ETH zürich

# Federated data services with abundant compute resources

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@Forschungszentrum Jülich: Katrin Amunz, Timo Dickscheid, Sonja Grün, Alex Peyser + team

# Deep Learning toolkits on Cray XC system @ CSCS

| DL Toolkit | C++ & GPU backend | MPI | Working on Cray XC | Fully supported @ CSCS |
|---|---|---|---|---|
| TensorFlow | yes | no | yes | yes |
| TensorFlow+MPI | yes | yes | yes | in progress |
| MXNet | yes | no, ext. to use MPI | yes | in progress |
| Caffe-MPI | yes | yes | yes | in progress |
| CNTK | yes | yes | yes | in progress |
| Spark | no (Java + ext. to use GPUs) | no | yes | in progress |

- Installing a DL toolkit on Cray XC is similar to installing any HPC application
  - few extra libraries are needed to satisfy dependencies
- Staging a toolkit can be done with SLURM (our resource manager at CSCS)
  - some toolkits (like Spark) require SSH to be available on compute nodes

# DL toolkits on CSCS's Cray XC systems

- Many toolkits use familiar HPC technology
  - developed in C++
  - CUDA/GPU-aware libraries
- HPC filesystems like Luster provide high throughput and data resilience
- MPI enables access to high performance network such as Cray Aries
  - low latency, high bandwidth
- Running a toolkit at scale requires a large amount of GPU accelerated nodes
  - HPC platforms are providing this capacity
- At scale the toolkits face common issues of HPC applications:
  - network and synchronisation boundedness
  - I/O and data access issues

**HPC systems are very well suited platforms for running Deep Learning workloads at scale**

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# Cray Takes on Fourth Paradigm

**XC50 supercomputer plus Microsoft's Cognitive Toolkit was used to scale up training**

Michael Feldman | December 19, 2016 18:09 CET

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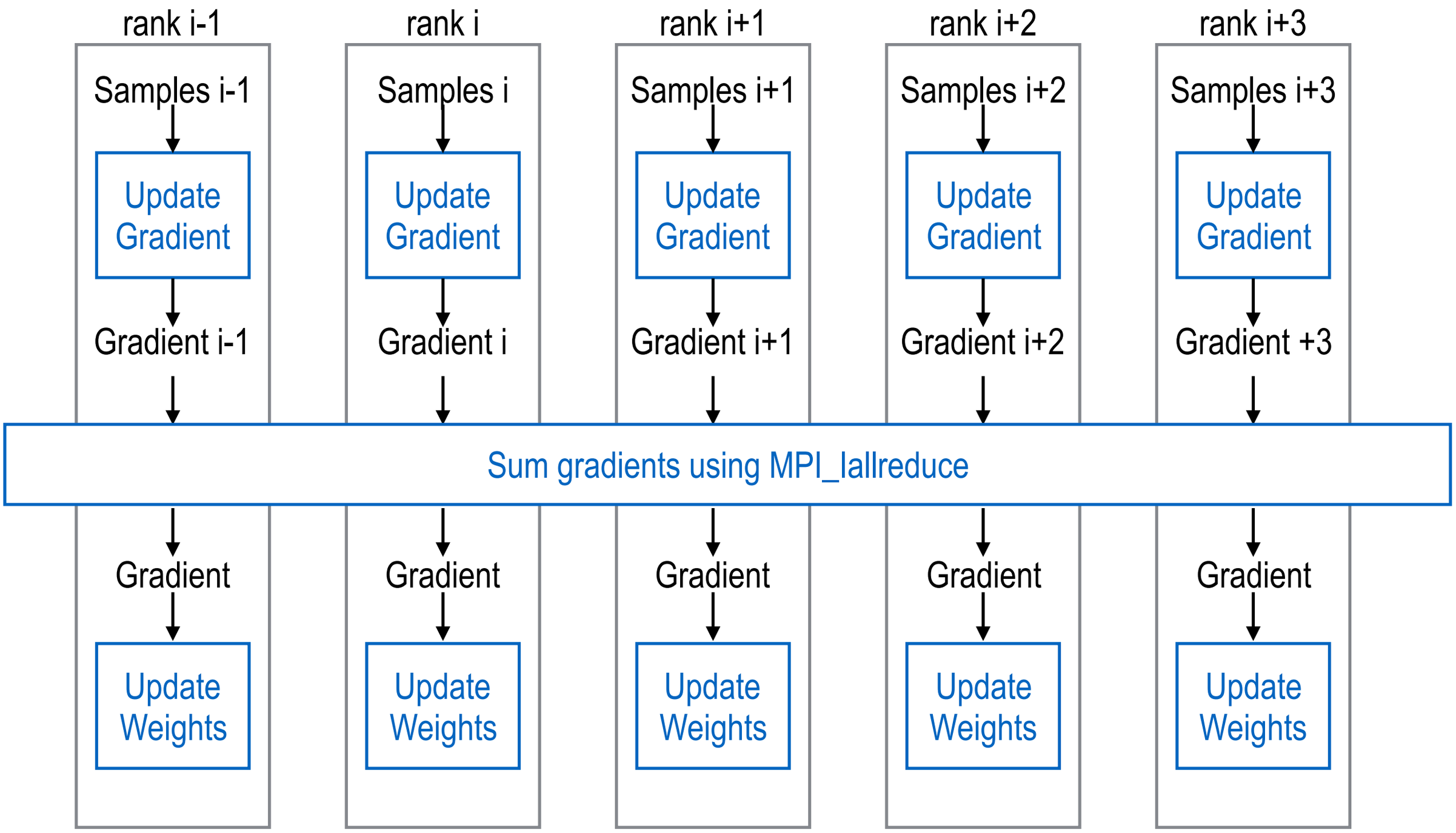
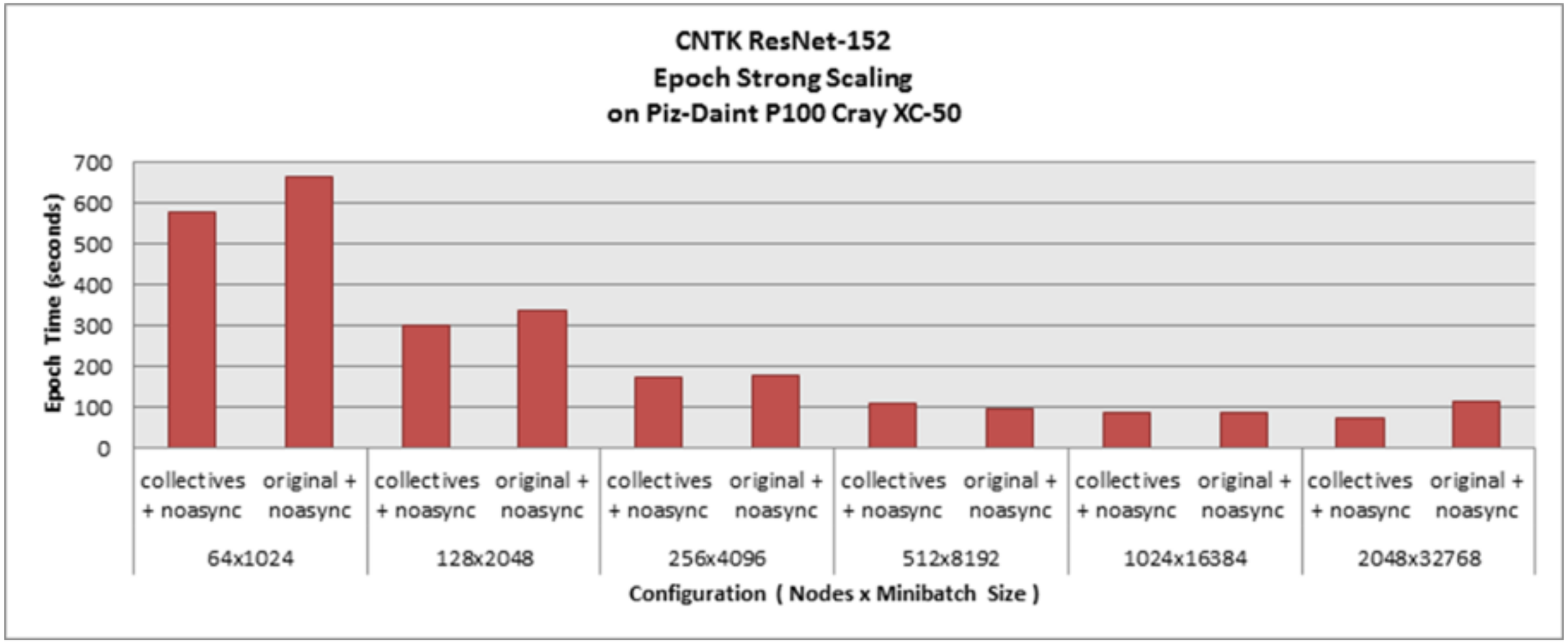
Cray's recent announcement about how its XC50 supercomputer plus Microsoft's Cognitive Toolkit was used to scale up training of a neural network serves as a proof point on how topflight HPC technologies can be used to push the boundaries of deep learning. But the company's long game is to bring supercomputing into the realm of deep learning and the broader category of data analytics in a more generalized fashion.

