Hartree Centre

Science & Technology Facilities Council

Tackling industry challenges with HPC, Big Data and Cognitive Computing

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STFC Hartree Centre

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@iainbethune @HartreeCentre

Who are we?

STFC's high performance computing, data analytics and cognitive technology centre

Provides businesses and researchers with access to powerful technologies, facilities and scientific computing expertise

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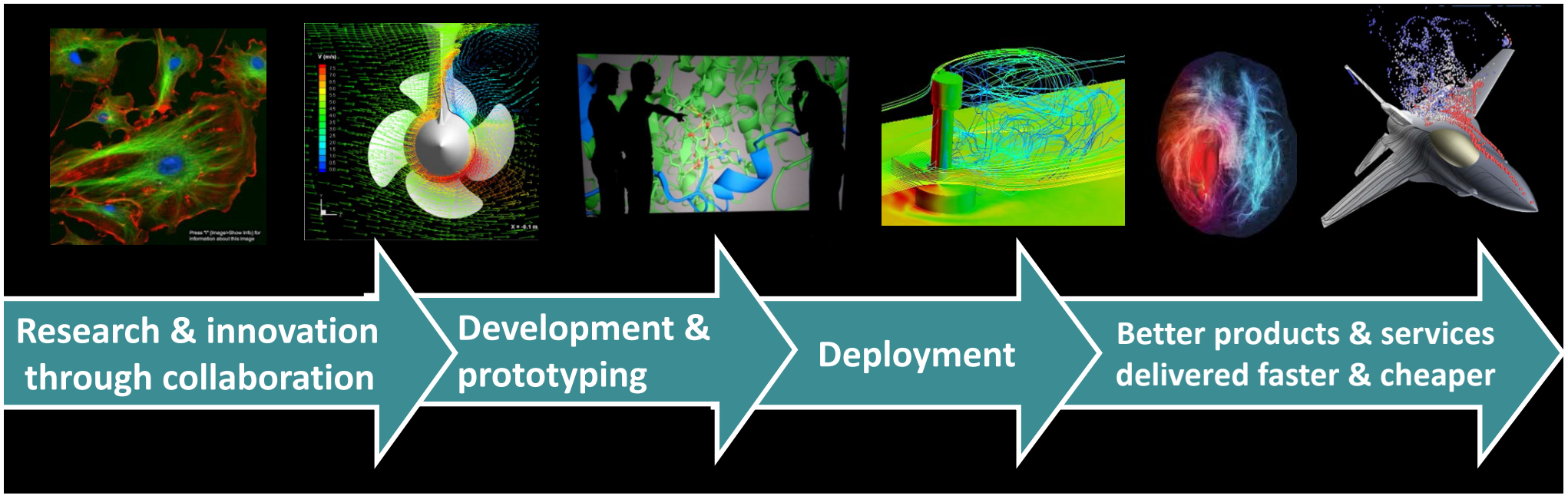
Our mission

To transform UK competitiveness by facilitating and accelerating the adoption of high performance computing, data-centric computing and cognitive technologies.



Hartree Centre Clients

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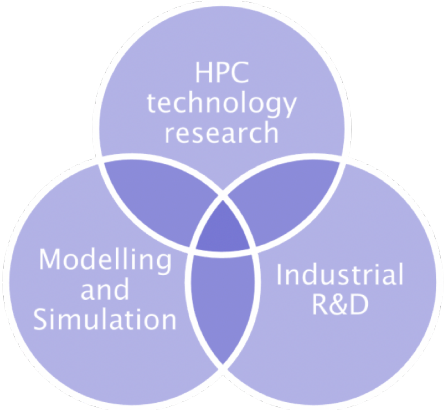
A Brief History

- Hartree Centre builds on STFC's long heritage and expertise in High Performance Computing
- 2012 focus on economic impact through software & modelling



- 2015 major investment in collaborative research (IROR)
  - Additional focus on data centric and cognitive computing
  - Embedded IBM Research Centre
  - Extended industrial & scientific reach
- 50 staff + 30 IBMers

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Our machines

Intel platforms

Bull Sequana X1000 | 846 SKL nodes + 840 KNL

Lenovo NeXtScale | 8,192 cores

Lenovo System x iDataPlex system | 2048 cores

Intel Xeon Phi | Knight's Corner

IBM Big Data Analytics cluster | 288TB

IBM data centric platforms

IBM Power8 + NVLink + Tesla P100 ”Paragon”

IBM Power8 + Nvidia K80 “Panther”

Energy-efficient & Emerging Tech

Maxeler FPGA system

ARM 64-bit platform

Clustervision novel cooling demonstrator

Academic HPC platform (Tier 2)

