CompBioMed
A Centre of Excellence in Computational Biomedicine

e-Seminar #30

nUCLeus: Creating and Running a Successful Adaptable, Portable HPC Education Environment

Presenter:
Cristin Merritt
(Alces Flight)

22 March 2023

The e-Seminar will start at 2pm CET / 1pm GMT

Moderator:
Tim Weaving
(University College London)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823712

INSILICO WORLD

https://insilicoworld.slack.com/archives/C0151M02TA4

The e-Seminar series is run in collaboration with:

VPH Institute
Building the Virtual Physiological Human

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Welcome!

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nUCLeus:

Creating and Running a Successful Adaptable, Portable HPC Education Environment

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Hello!

Cristin Merritt

Chief Marketing Officer (CMO)

cristin.merritt@alces-flight.com

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Team nUCLeus

Andrea Townsend-Nicholson
David Gregory
Art Hoti
Marcellus Augustine

UCL

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Cristin Merritt
Stu Franks

Andrew Narracott
Guillaume Hautbergue

The University Of Sheffield.

The glue that holds HPC together.

Alces Flight builds, manages and grows cloud-native solutions in High Performance Computing.

1.
March, 2020

It was the worst of times,
it was the worst of times.

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HPC Education Needed!

CompBioMed had secured HPC education for medical students but…

How do we educate?

The students were now distributed and working virtually.

Virtual learning was untested at scale

High uncertainty around if, or how things would work.

Resources were nebulous

How would students get access to HPC resources?

To the cloud!

UCL, Alces Flight + Sheffield decide to go in for a long term, portable solution.

2.

June - Sept, 2020

Building a minimum viable cluster environment

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HPC in Three (Semi-Easy) Steps

How to approach a portable HPC project.

Collate and Clean

Everything known or used on prior projects around QIIME + QIIME2 was brought into a single location and cleaned up.

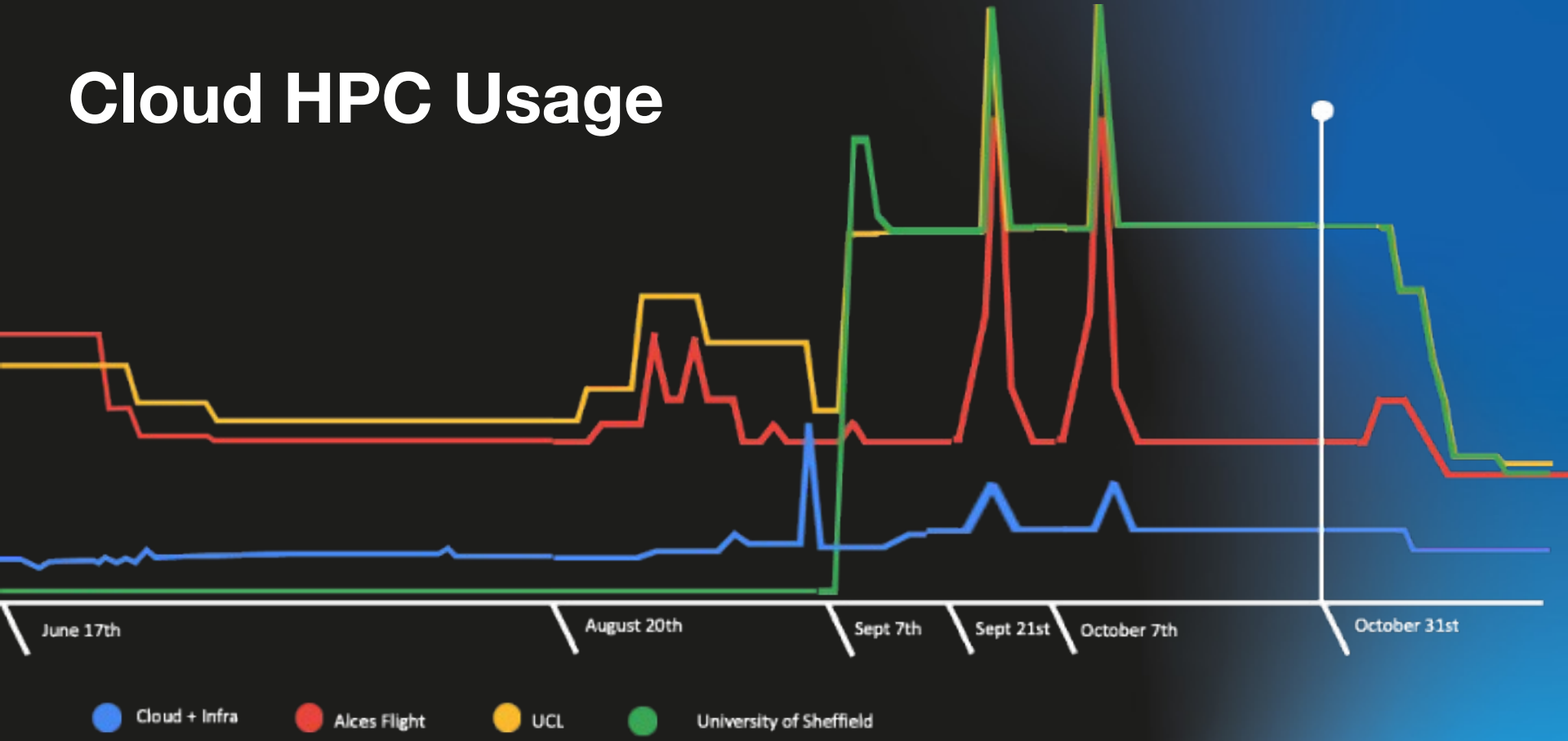
Build a Minimum Viable Cluster (MVC)