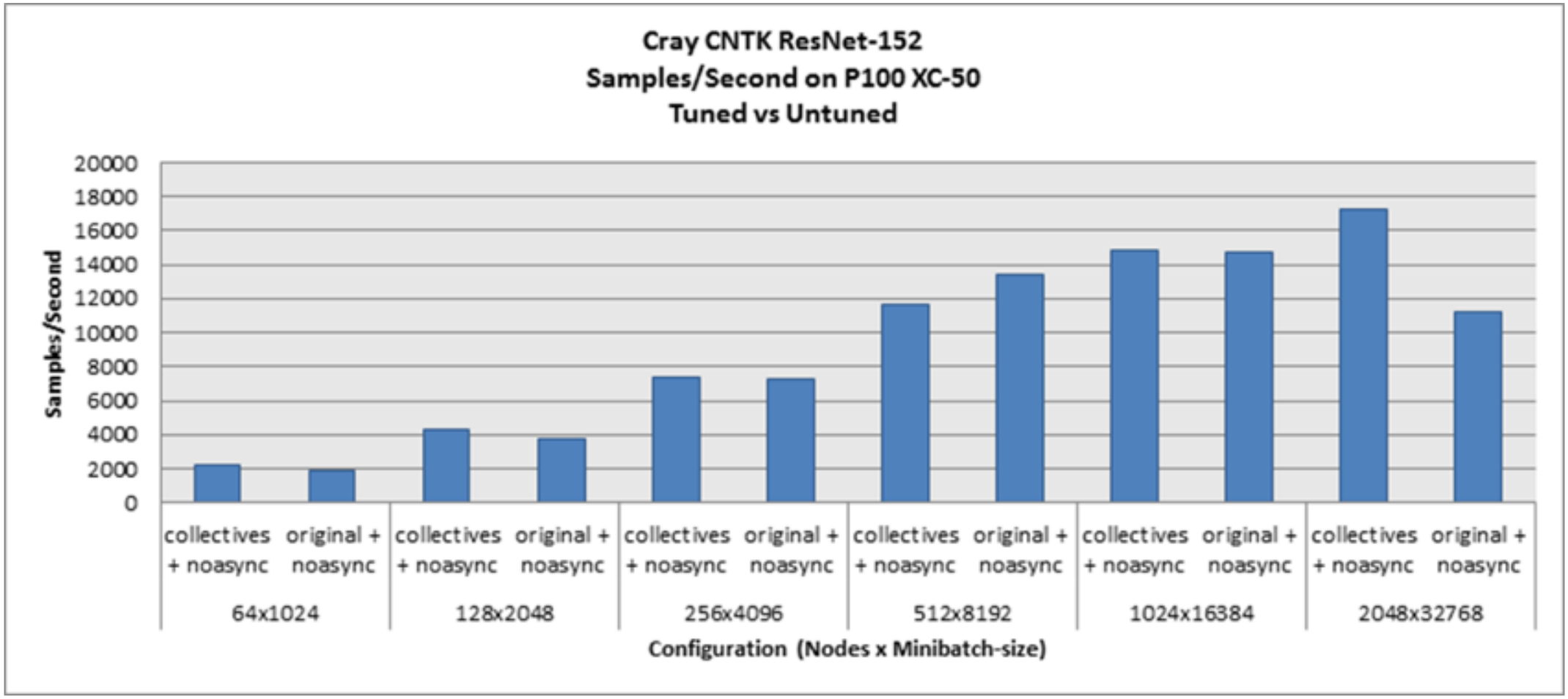

The XC50 in question is "Piz Daint," the 9.8-petaflop system housed at the Swiss National Supercomputing Centre (CSCS), which was recently upgraded with 4,500 of NVIDIA's new P100 GPUs. Each of those GPUs is able to deliver over 5.3 teraflops of double precision floating point performance, 10.6 teraflops of single precision performance, or 21.2 teraflops of half precision performance. Those lower precision flops make these devices especially useful for deep learning codes, where 64-bit float pointing operations are, for the most part, overkill.