JADE Nvidia DGX-1

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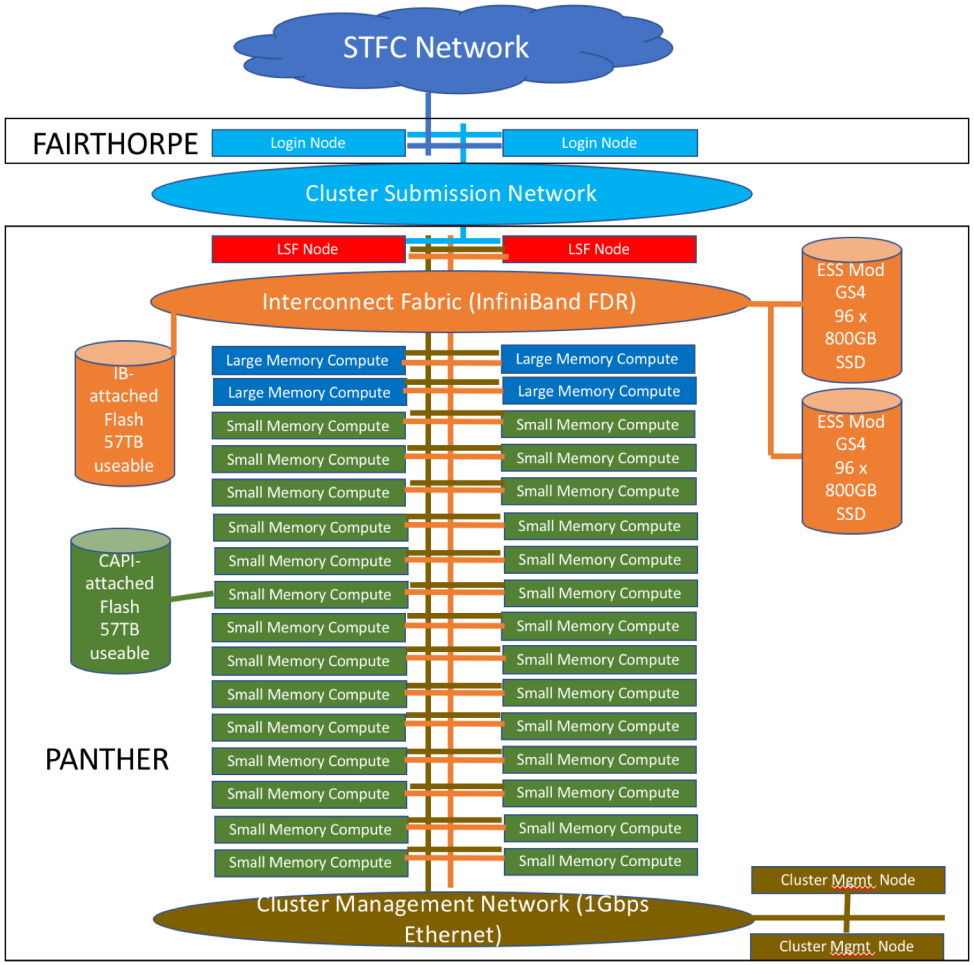
Panther: Current Architecture



SERVER SPECIFICATIONS

Login Node
- S822LC (8335-GTA)
- Bare metal RHEL 7.2 LE
- 16 x 3.3 GHz cores
- 1TB RAM
- 2 x 1TB 7.2k RPM drives
- 2 x nVidia K80 GPUs

LSF Node
- S822LC (8335-GCA)
- Bare metal RHEL 7.2 LE
- 16 x 3.3 GHz cores
- 512GB RAM
- 2 x 1TB 7.2k RPM drives

Large Memory Compute
- S822LC (8335-GTA)
- Bare metal RHEL 7.2 LE
- 16 x 3.3 GHz cores
- 1TB RAM
- 2 x 1TB 7.2k RPM drives
- 2 x nVidia K80 GPUs

Small Memory Compute
- S822LC (8335-GTA)
- Bare metal RHEL 7.2 LE
- 16 x 3.3 GHz cores
- 512GB RAM
- 2 x 1TB 7.2k RPM drives
- 2 x nVidia K80 GPUs

Cluster Mgmt. Node
- S822LC (8335-GCA)
- Bare metal RHEL 7.2 LE
- 16 x 3.3 GHz cores
- 512GB RAM
- 2 x 1TB 7.2k RPM drives

- 32x compute nodes
- LSF Data Manager – stage to/from CDS
- LSF Batch job scheduler

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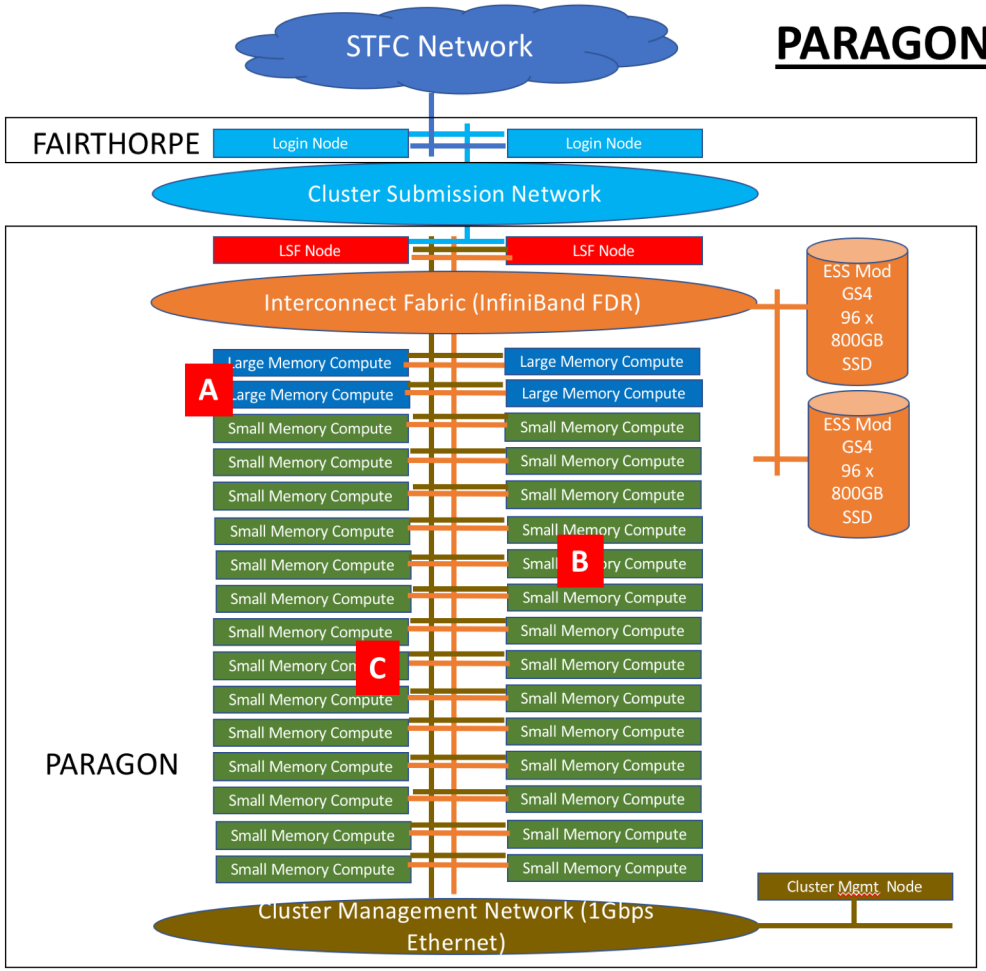
Paragon: Current Architecture



