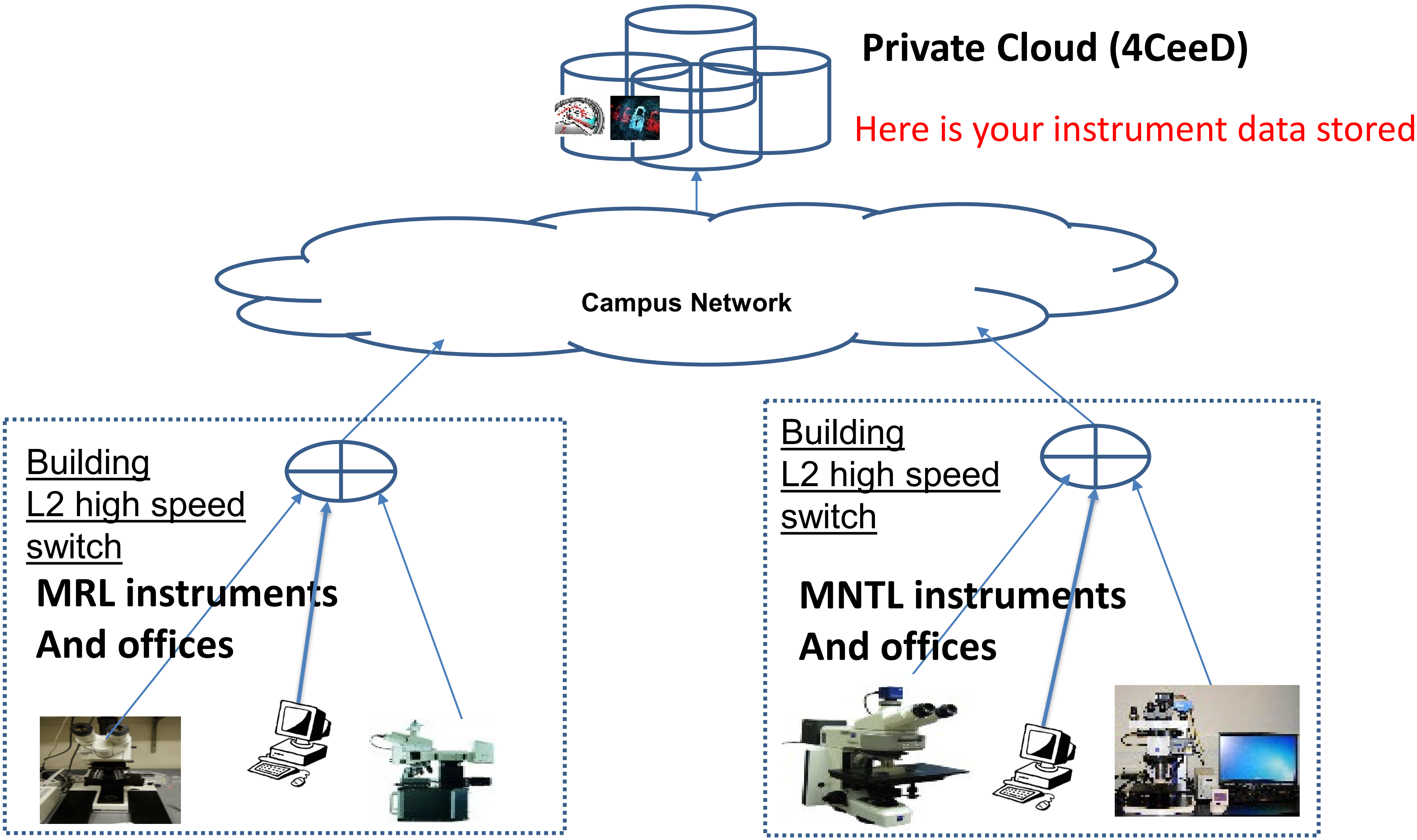
- *Key enabling factor*: Network connected scientific instruments capable of real-time data capture



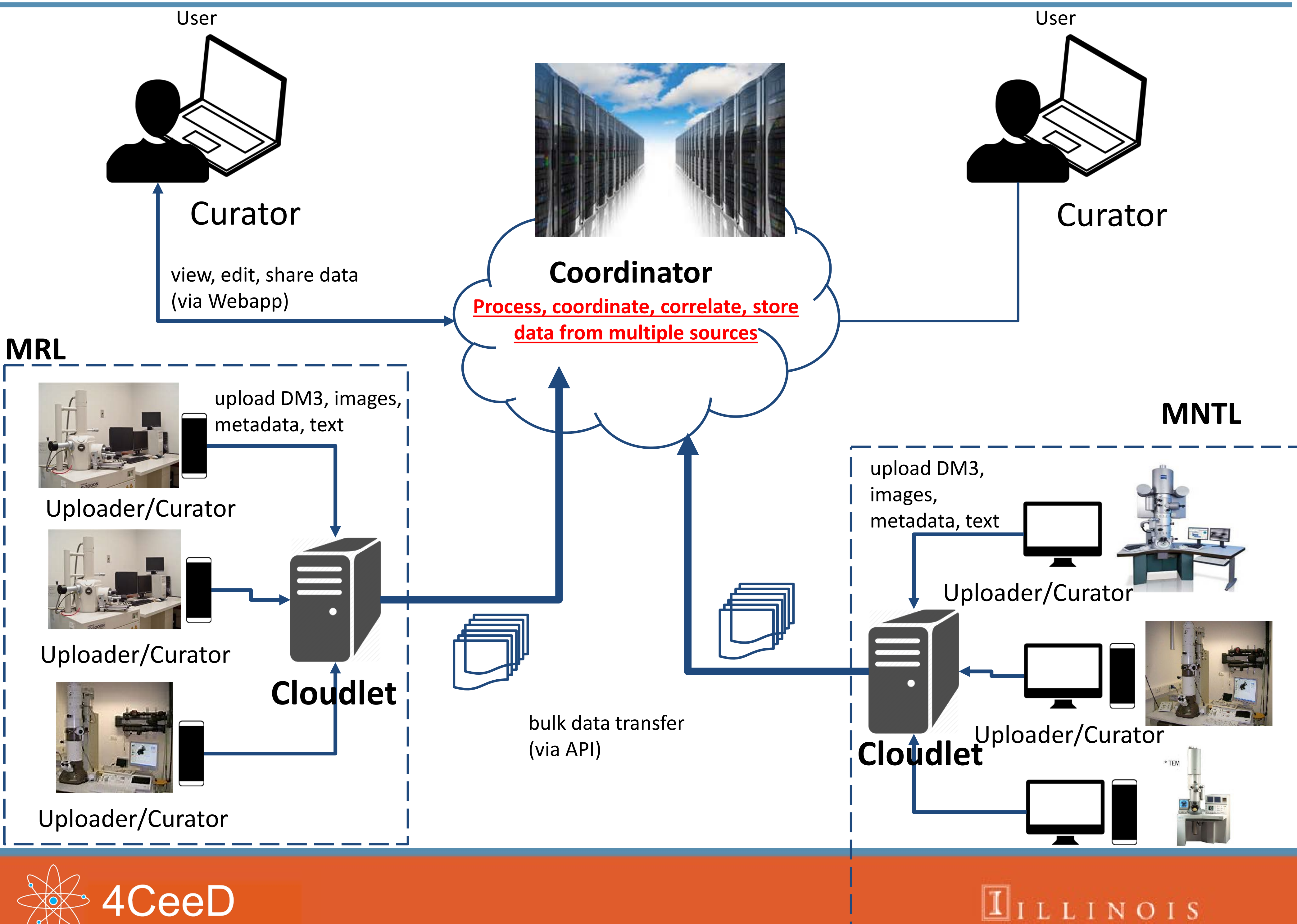


Digital microscope

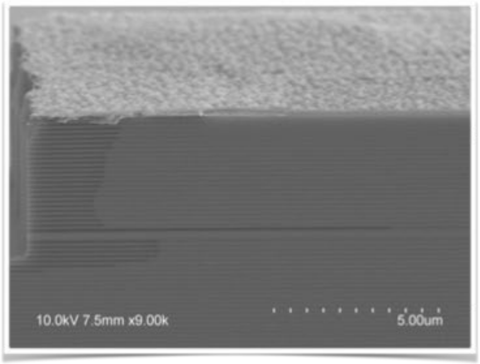
4CeeD Design Considerations - Distributed View



4Ceed Design Considerations – Component View



4CeeD Design Considerations - Multimodal data format View



Result image of 07302013-Oxidation experiment

Experimental setting:

Time 13min
Temp 425 C

(Structured meta data)

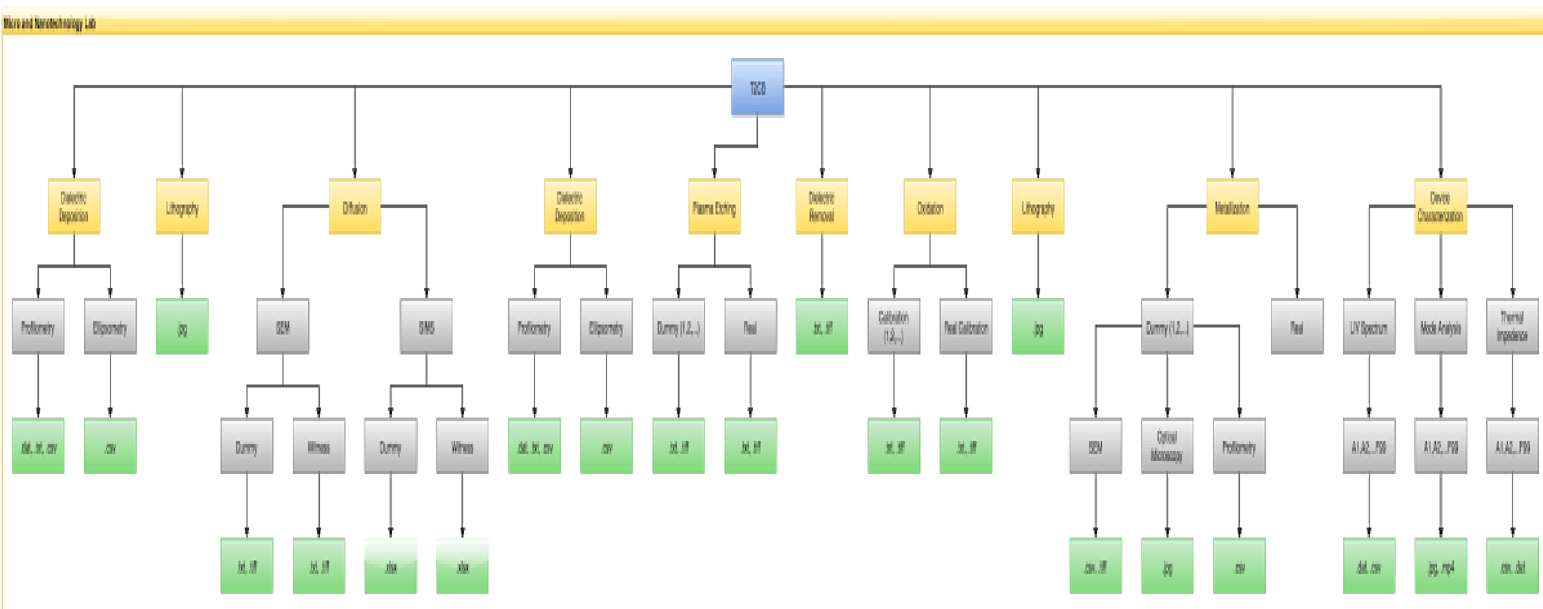
Notes:

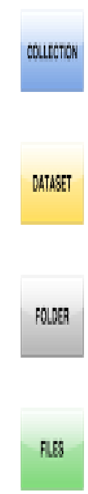
Oxidation depth is about 12um. Oxidation layer composed of Al(0.98)GaAs with thickness of 30 nm. Furnace in 2111 MNT L, 2" diameter quartz.