Despite all this concentrated performance, training neural networks is so computationally intense that many GPUs are often needed to in train these models in a reasonable amount of time – minutes or hours, rather than weeks or months. The problem is that with conventional compute clusters and first-generation deep learning frameworks, it's hard to scale these applications without running into some rather daunting bottlenecks.

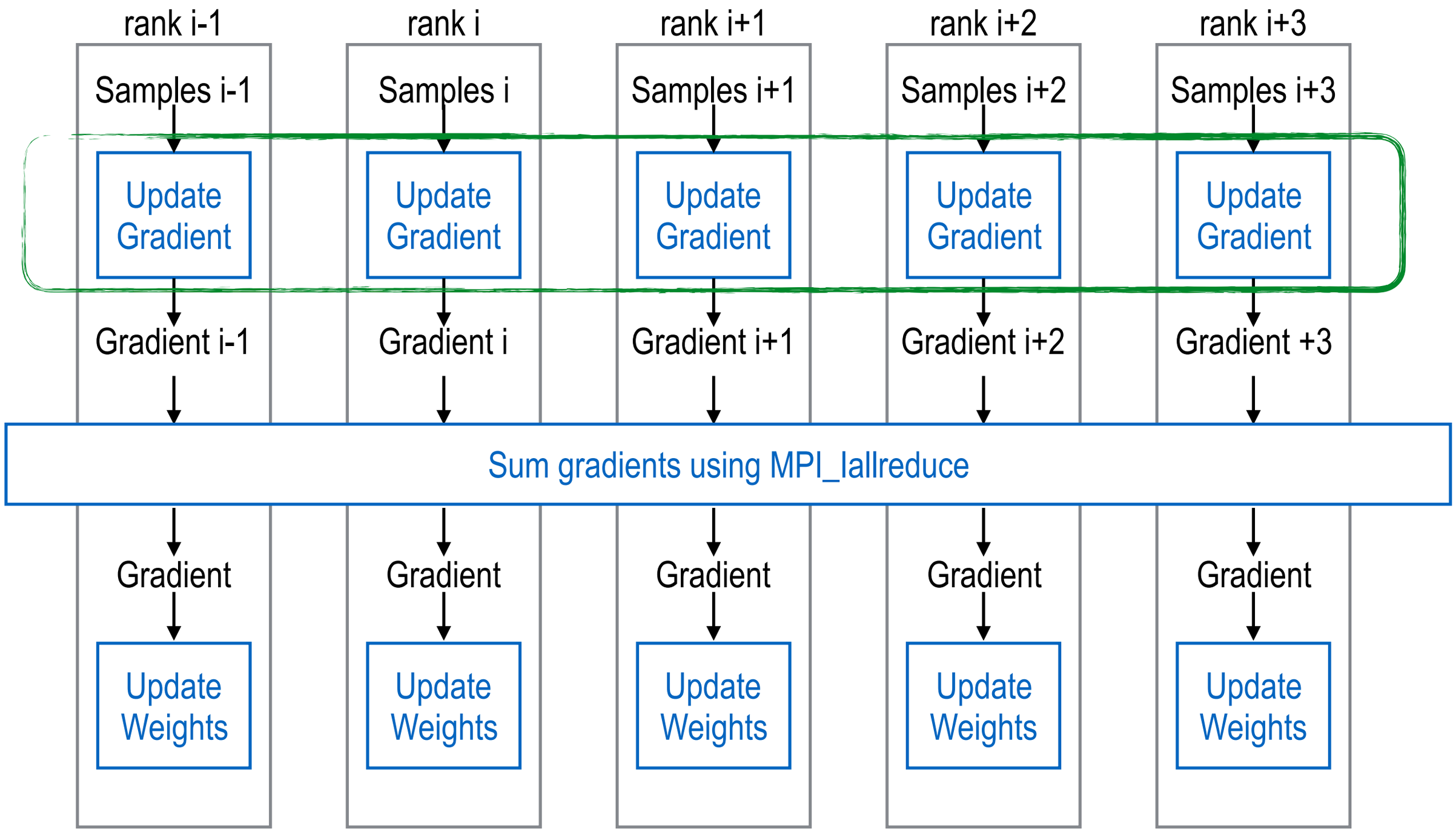
# Scaling CNTK with MPI




CNTK ResNet-152
Epoch Strong Scaling
on Piz-Daint P100 Cray XC-50
Epoch Time (seconds)
700
600
500
400
300
200
100
0
collectives + noasync
original + noasync
64x1024
128x2048
256x4096
512x8192
1024x16384
2048x32768
Configuration ( Nodes x Minibatch Size )


Cray CNTK ResNet-152
Samples/Second on P100 XC-50
Tuned vs Untuned
Samples/Second
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
collectives + noasync
original + noasync
64x1024
128x2048
256x4096
512x8192
1024x16384
2048x32768
Configuration (Nodes x Minibatch-size)

# Scaling CNTK with MPI



“We develop algorithms, we don’t have time to deal with C/C++ or MPI”