PARAGON 2017 EXTENSIONS

A 1 x new Large Memory Compute node added (to bring number to 5)

B 7 x new Small Memory Compute nodes added (to bring number to 35)

C 3.2TB NVMe PCIe flash added to all Compute Nodes (only included in Large Memory Compute nodes at initial deployment)

- 40x compute nodes
- NVIDIA Tesla P100 GPUs

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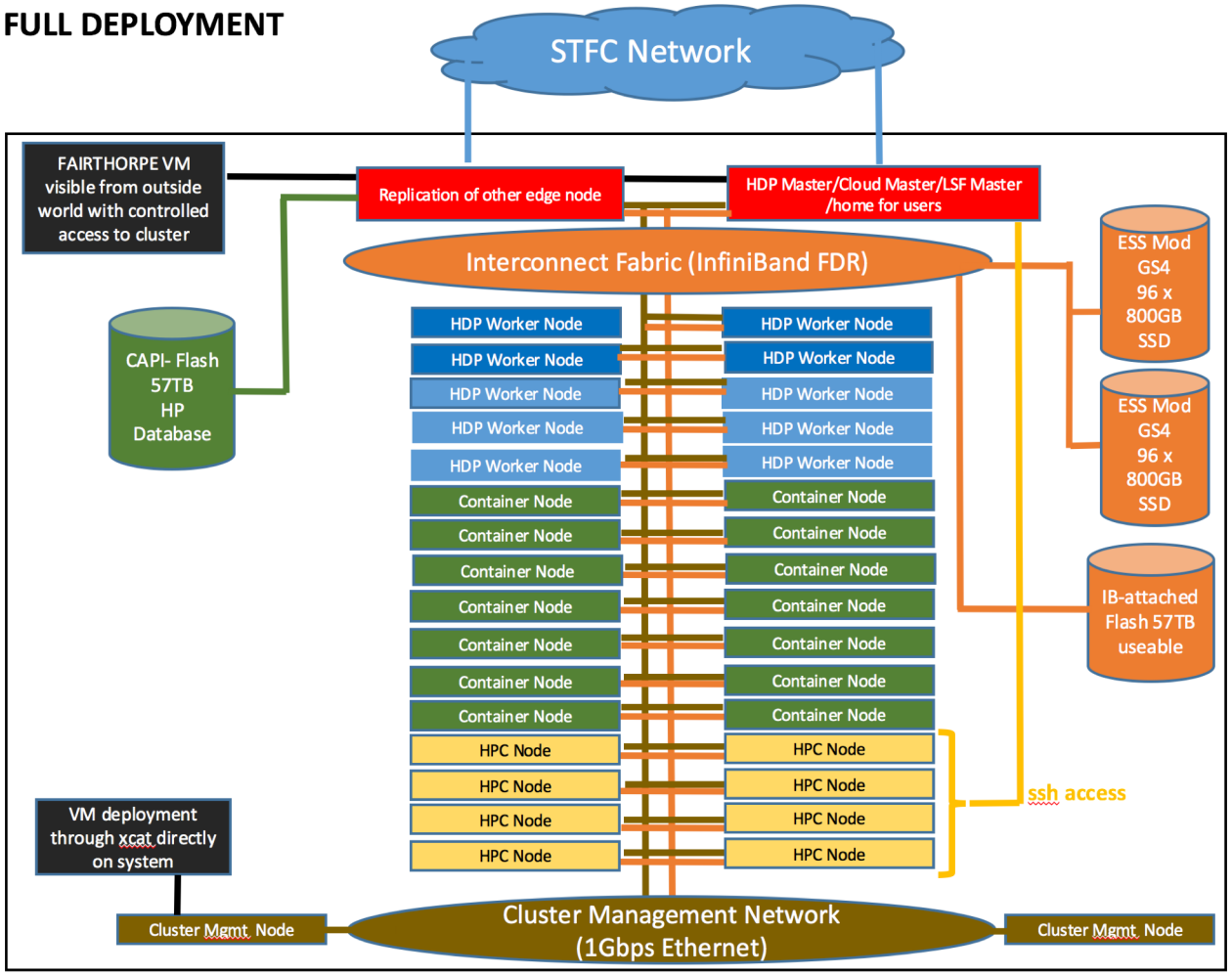
Towards a converged architecture for HPC, Big Data & Container/cloud workflows

PHASE 2
FULL DEPLOYMENT



- HDFS-GPFS adaptor
- HPC Nodes (LSF)
- Hortonworks Data Platform Worker Nodes (Yarn)
- Container Nodes (Kubernetes / IBM Cloud Private)

- VMs for web-services

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IROR: Innovation Return on Research

- £115m investment by BEIS (2015-2020)
- Collaborative R&D programme with IBM Research
- Developing ‘Digital Assets’ to benefit key sectors of UK Economy
  - Chemistry & Materials, Life Sciences, Science/Engineering/Manufacturing
- Projects developed with major UK companies
  - Sectoral approach -> wider benefits

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Chemistry

- Parameterisation Engine
- Chemistry Workflow for HPC
- Cognitive Accelerator for Chemistry
- Consumable Computing for Chemistry
- Particle Dynamics Modeller

Life Sciences

- Membrane Binding & Permeation Assay
- Electronically Coarse Grained Biomolecular Simulation Method
- Omics analytics Catalogue
- HPC omics workflows as a service
- Precision Agriculture

Sci,Eng,Man

- Multiscale & Multiphysics Code Coupler
- Cognitive Uncertainty Quantification Toolkit
- Simulation Methods for Engineering Applications
- Intelligent Manufacturing

Enabling Technologies

- Code analysis & generation for HPC
- Cognitive Technical Computing as a Service
- Machine Learning at Scale
- Cognitive Knowledge APIs
- Cognitive Transportation Technology
- Cybersecurity at Scale
- Data Technology Platform


Converting physical experiments to a simulation workflow
Reducing the innovation cycle and time to market
Putting the tools in the hands of the formulation chemist
Ch
L
S
S
E
M
ET
Unilever – Computer Aided Formulation