(Free text)

A lot of useful information is hidden in unstructured text

Example of multimodal experimental d



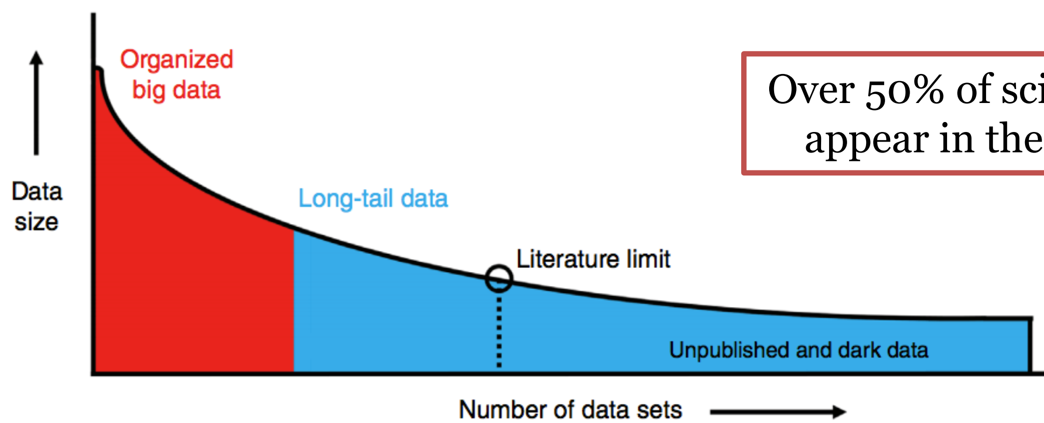


Heterogeneity of experimental data (Spaces, Collections Datasets)

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

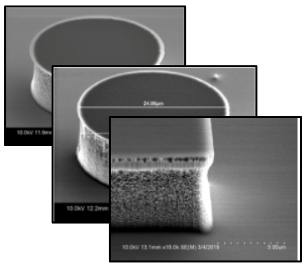


Over 50% of scientific findings do not appear in the published literature

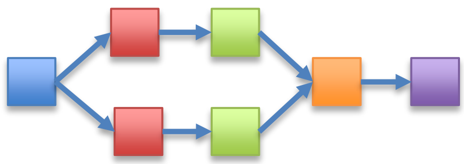
Long-tail scientific data
Source: Ferguson et al. *Nature neuroscience* 17.11 (2014)

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

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



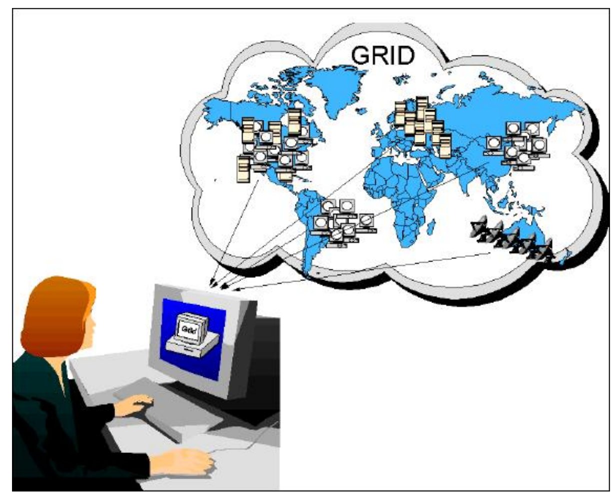
Raw data



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

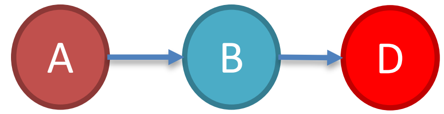


Executing workflows on grid infrastructure

4CeeD Design Considerations – Task Workflows

- Application is a Computational Workflow

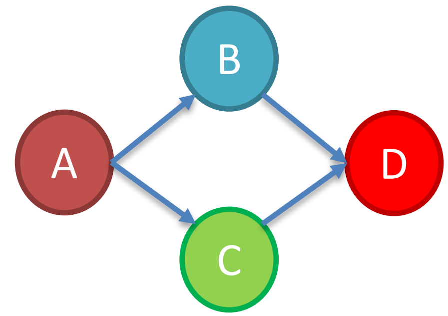
- Workflow is Set of Tasks (e.g., A, B, C, D) executing over materials data



Workflow type 1

1. Example of a Task C: "Plotting a graph"

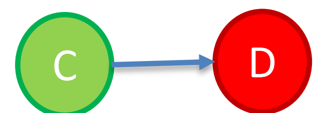
```
In [5]: metadata = py4ceed.get_metadeta()
        metadata.plot(x='Pressure', y='Etch_Rate')
        plt.show()
```



Workflow type 2

2. Example of a Task D: "Filter Data"

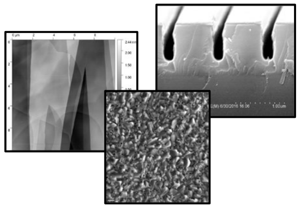
In [6]: metadata[metadata ['Pressure'] >=7]



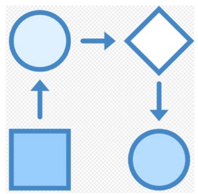
Workflow type 3

- 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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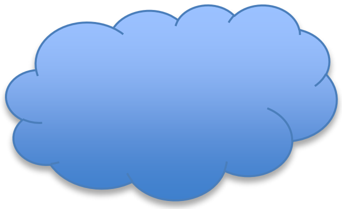
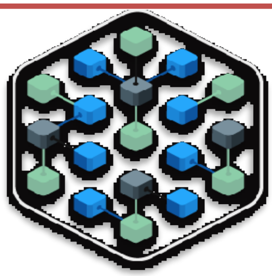
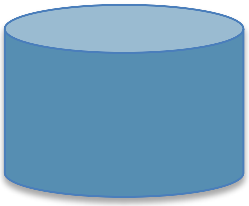
4CeeD Cloud Design