–a famous computer science colleague working in machine learning

# … echoed by many scientists working with data

## Interactive Notebook

Import TensorFlow and start an interactive session

In [1]:
```
import tensorflow as tf
sess = tf.InteractiveSession()
```

Build a computation graph

In [2]:
```
matrix = tf.constant([[1., 2.]])
negMatrix = tf.neg(matrix)
```

Evaluate the graph

In [3]:
```
result = negMatrix.eval()
print(result)
```

```
[[-1. -2.]]
```

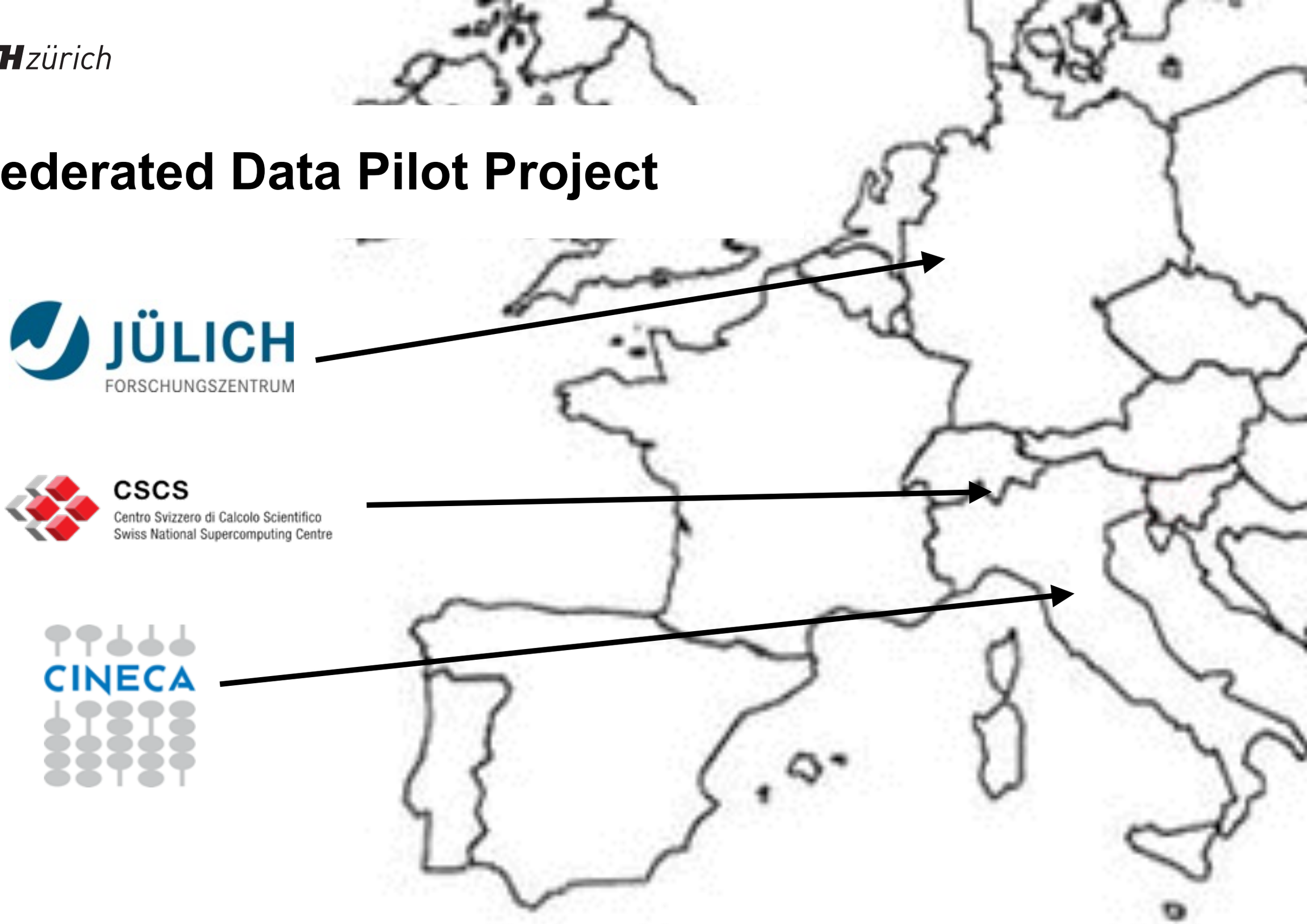
Nishant Shukla (2017)

# Using Jupyter to get our heads around interactive supercomputing

- Jupyter allow users to
  - integrate development, execution of computation, pre- and post processing with visualisation into one “workflow”;
  - share these workflows in a team; and
  - document their work
- Need to provide an environment where web-based front-end of the notebook is separated from the computation backend
  - run some of the computation on a supercomputer
- Interactive simply means sub-second response time
  - this requires properly organising data in memory/storage sub-system