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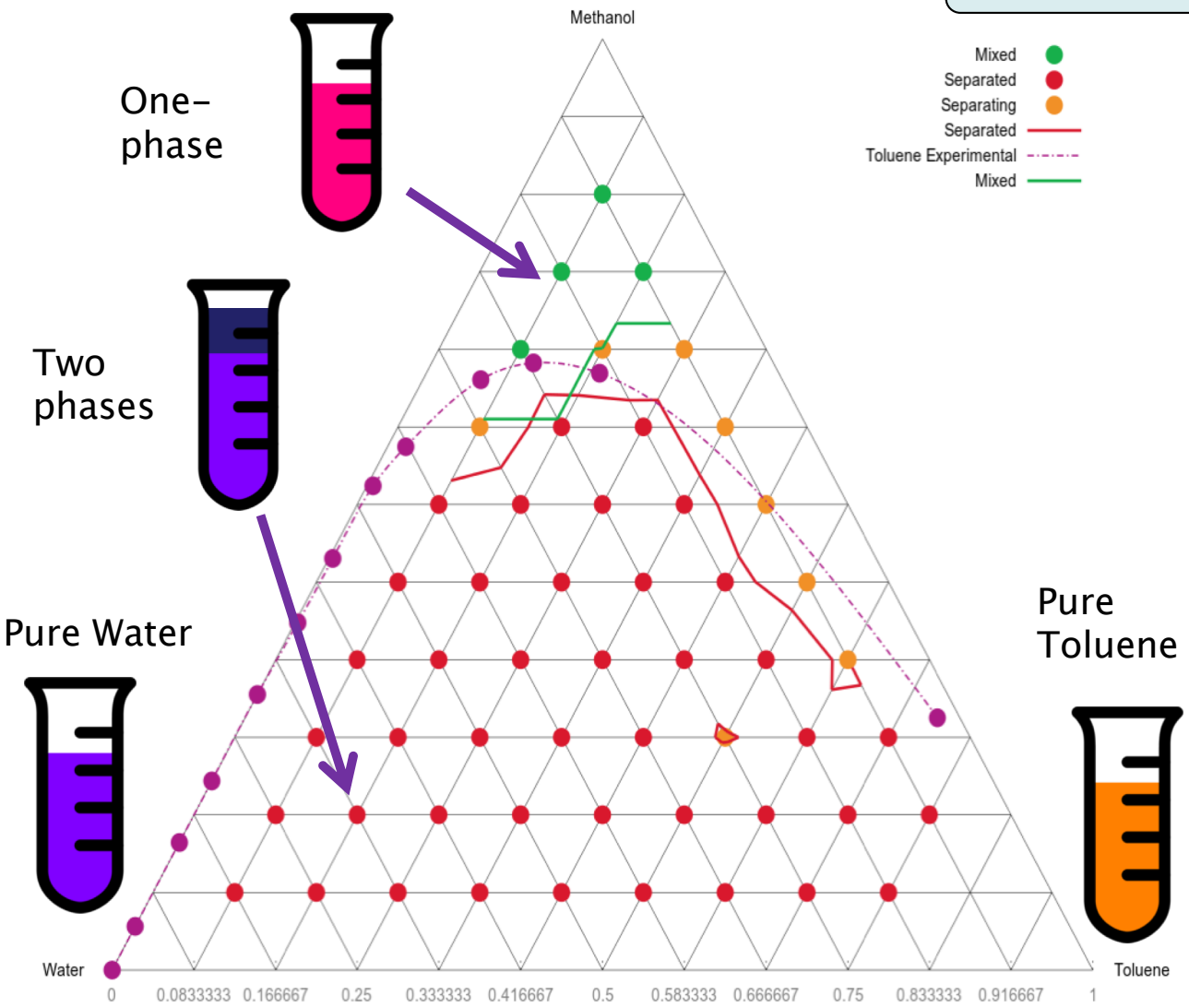
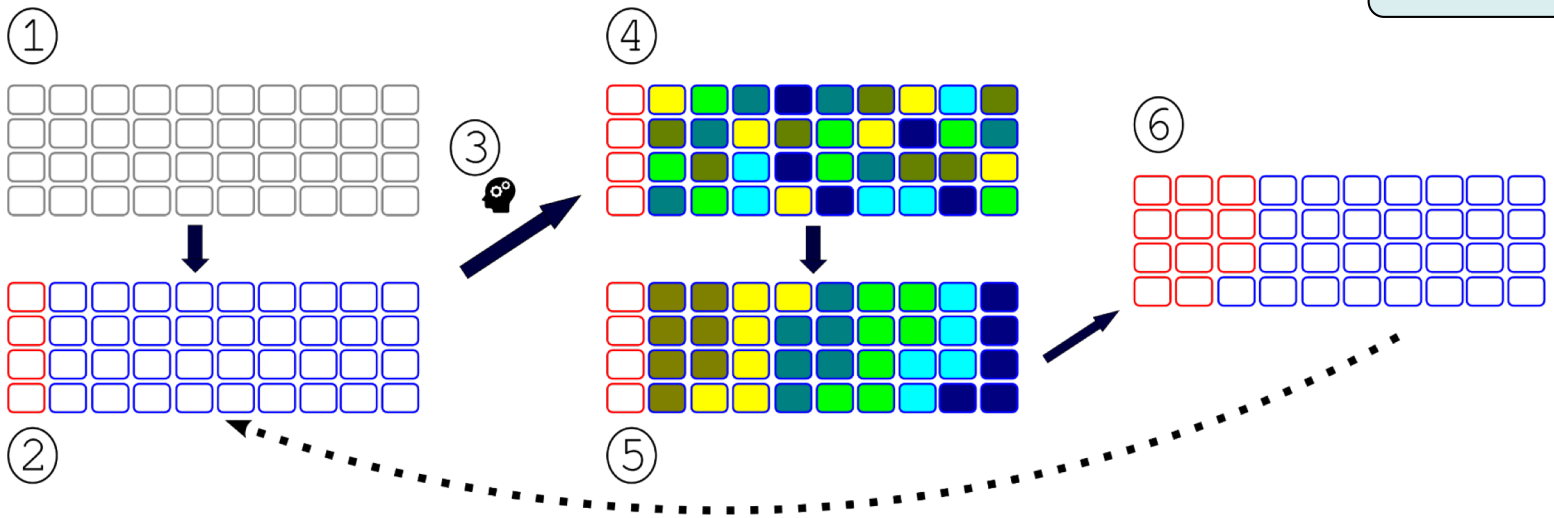
Ternary Phase Diagram