✓ Cloud Concept

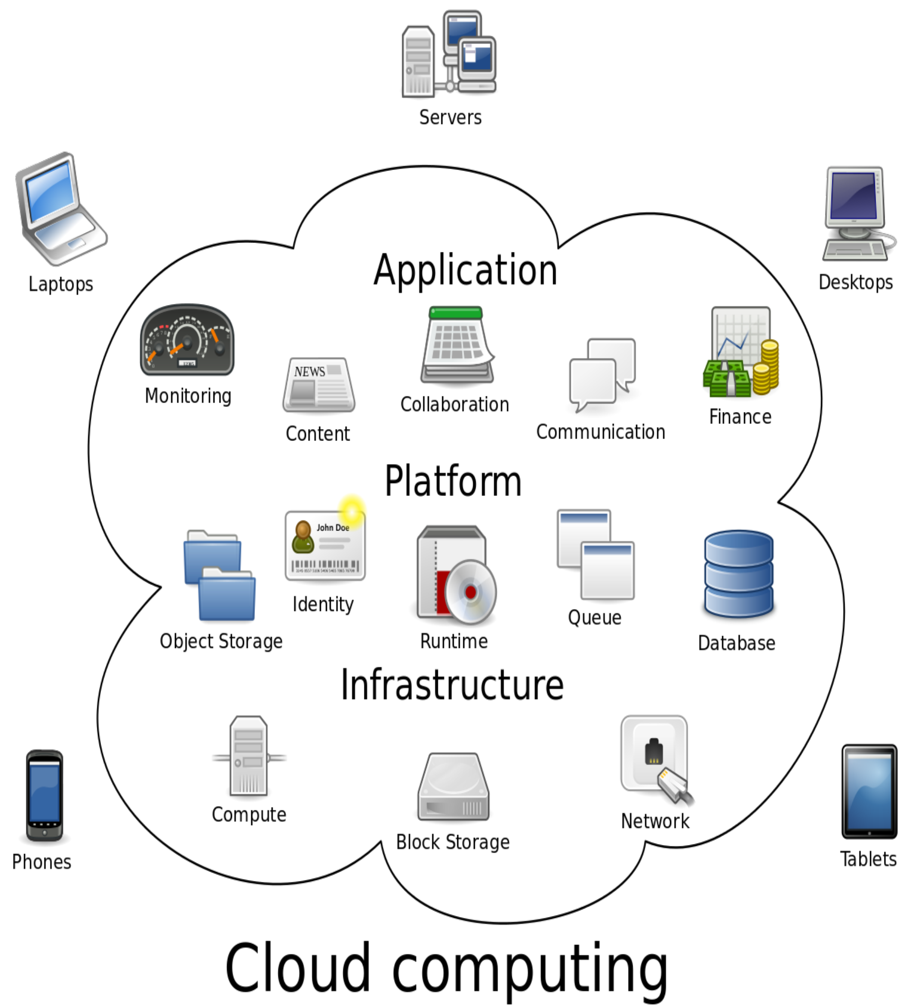


✓ Micro-service execution environment



✓ Data Management

Cloud Computing Concept



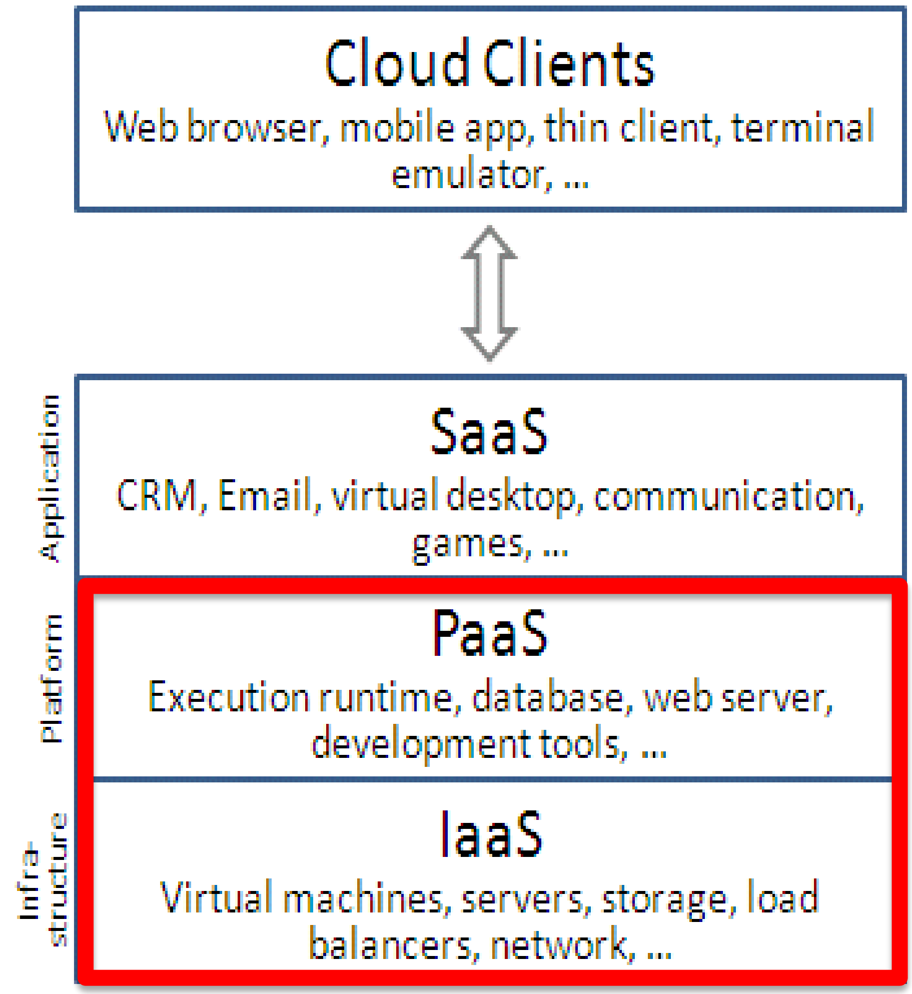
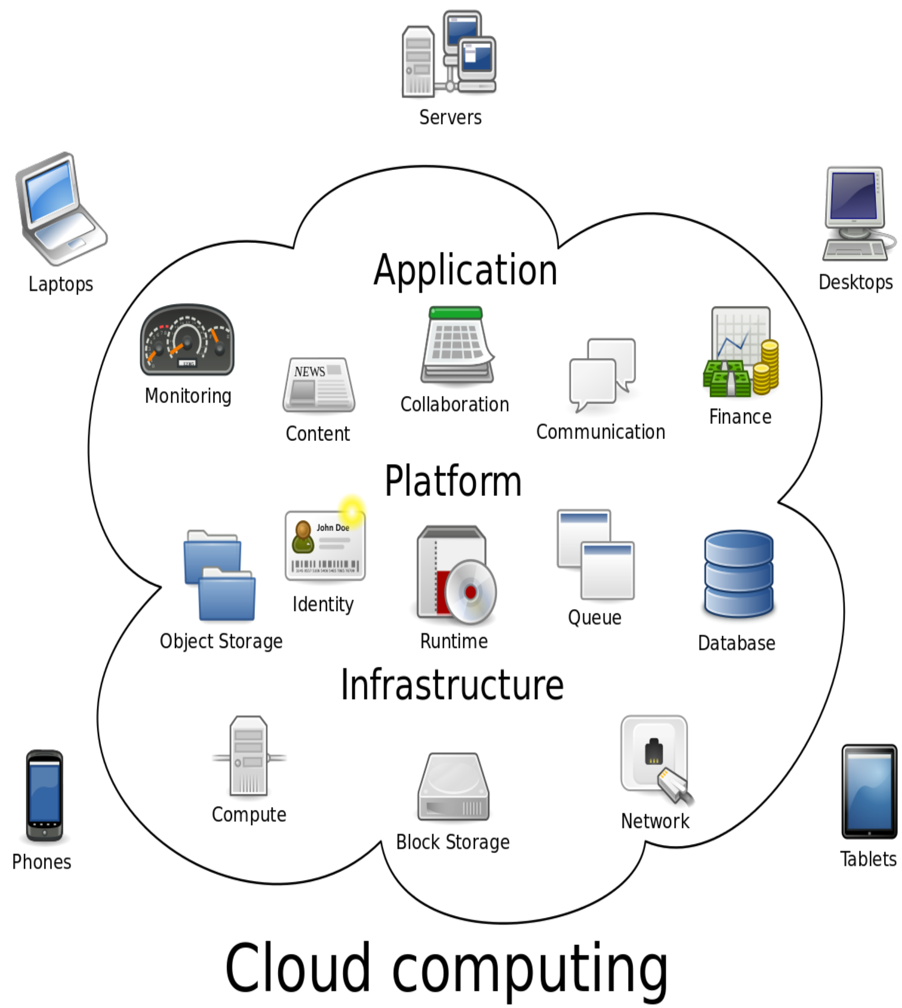
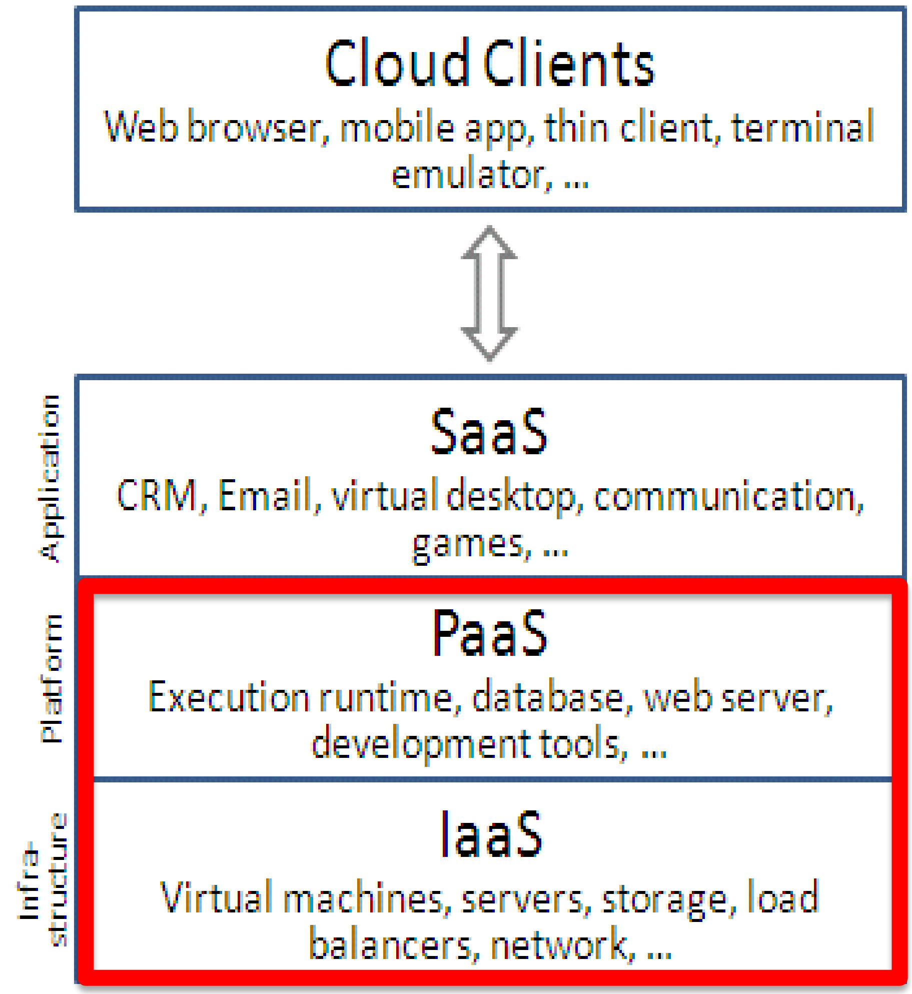