# … and the service should be up most of the time (like 99+ %)

# Federated Data Pilot Project

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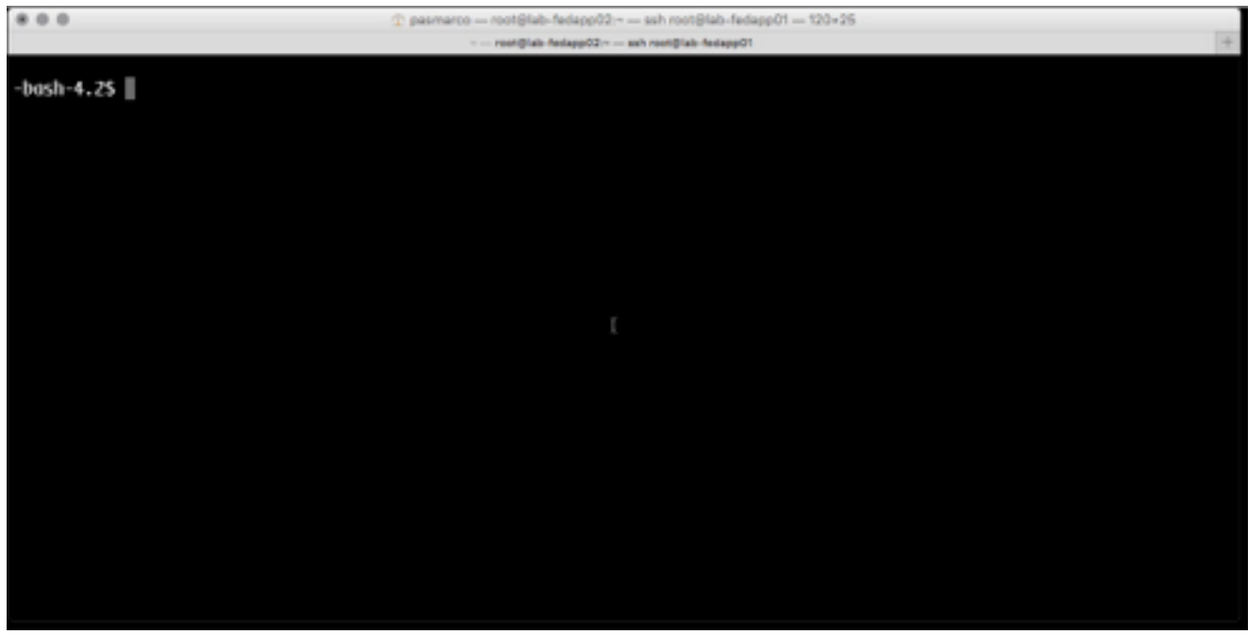
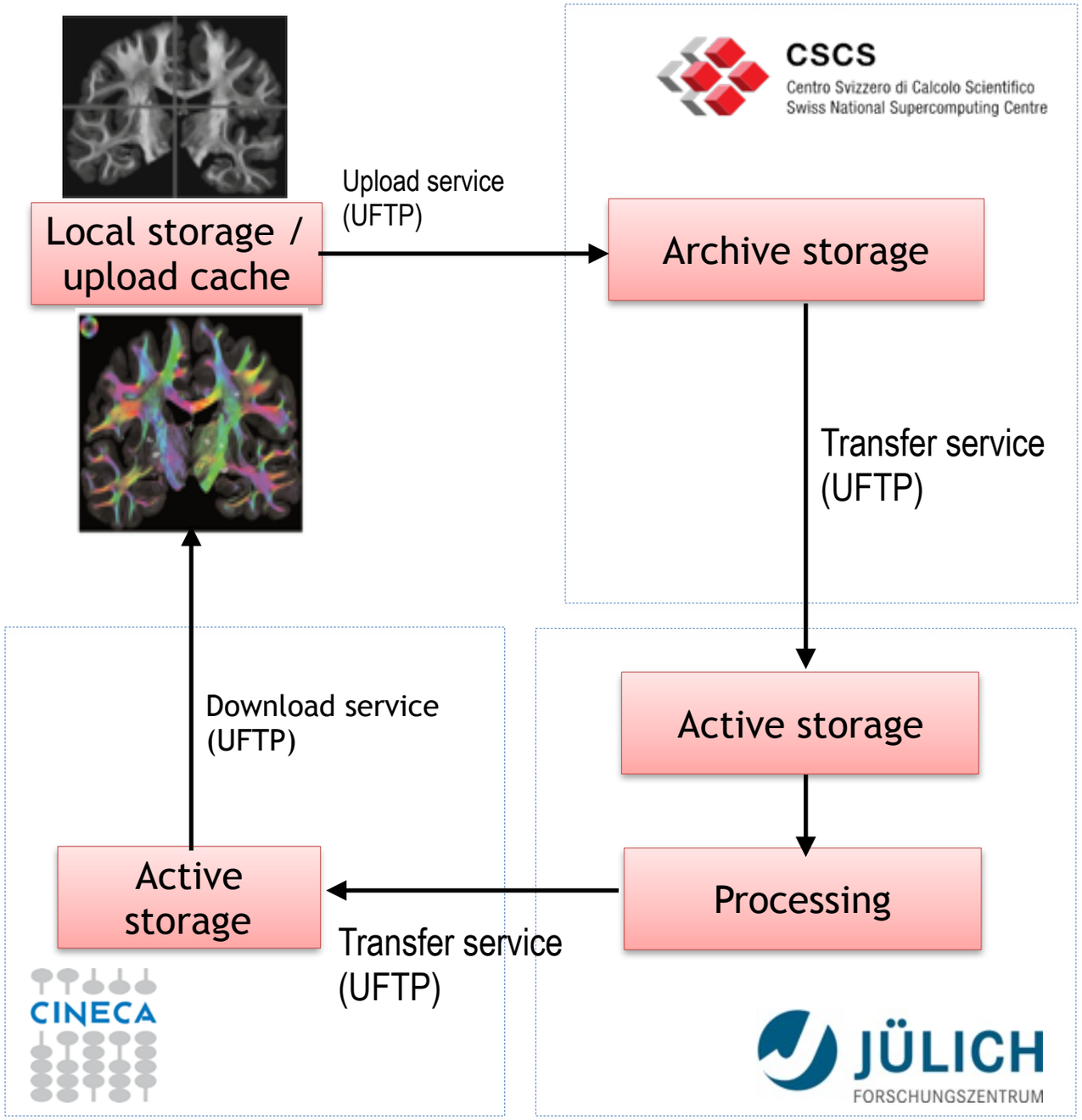
# Federated data infrastructure – proof of concept