- Simulations of solutions of three different molecule types:
  1. Water
  2. Methanol
  3. Toluene
- Solutions will become either phase separate into two liquids or remain mixed



Smarter Simulations by Machine Learning



- Speedup attained in two different ways:
  - Choosing the calculations intelligently (**less calculations**)
  - Interpolating between the calculations performed in a sophisticated manner
- Gaussian process used for both tasks
  - Bayesian operation, so it **knows what it doesn't know**
- Maximum entropy sampling used to choose next calculations
  - Minimizes redundant information from calculations
- Non-parametric interpolation increases the resolution by 6 orders of magnitude

Getting HPC to “work smart, not hard”

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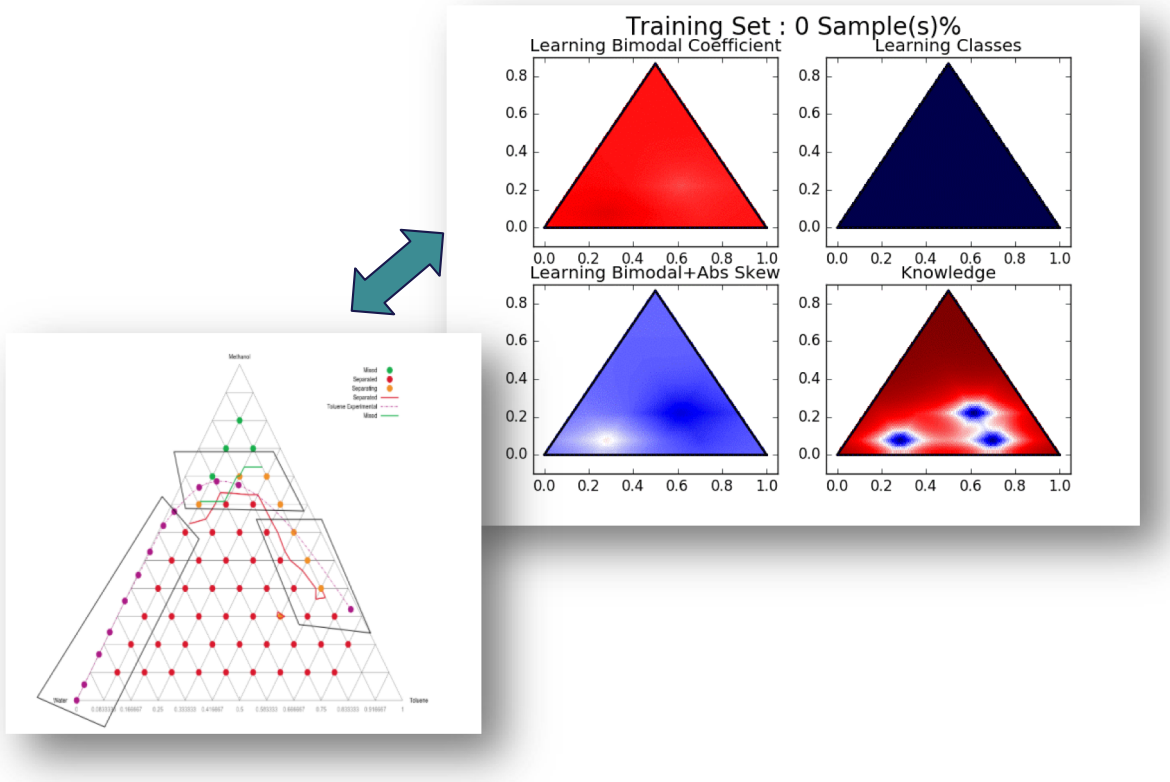
- Typically HPC development is focused on increased speed.
  - The fastest calculation is the one which you don’t run!
- We can use machine learning to make better decisions on **which simulations give the most value**
- We can use machine learning to **improve resolution of information**



Cognitive workflow uses 1/3 of the calculations to achieve 4 orders of magnitude resolution increase