Figure Source: Wikipedia

Cloud Computing Concept





4CeeD Cloud

Private and Public Clouds

4CeeD is Private Cloud

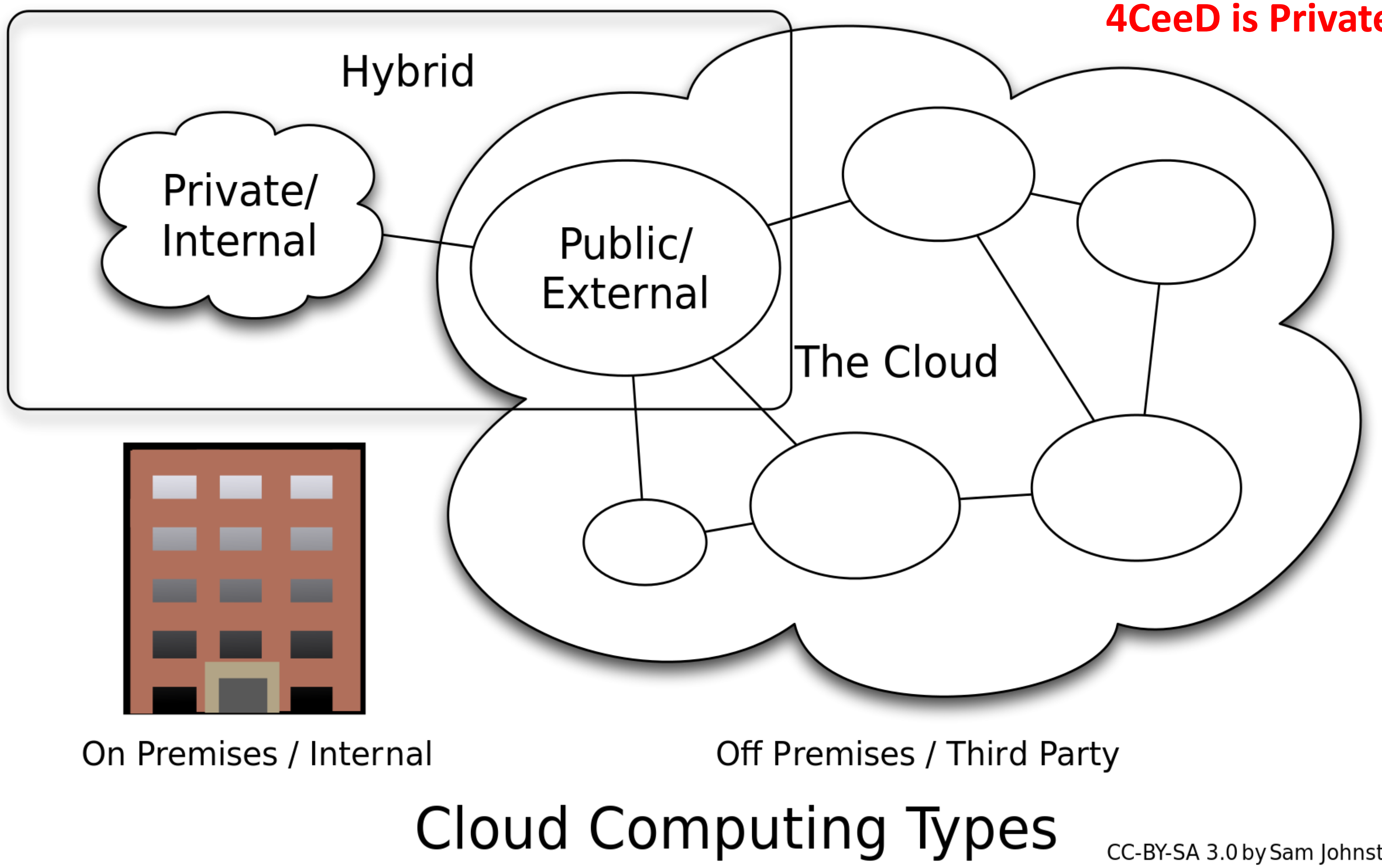
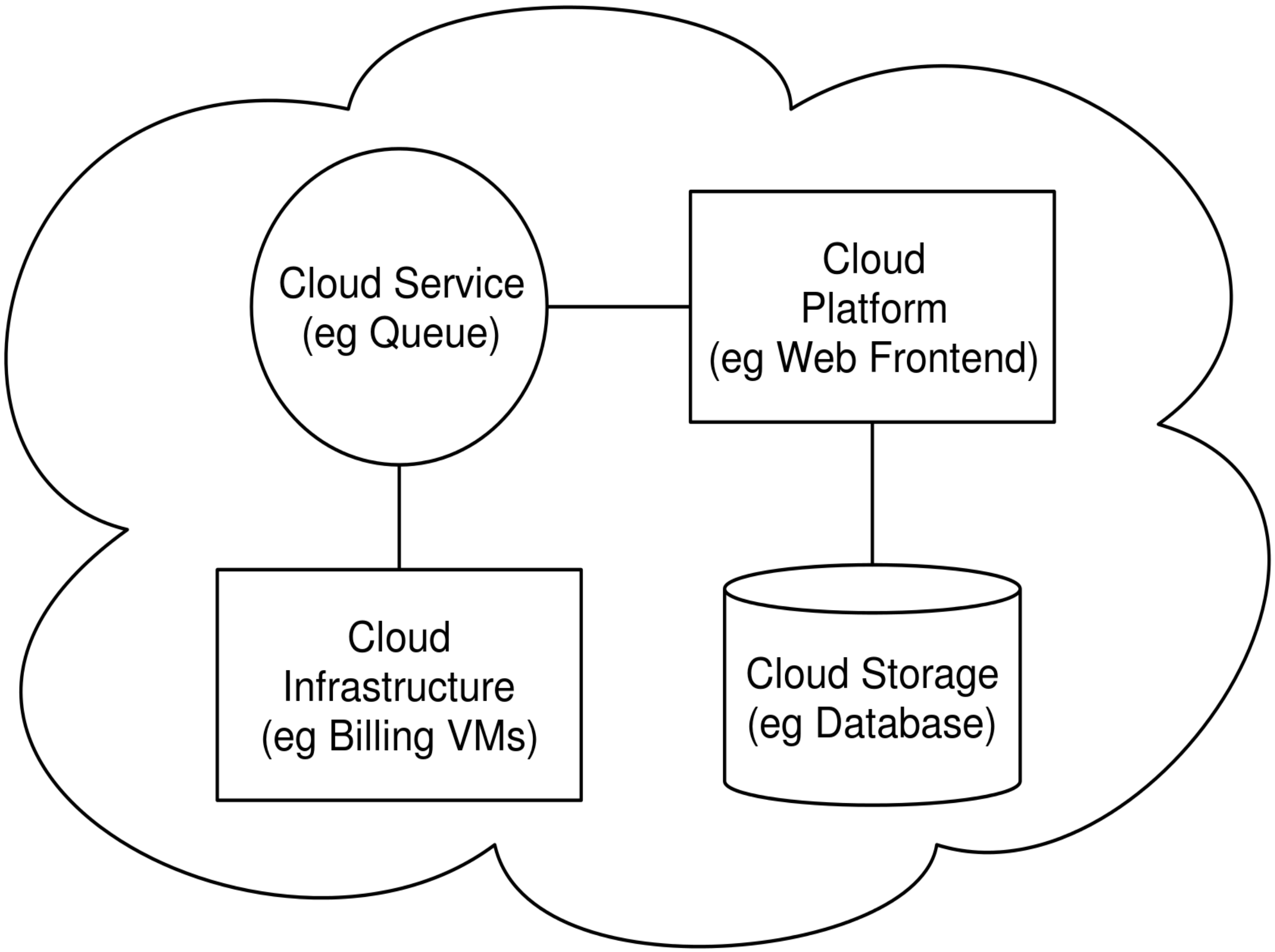


Figure Source: Wikipedia

Example of Cloud Components

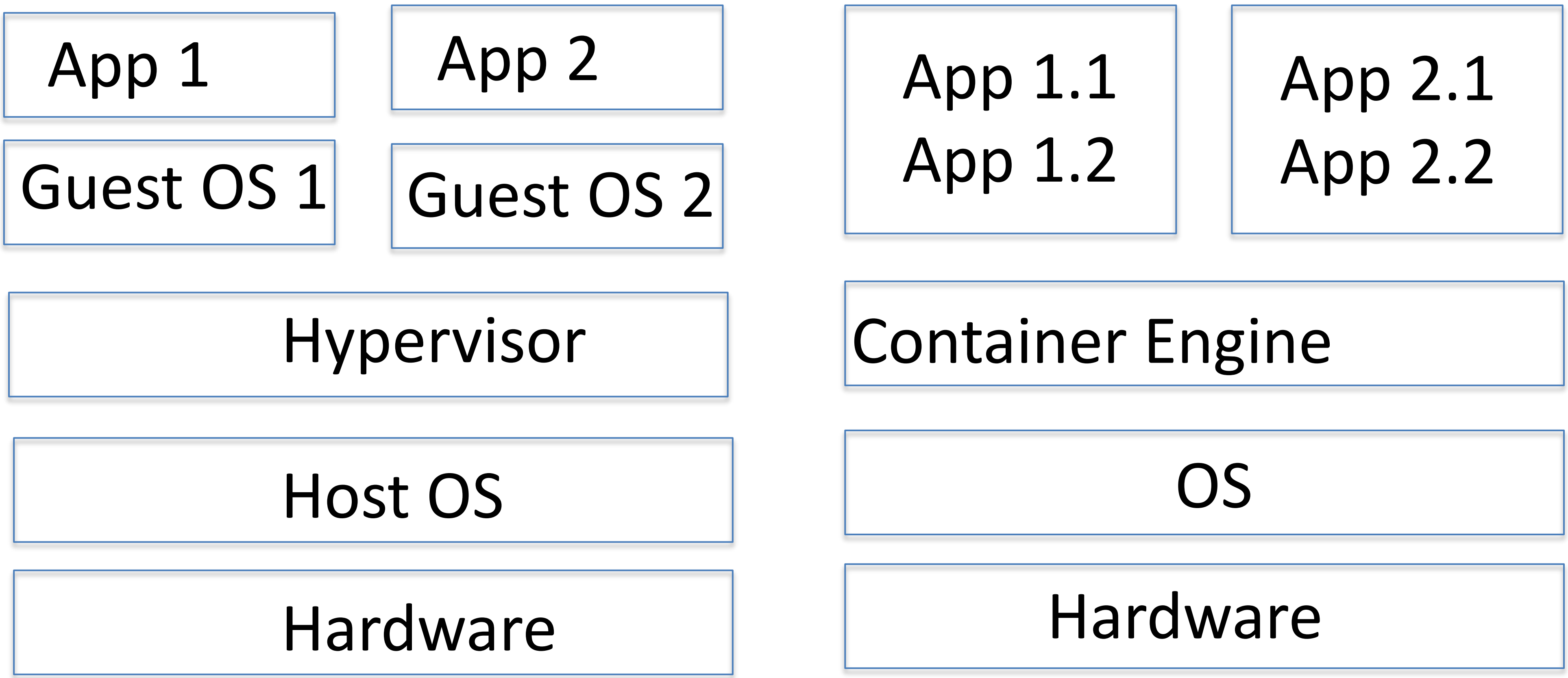


- 4CeeD is **Web-based**,
- 4Ceed uses **Containers And Micro-service** Infrastructure (Docker and Kubernates/Docker Compose)
- 4CeeD uses **Queue** (RabitMQ)
- 4CeeD uses **Database** (MongoDB) and Filesystem (HFS)

Figure Source: Wikipedia

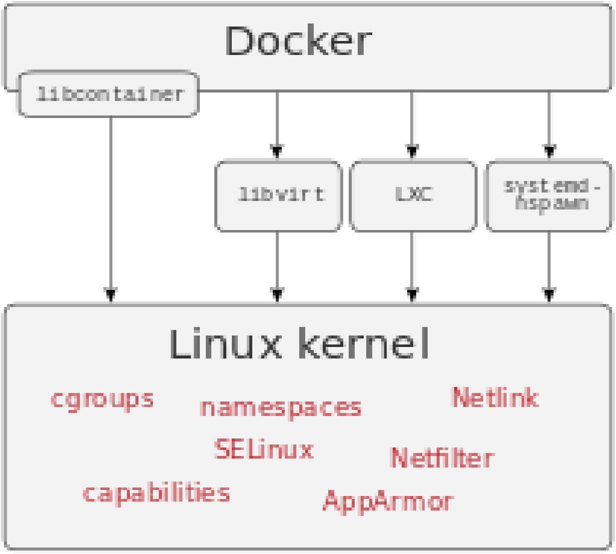
Hardware Virtualization

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



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.