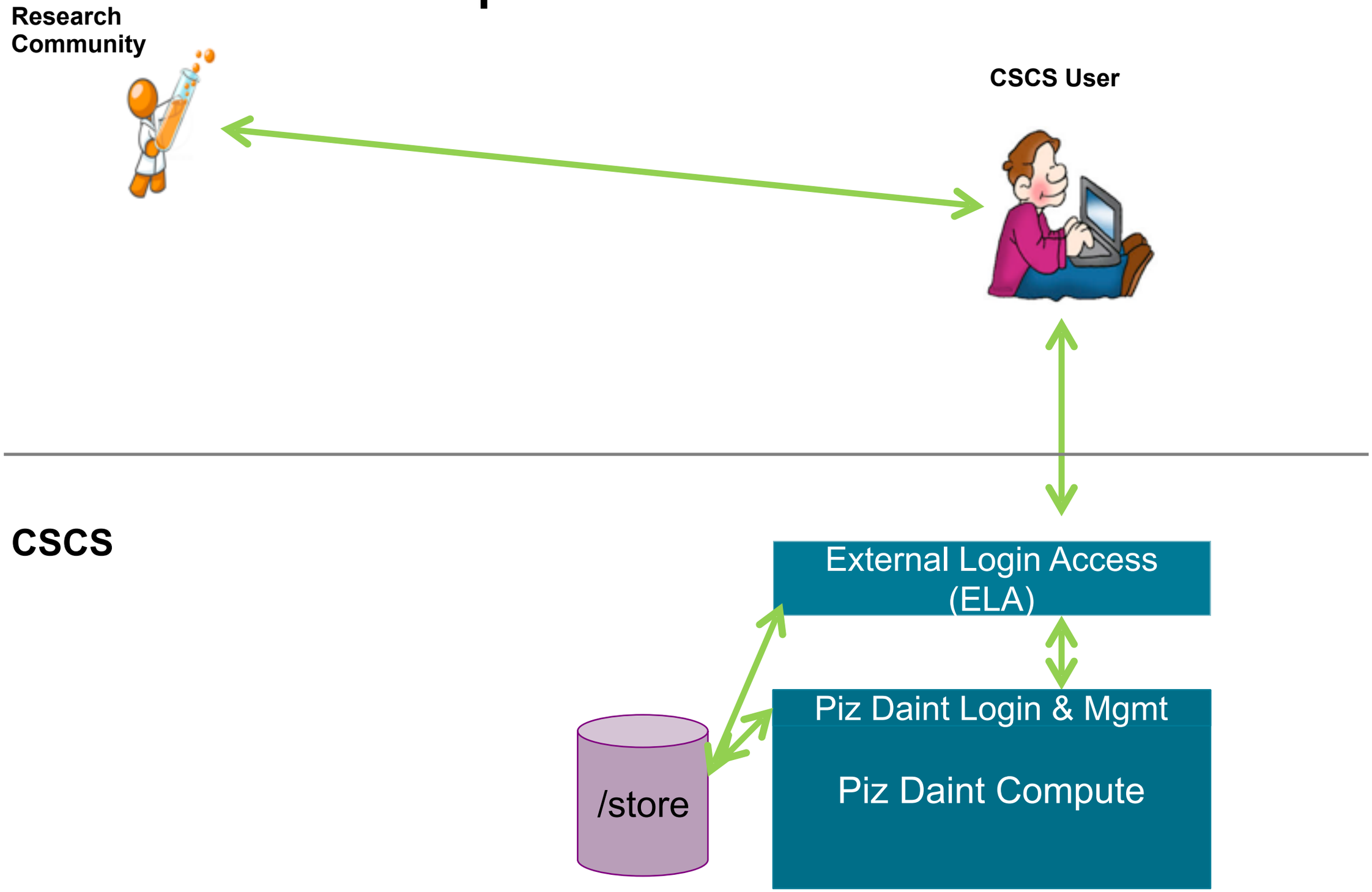


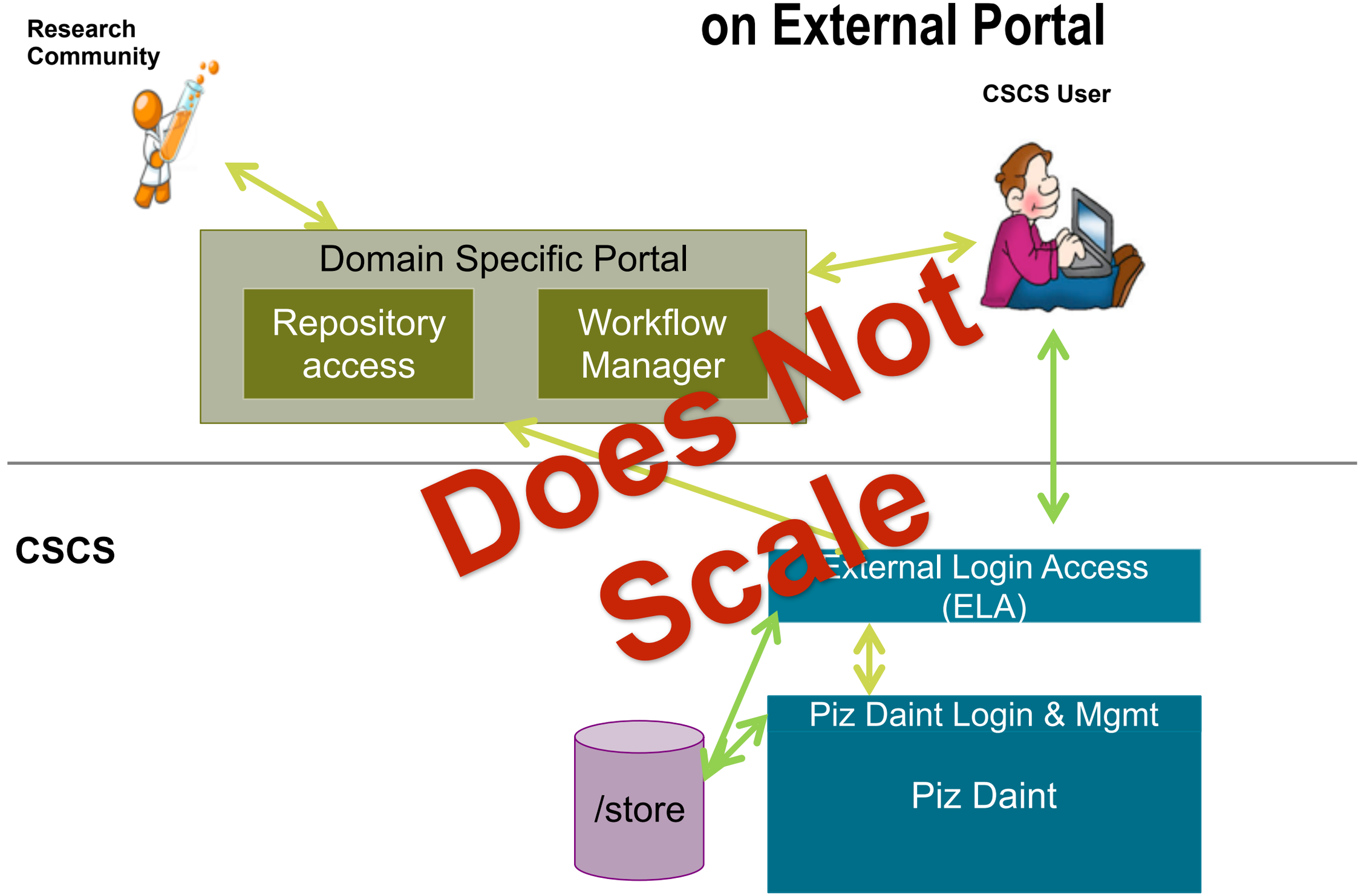
# A few more practical things …

- Scientists, not system administrators will want to manage teams and access to data
  - this poses a fundamental challenge to POSIX style file systems
  - so we have to map between object-store approaches that give users control and POSIX file systems with appropriate performance and in use on supercomputers
- Software deployment needs to be easy
  - virtual machines; or
  - light-weight VMs: Docker / Shifter as a service