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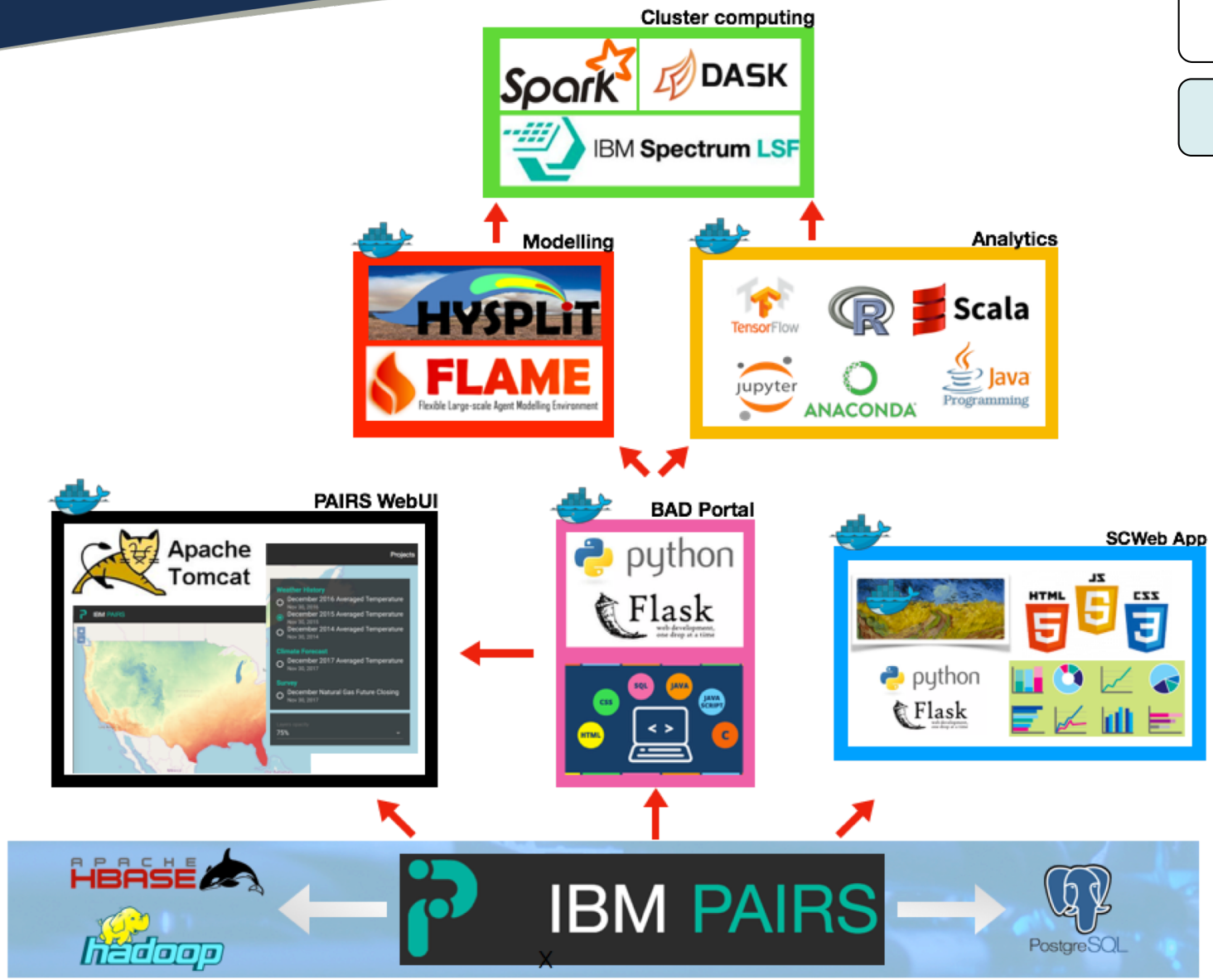
Smart Crop Protection using Big Agricultural Data

- Large quantities of geospatial data exist
  - Public (open data) / private
  - Static / dynamic
  - Raster / vector
- Can we store, access and query the data?
- Can we use the data for agriculture applications?
- PoC with Rothamsted Research
  - Moth migration

30% crop loss worldwide due to pests, pathogens and weeds!

ROTHAMSTED RESEARCH 175


Cluster computing
Spark
DASK
IBM Spectrum LSF
Modelling
HYSPLIT
FLAME
Flexible Large-scale Agent Modelling Environment
Analytics
TensorFlow
Scala
jupyter
ANACONDA
Java Programming
PAIRS WebUI
Apache Tomcat
BAD Portal
python
Flask
SCWeb App
HTML
python
Flask
APACHE HBASE
hadoop
IBM PAIRS
PostgreSQL

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IBM PAIRS geospatial database platform

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‘SCApp’ web app for farmers

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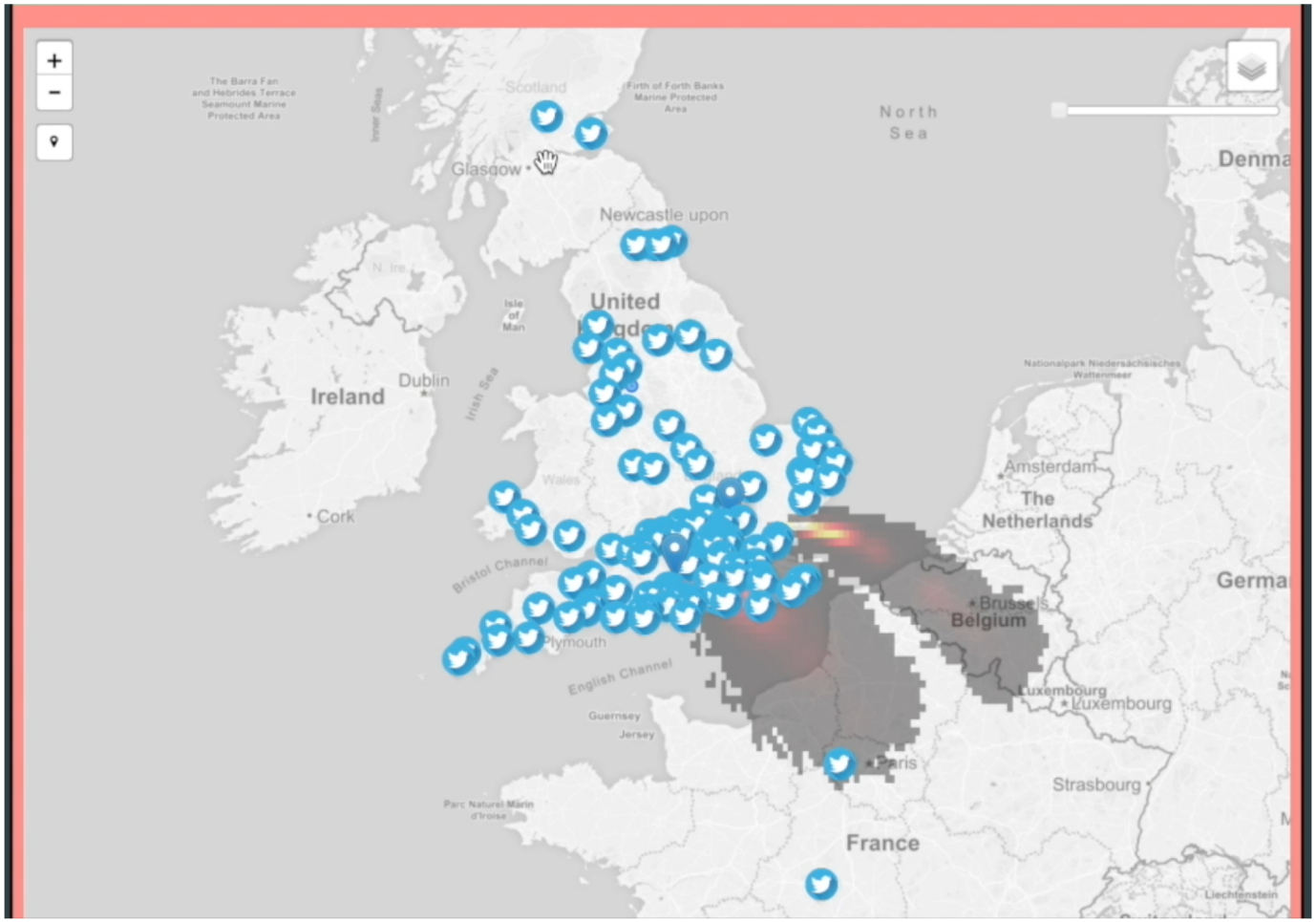
Agent-based modelling based on weather and Twitter-sourced sighting data