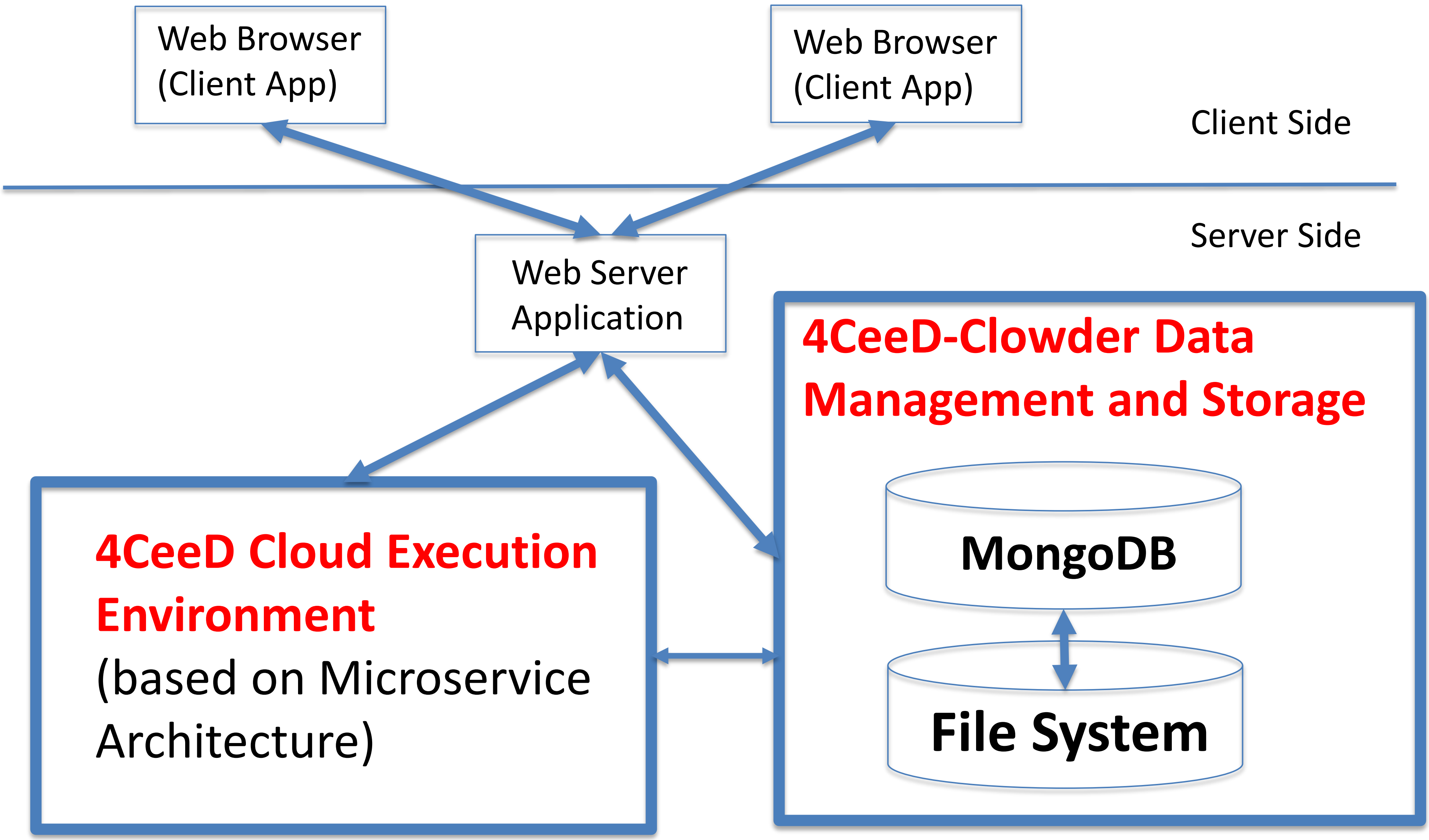


Source: Wikipedia

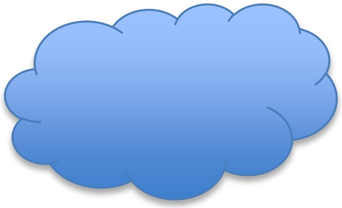
Micro-Service

- 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*.

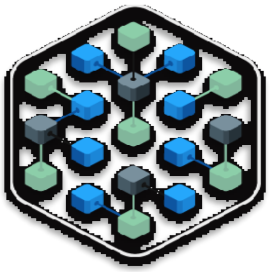
4CeeD Cloud Architecture Components – Putting it Together



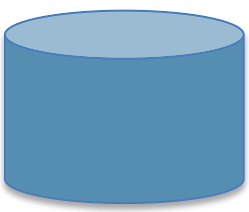
4CeeD Cloud Design



- ✓ Cloud Concept



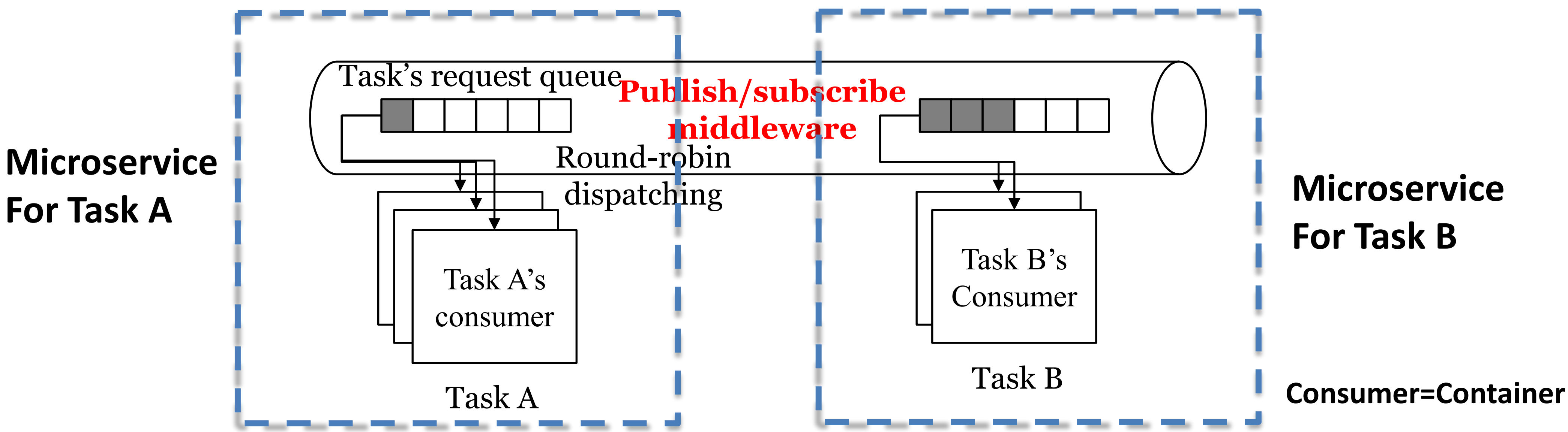
- ✓ Micro-service execution environment



- ✓ Data Management

Micro-service execution environment

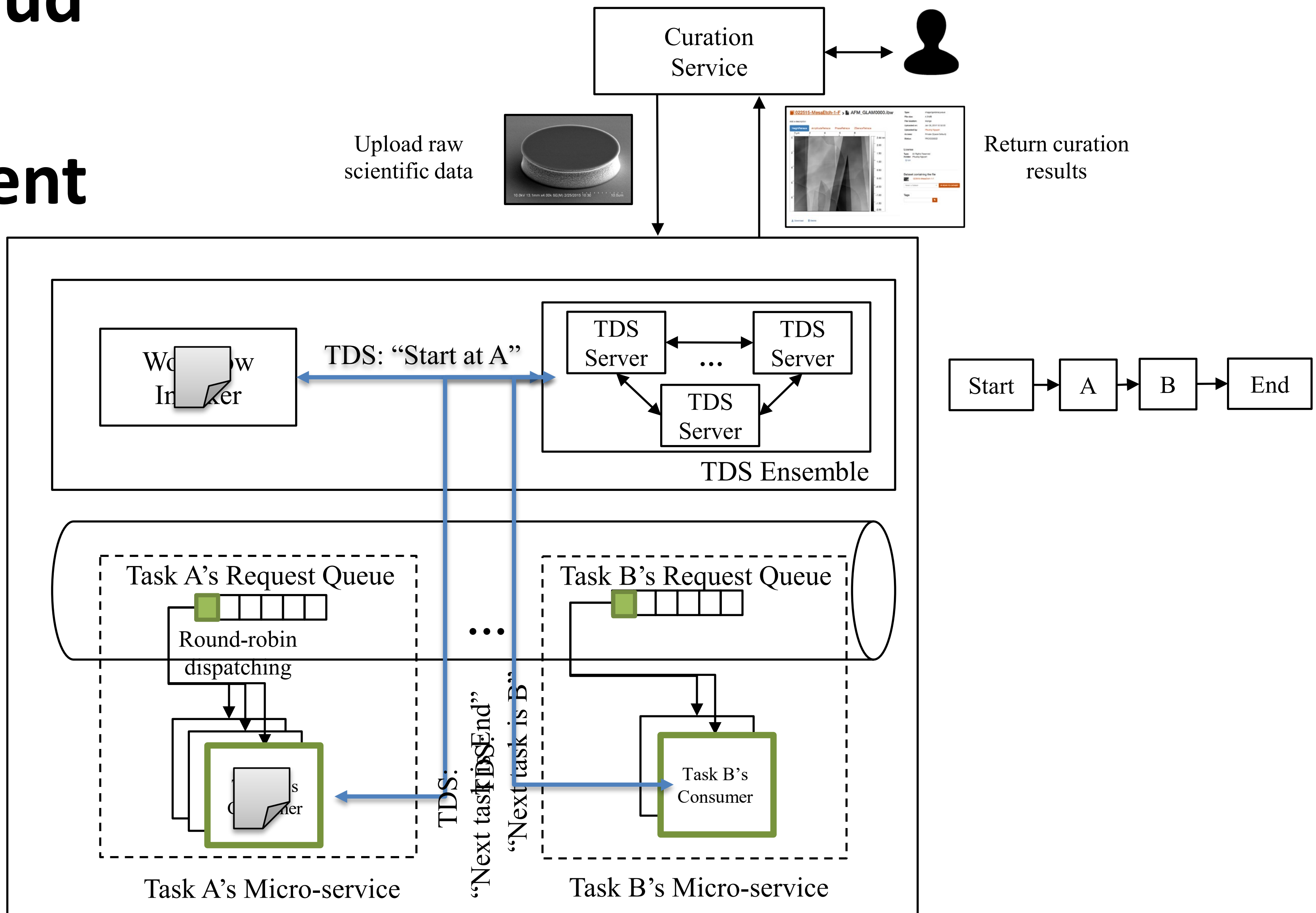
- ***Micro-services over monoliths***: Each task is modeled as a micro-service
  - Use publish-subscribe middleware to connect between micro-services



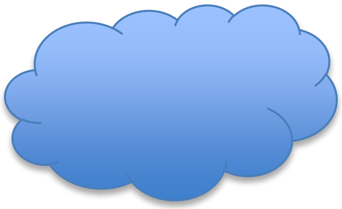
- **Separate task dependencies** from task implementation & deployment
  - Enable flexible workflow composition
  - Task-level resource provisioning