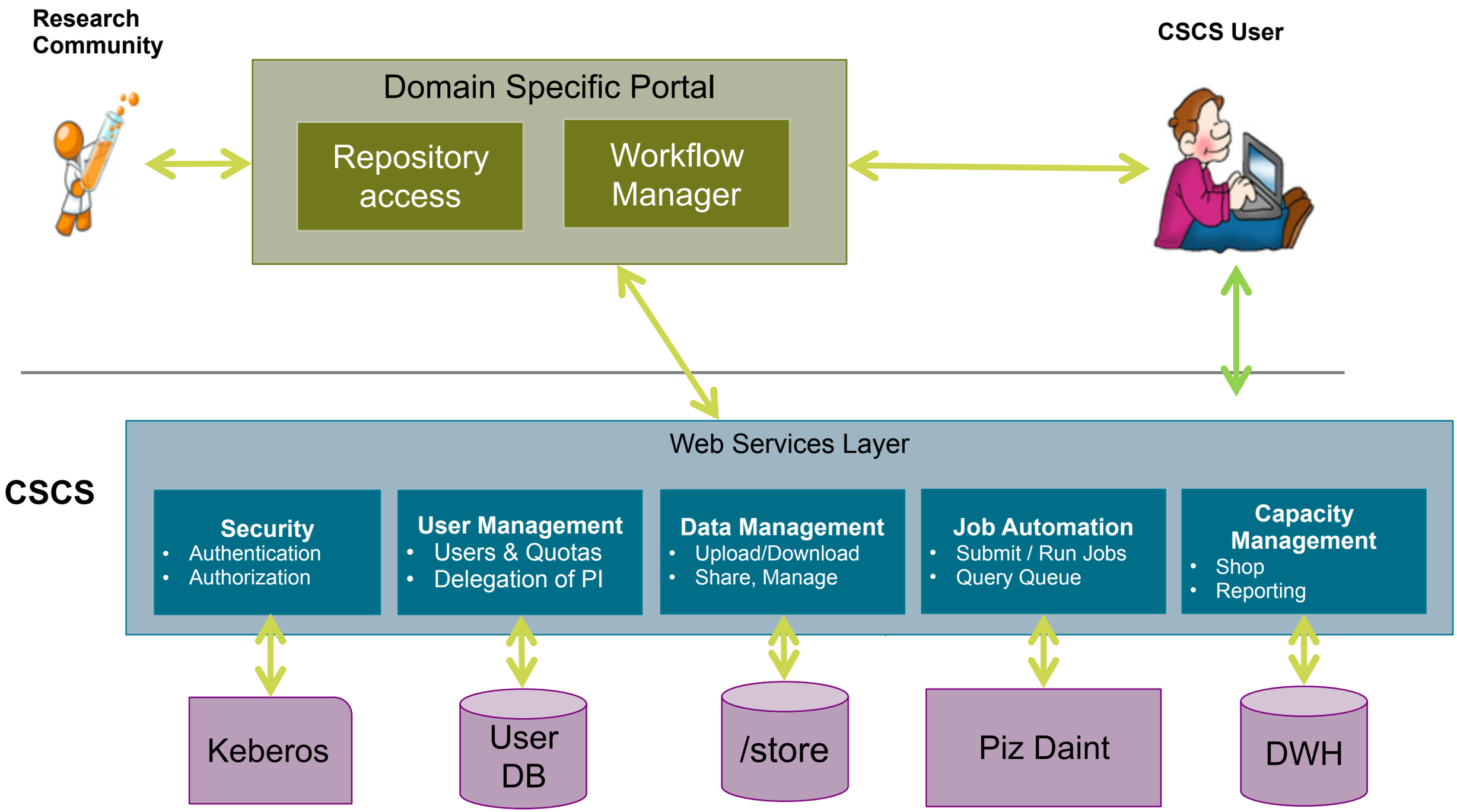
# Architectural Developments – Traditional Architecture