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Jupyter (+Spark) analytics portal

jupyter Demo_LandSatelliteNDVI Last Checkpoint: Last Tuesday at 1:14 PM (autosaved)

Logout

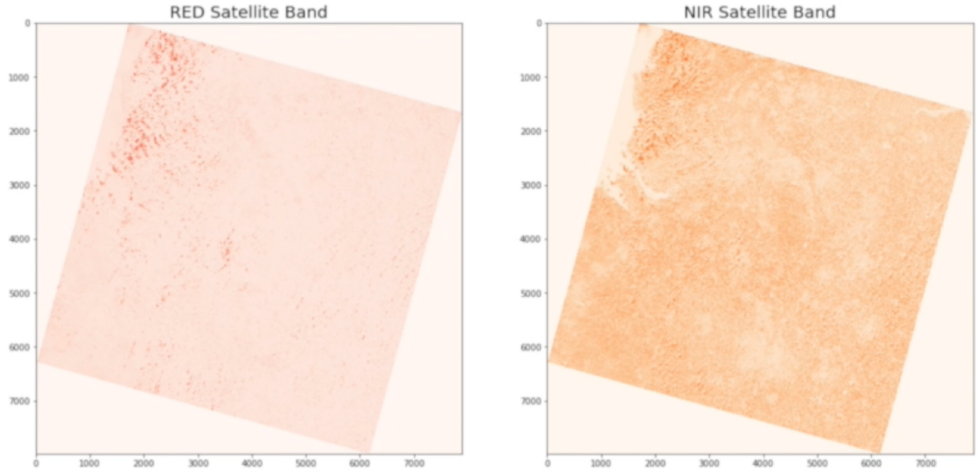
File Edit View Insert Cell Kernel Help Trusted Python 2

Code

1. NDVI Calculation from RED and NIR

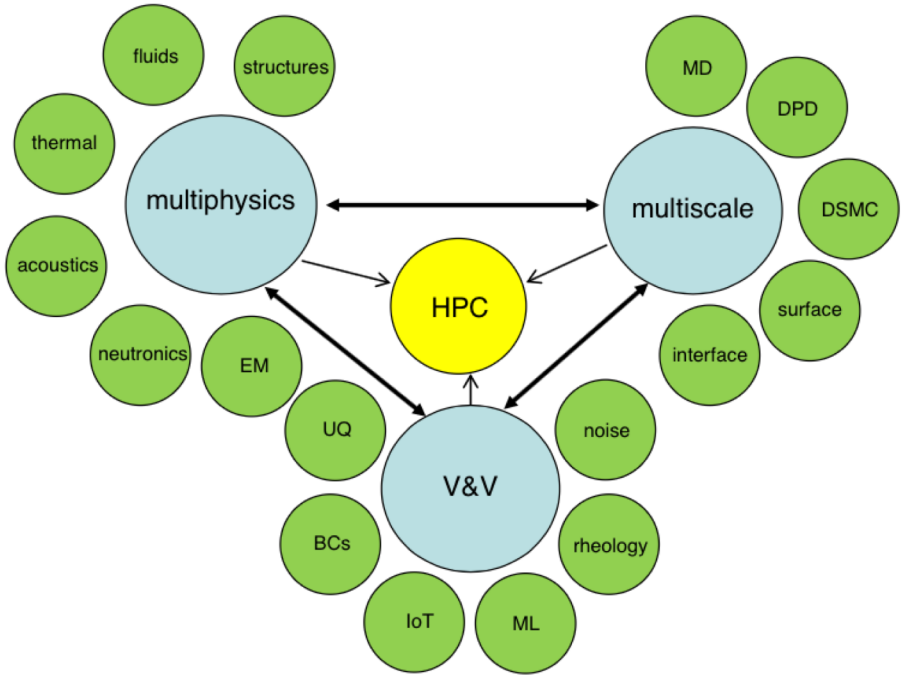
We first need to import the RED and NIR layer and convert the Geotiff into a numpy array. We can either import the data directly or get it from PAIRS instead.

In [8]:
```
#Read layers in from raw files:

def read_dat_layers(path,band):
    file_location = path+"LC08_L1TP_203023_20160504_20170325_01_T1_"+band+".TIF"
    ds = gdal.Open(file_location)
    return np.array(ds.GetRasterBand(1).ReadAsArray())

bandRed = read_dat_layers(path="ndvi/",band="B4")
bandNIR = read_dat_layers(path="ndvi/",band="B5")

#Explore what data looks like:
#print bandRed
plt.figure(figsize=(20,10))
plt.subplot(1, 2, 1)
plt.imshow(bandRed,cmap="Reds")
plt.title('RED Satellite Band',fontsize=20)
plt.subplot(1, 2, 2)
plt.imshow(bandNIR,cmap='Oranges')
plt.title('NIR Satellite Band',fontsize=20)
plt.show()
```



Virtual Product Design

- a.k.a. Digital Twinning
- Full product lifecycle
  - Design
  - Manufacture
  - Operation
  - Disposal