4CeeD Executing scientific data processing workflow

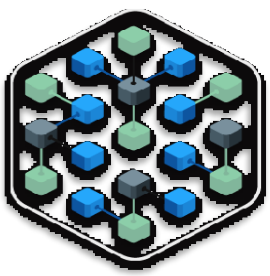
4CeeD Cloud Execution Environment



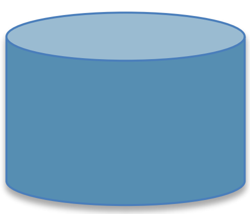
4CeeD Cloud Design



✓ 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)

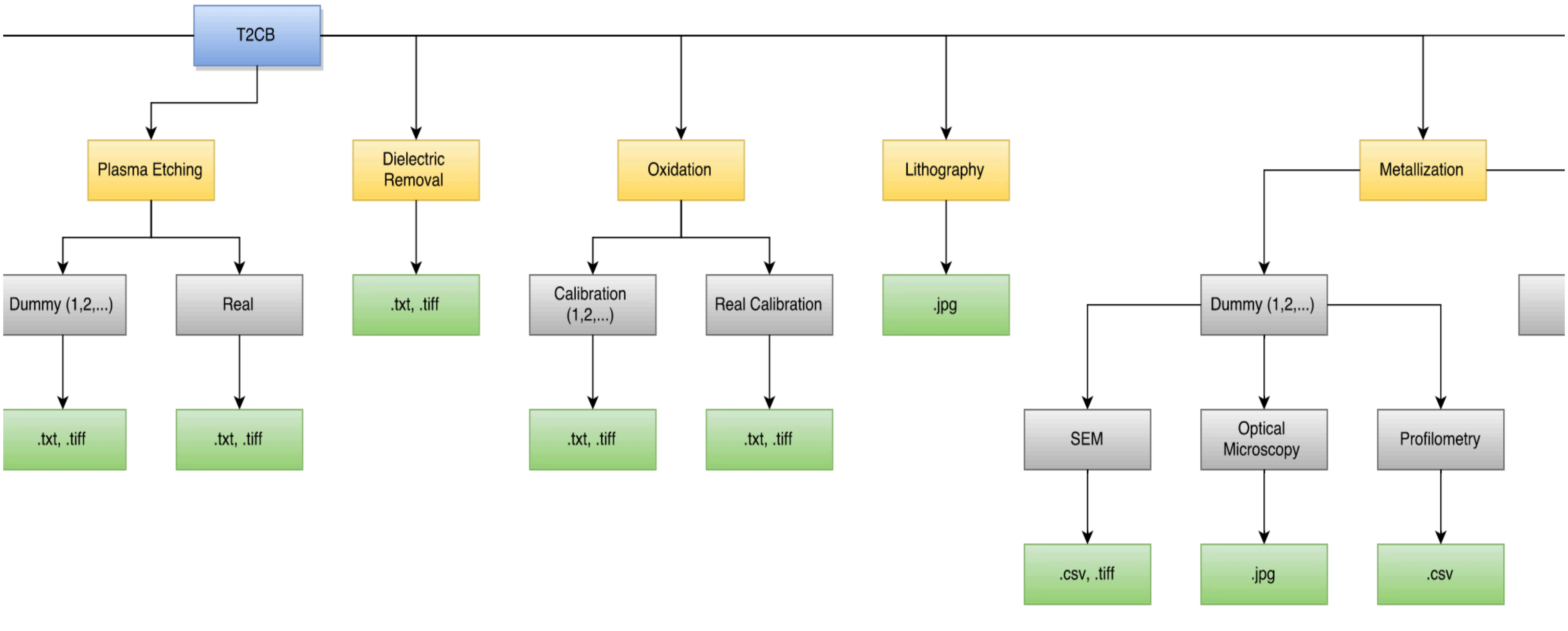
- 4CeeD uses MongoDB
- In MongoDB
  - Documents are stored in a JSON-like format
- Example of JSON-like Format
- 4CeeD Data Model organizes projects into collections, datasets, and files.
- These can then be shared in spaces. 4CeeD utilizes and modifies NCSA Clowder data management system.


```
{ "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, …



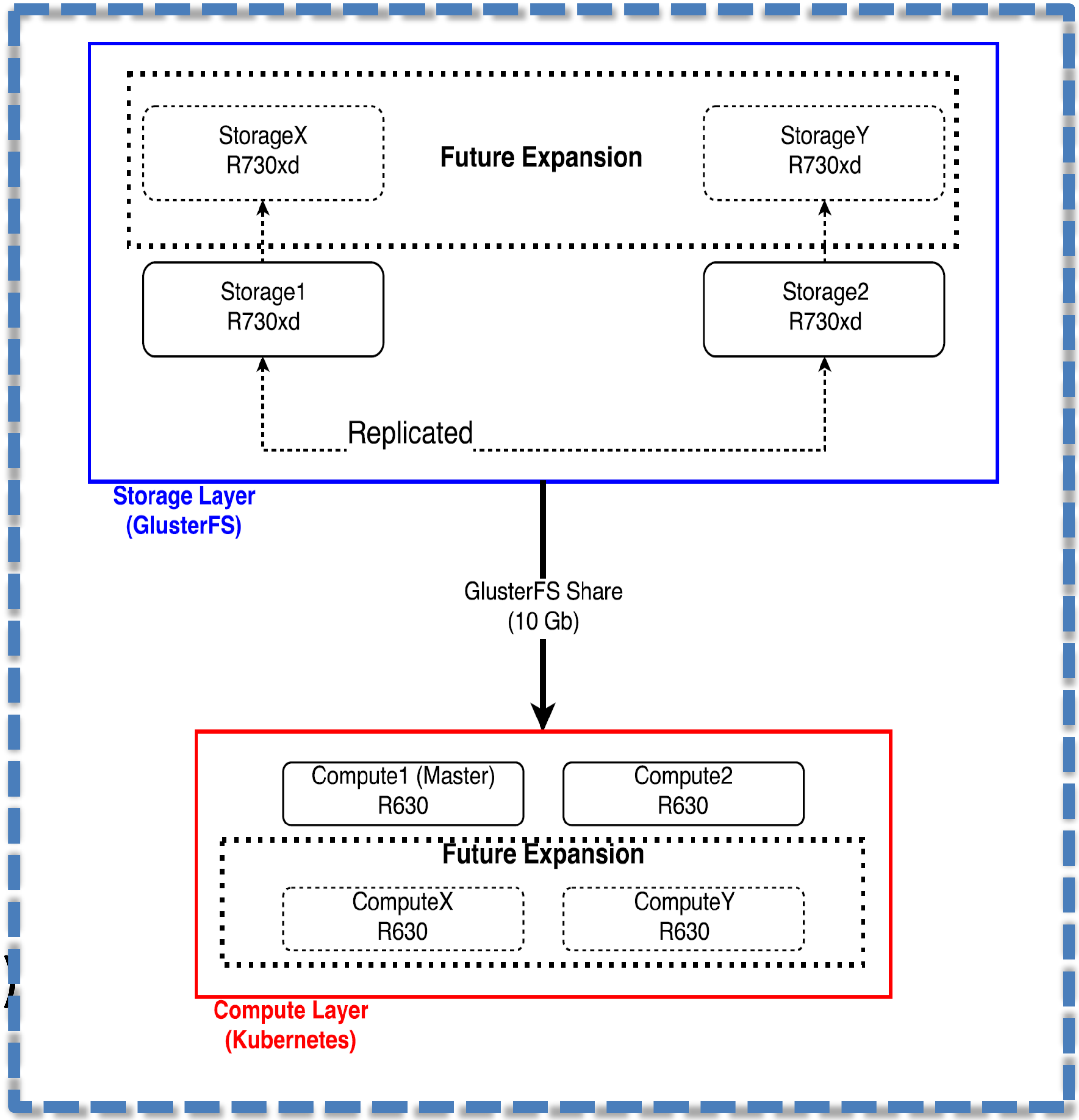
4CeeD Deployment – Cloud Production System

Goals:
- Redundancy
- Availability
- Scalability

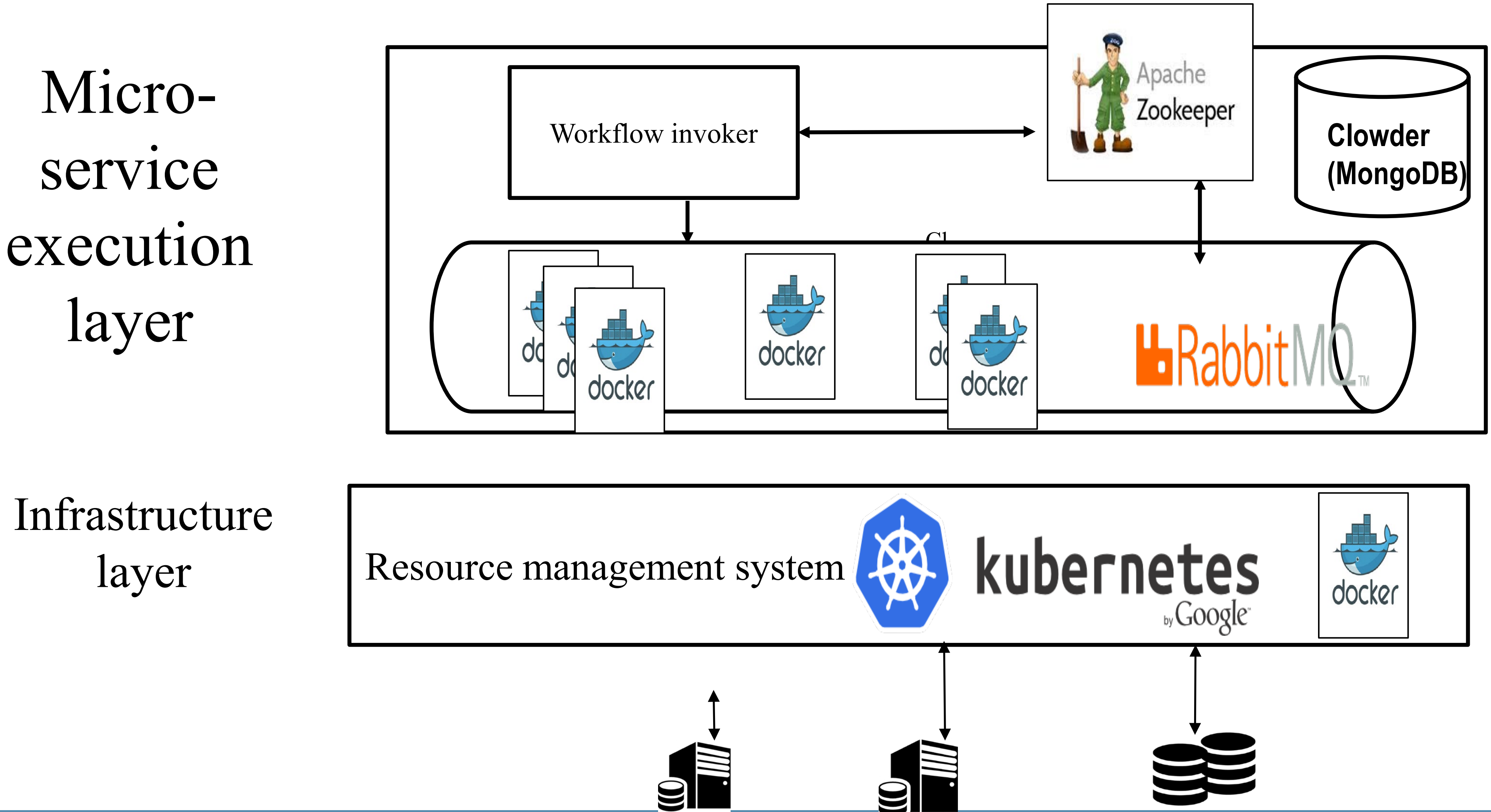