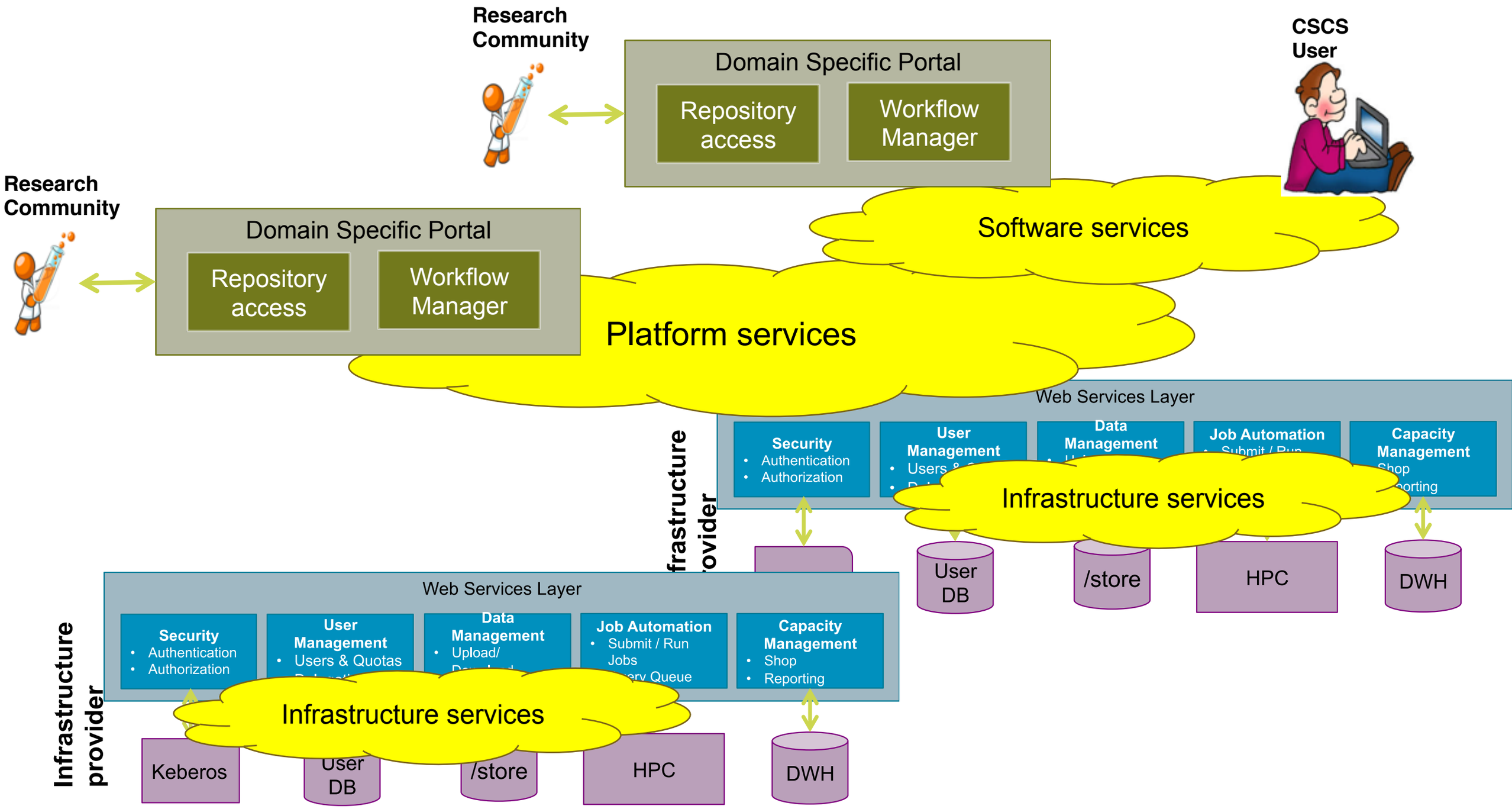
# Architectural Developments – Improved Architecture Based on External Portal



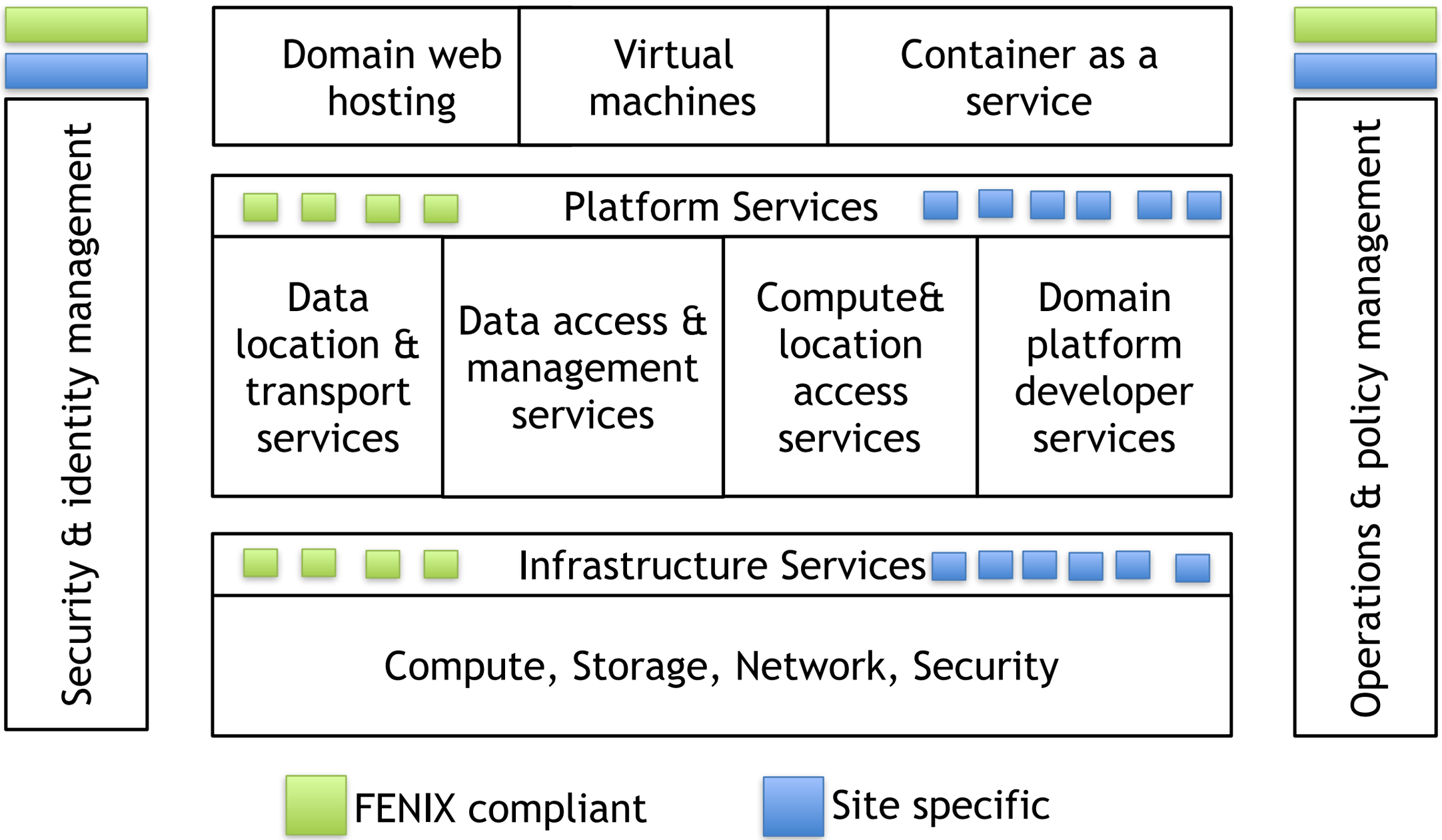
# Architectural Developments – Service Oriented Architecture (SOA)



# Supporting Federation using SOA



# The data center's concerns of SOA



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