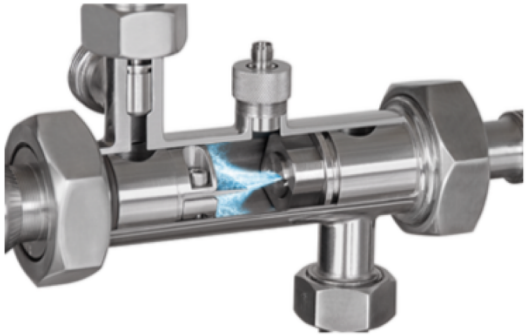


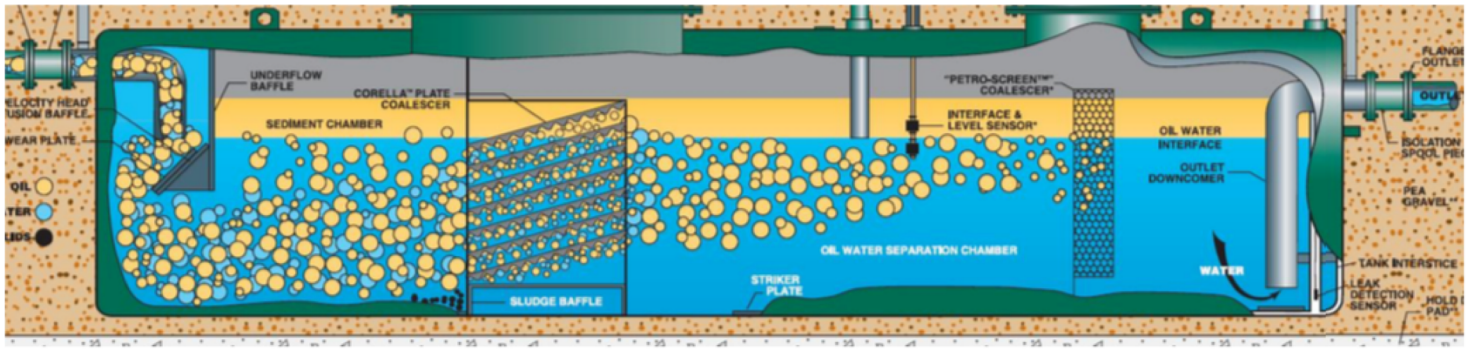
- Requires complex physics and understanding limitations

Mixing in industrial processes

Chemical engineering applications:

- oil and gas,
- food industry,
- personal-care products,
- paint and coating industry,
- effluent dispersion in wastewater.





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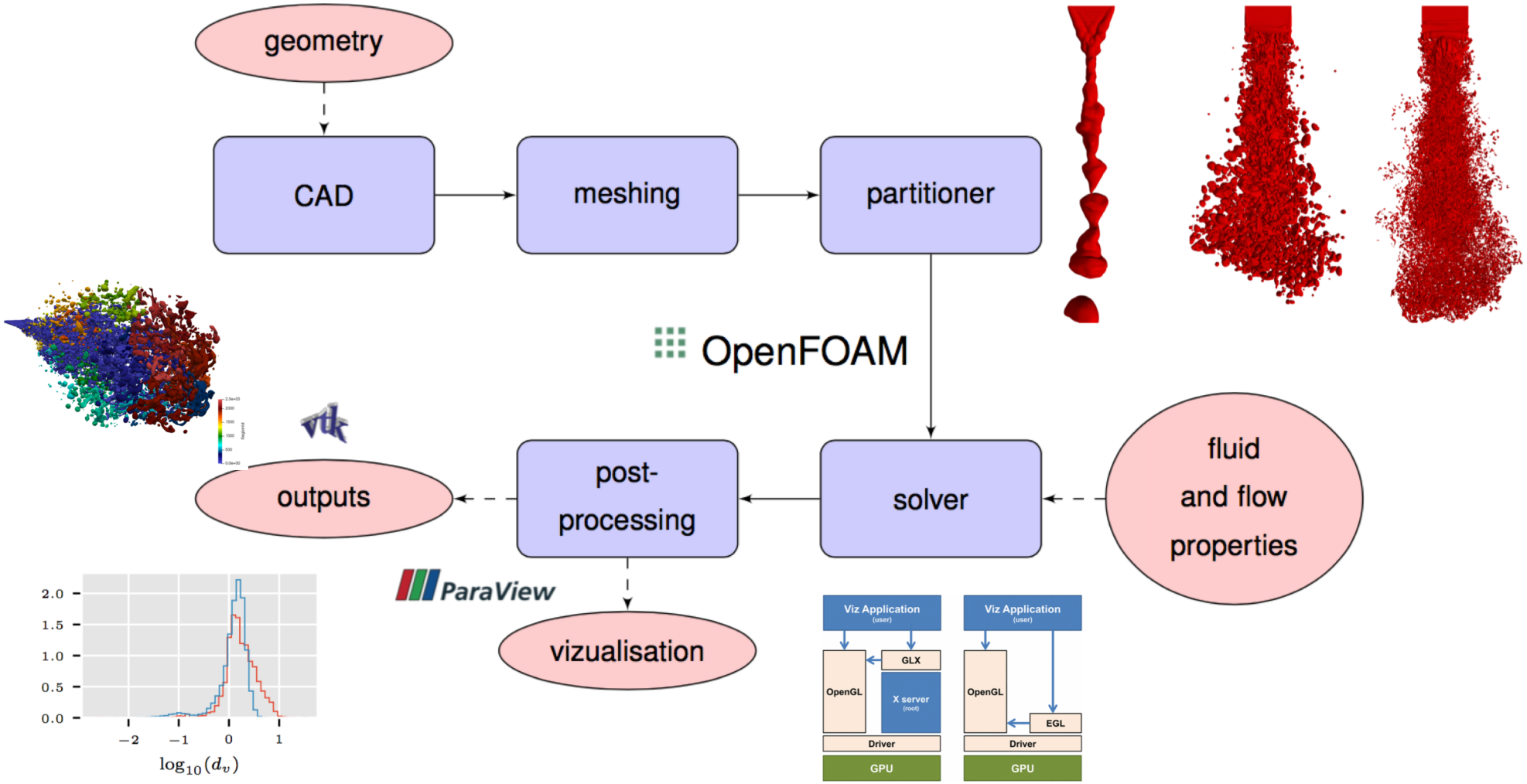
Classical HPC CFD workload



Thanks for listening!

Acknowledgments:
STFC & IBM Research Staff