Storage Layer:
- **40 TB (20 TB per investor)**
- Replicated for redundancy

Compute Layer:
- Docker container orchestration (Kubernetes)
- Single master (High Available masters in future)

4CeeD Cloud



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



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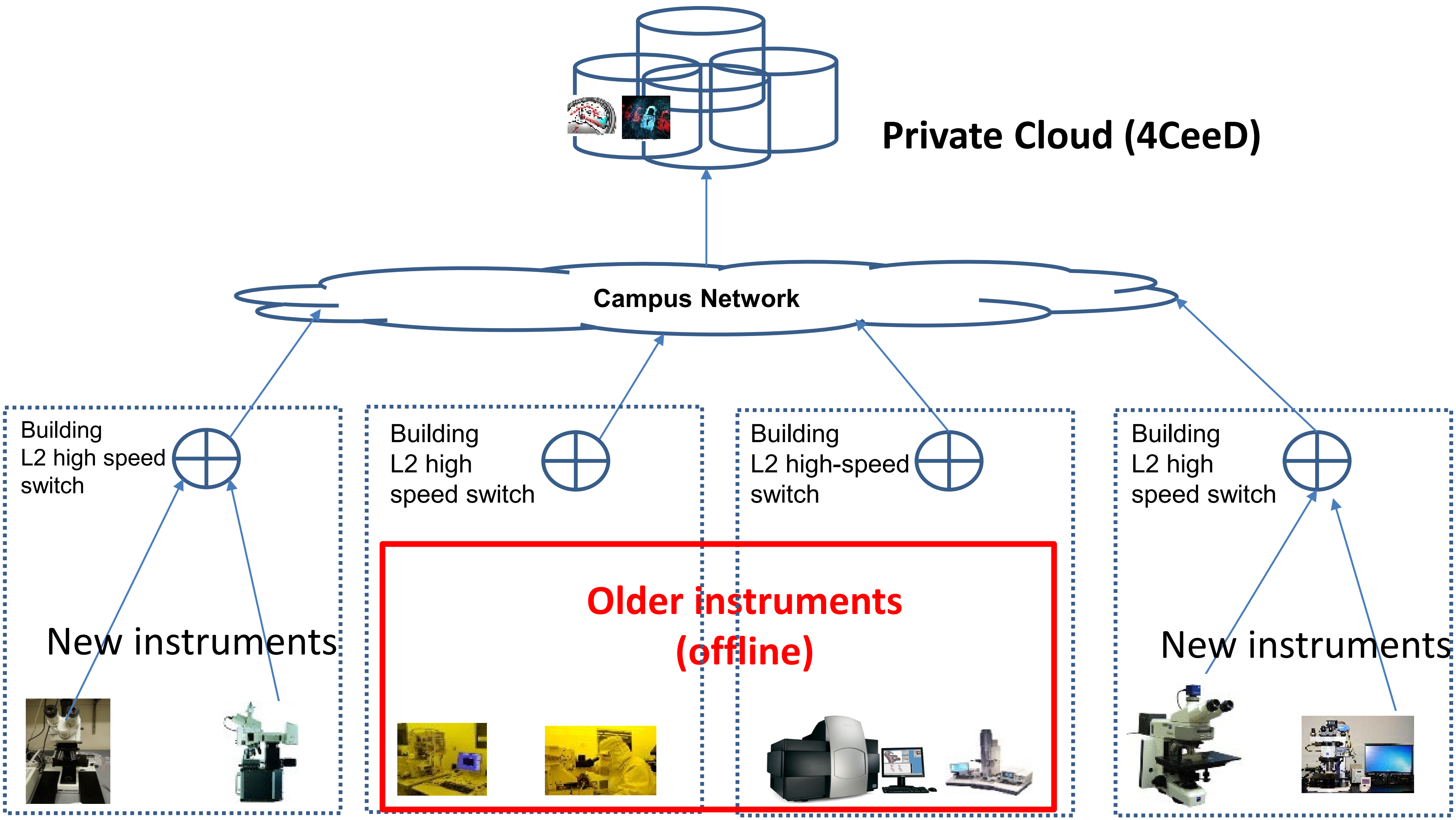
Current situation in campus cyberinfrastructure



Challenges of connecting offline older instruments

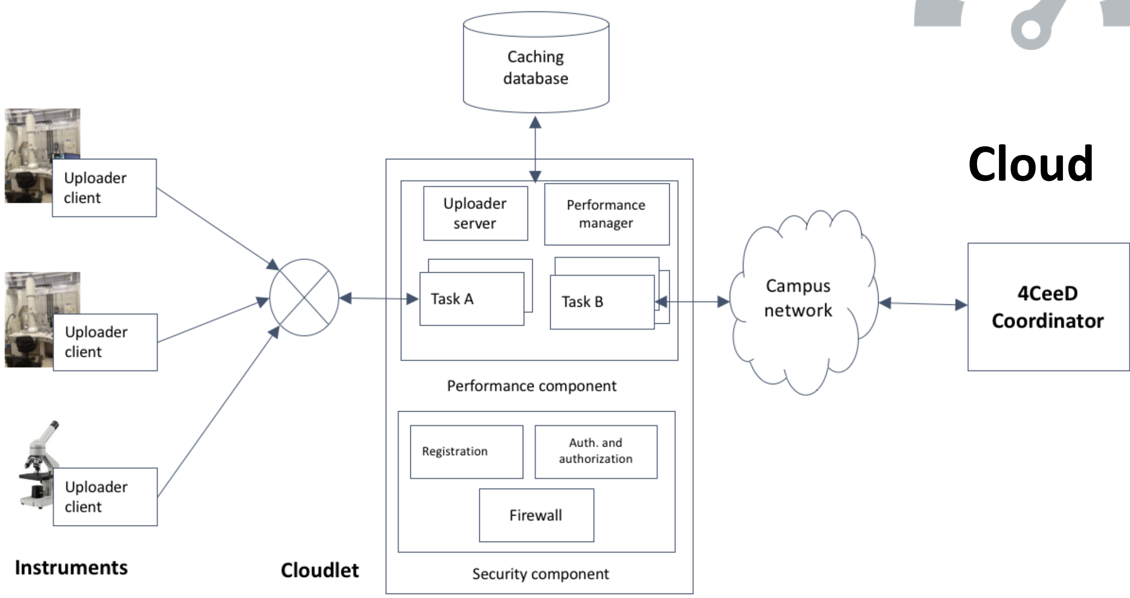
- **Performance mismatch**: Older instruments' Windows NT or XP runs network protocols at lower bandwidth speeds (10Mbps or 100Mbps)

- **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

Edge Server (Cloudlet)

Cloud



Performance:

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

BRACELET in 3-tier architecture

Security:

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

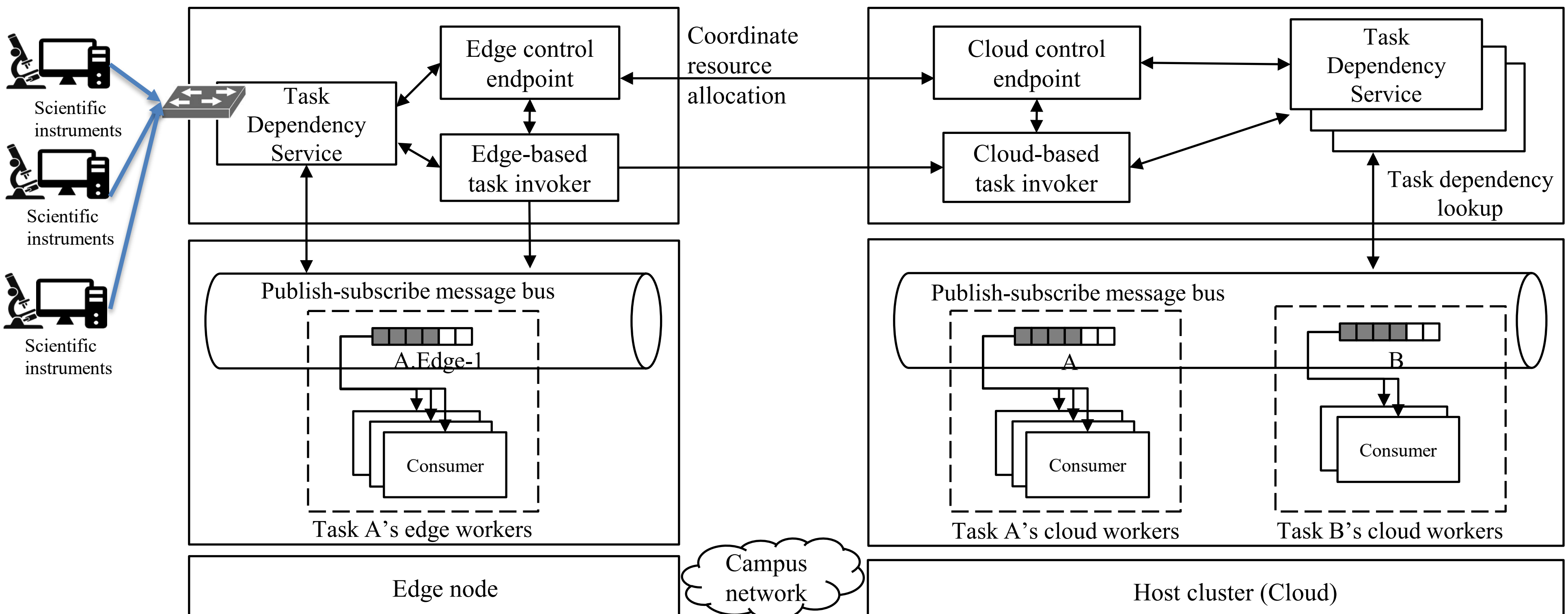
BRACELET Design

Edge Server

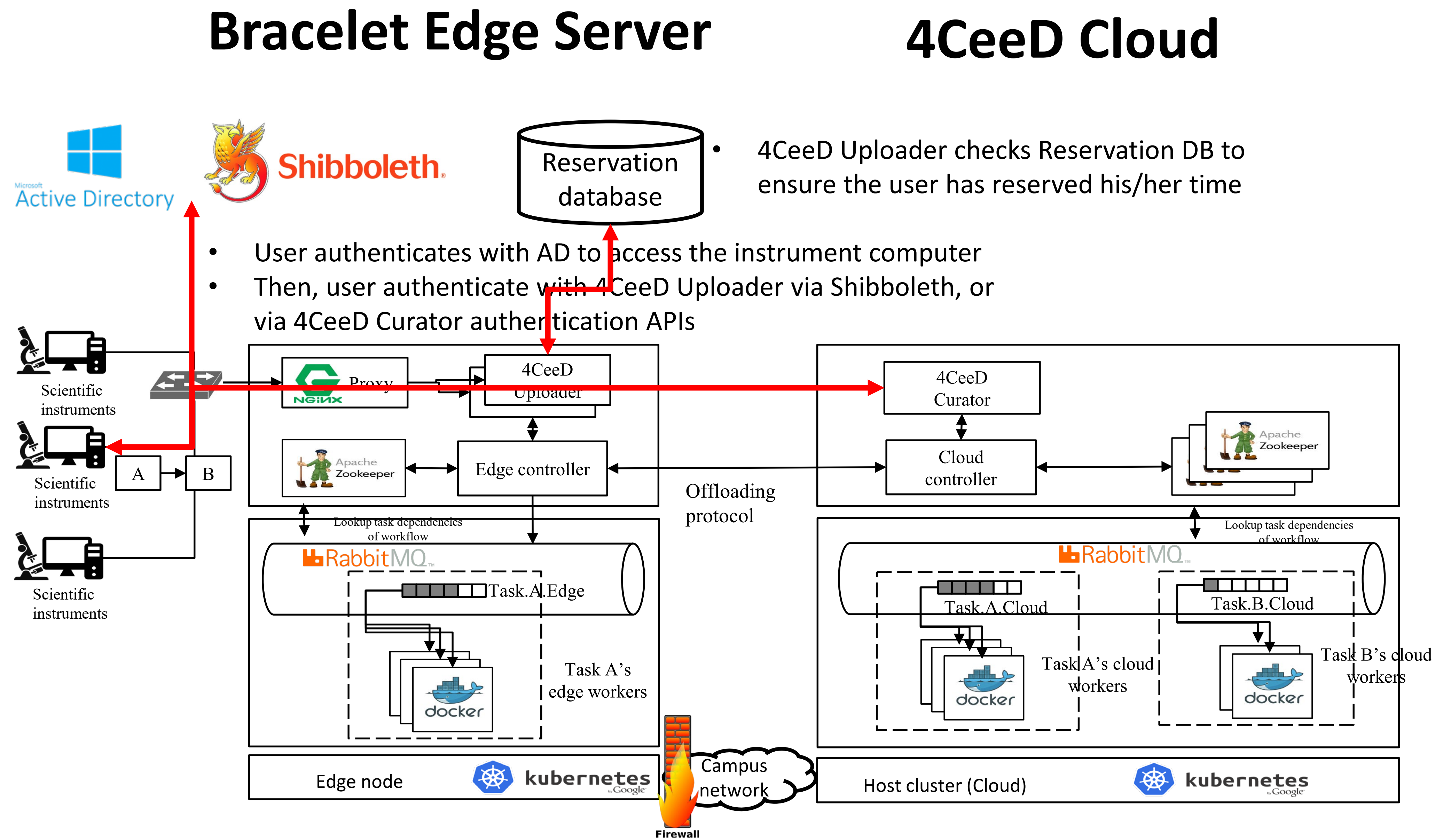
- Security service
  - Check equipment address
  - Authenticate user and his reservation
- Compute/Transport service
  - Forward and upload data

Cloud

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



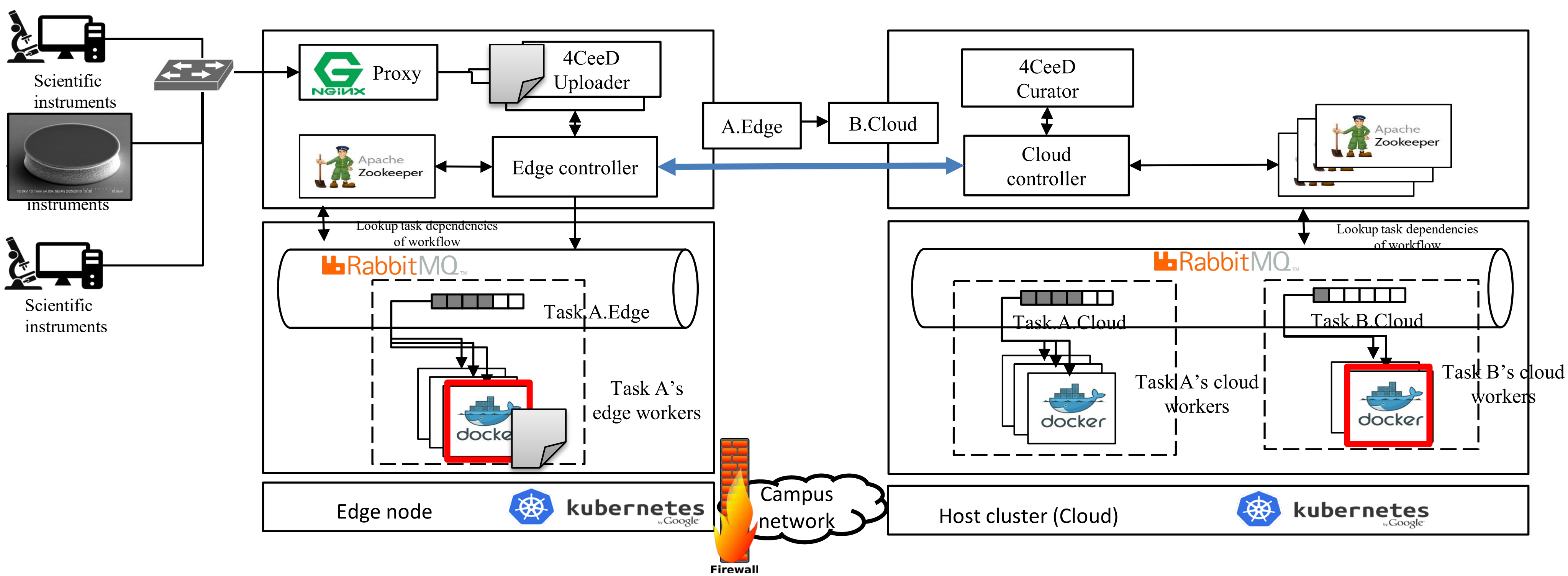
User authentication from instruments via BRACELET



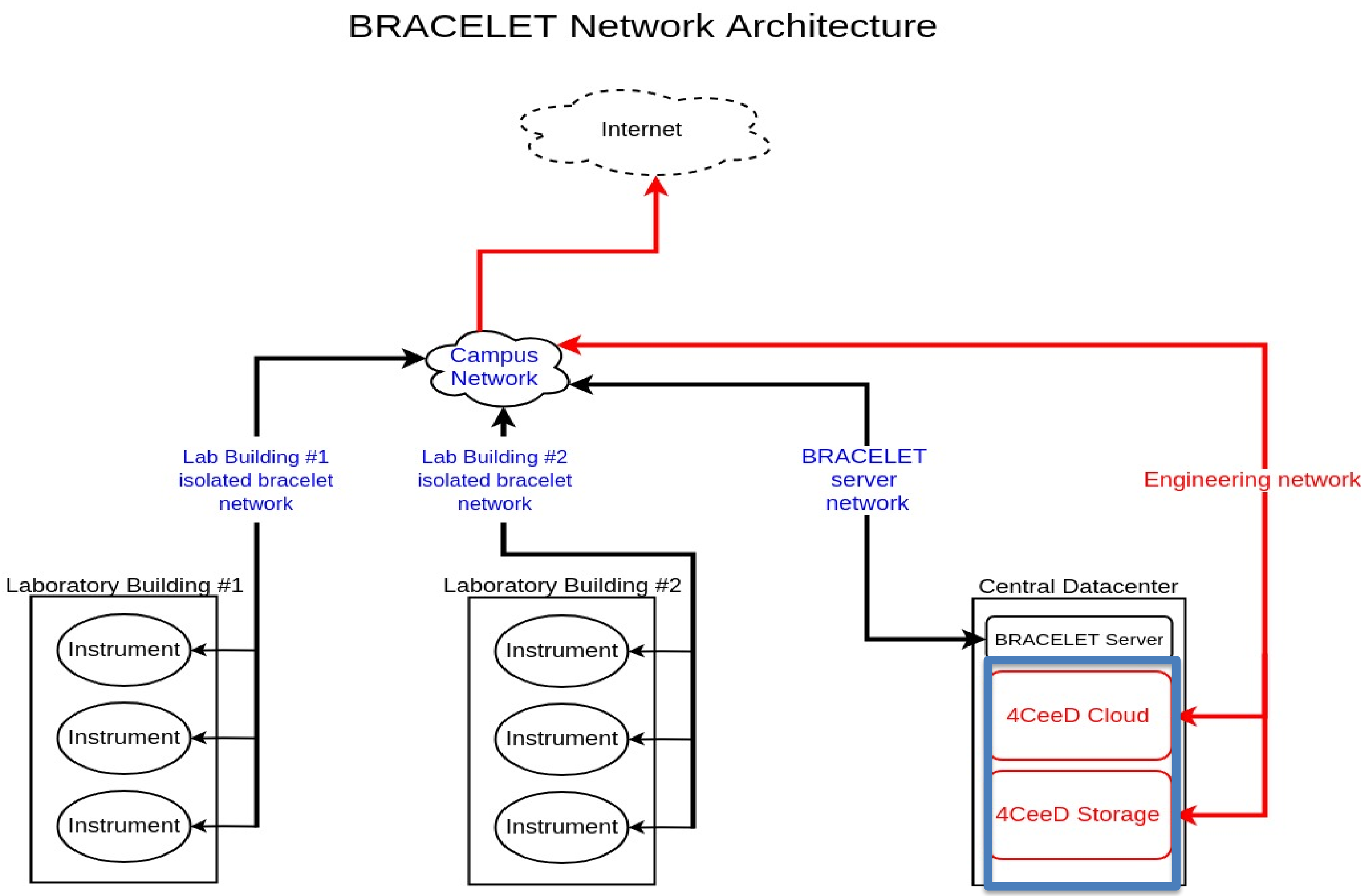
- 4CeeD Uploader checks Reservation DB to ensure the user has reserved his/her time
- User authenticates with AD to access the instrument computer
- Then, user authenticate with 4CeeD Uploader via Shibboleth, or via 4CeeD Curator authentication APIs

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.