What are the fastest, cheapest resources needed to run this course?

Teach a Cohort

Go through a cohort with rigorous review process overlaid on top.

Cloud HPC Usage



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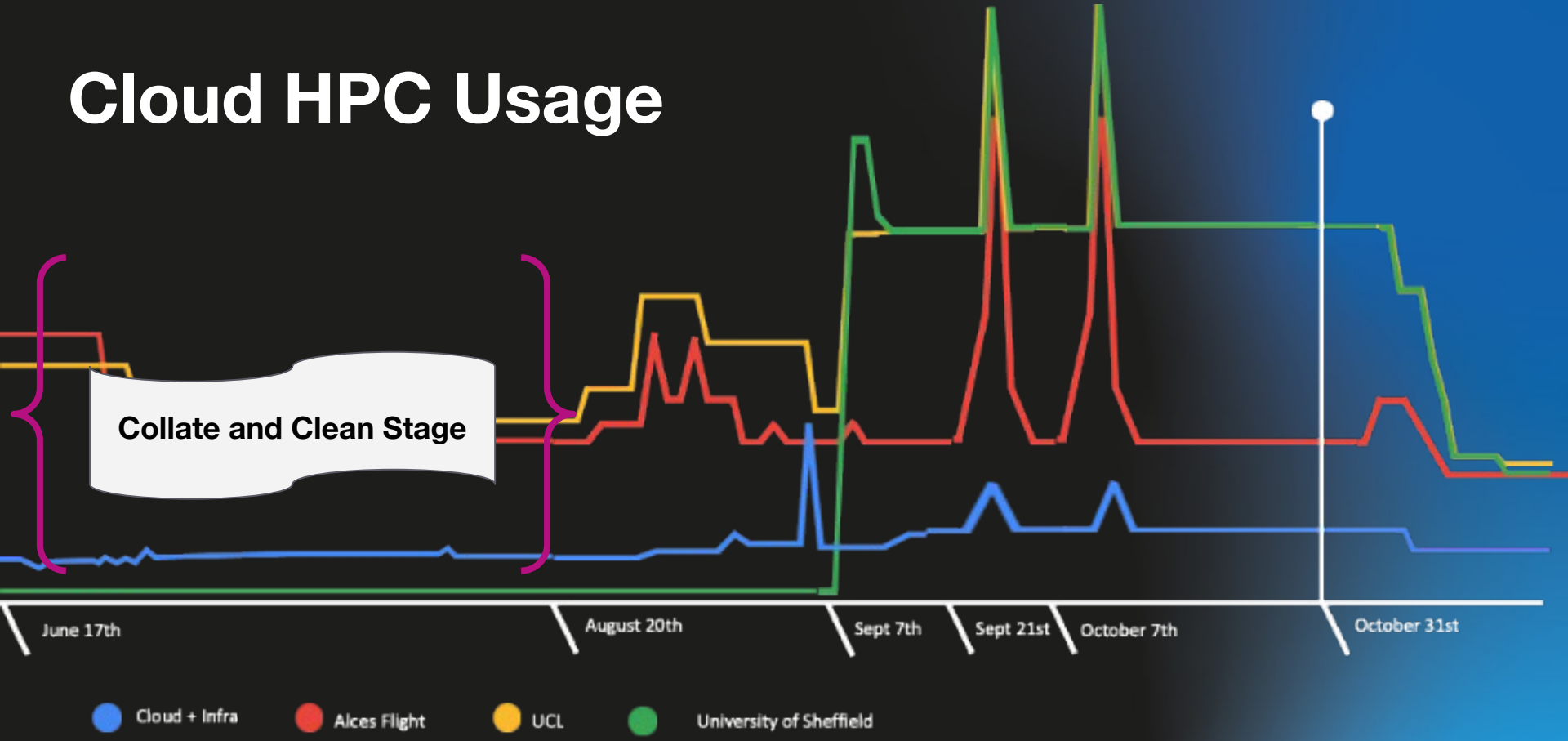

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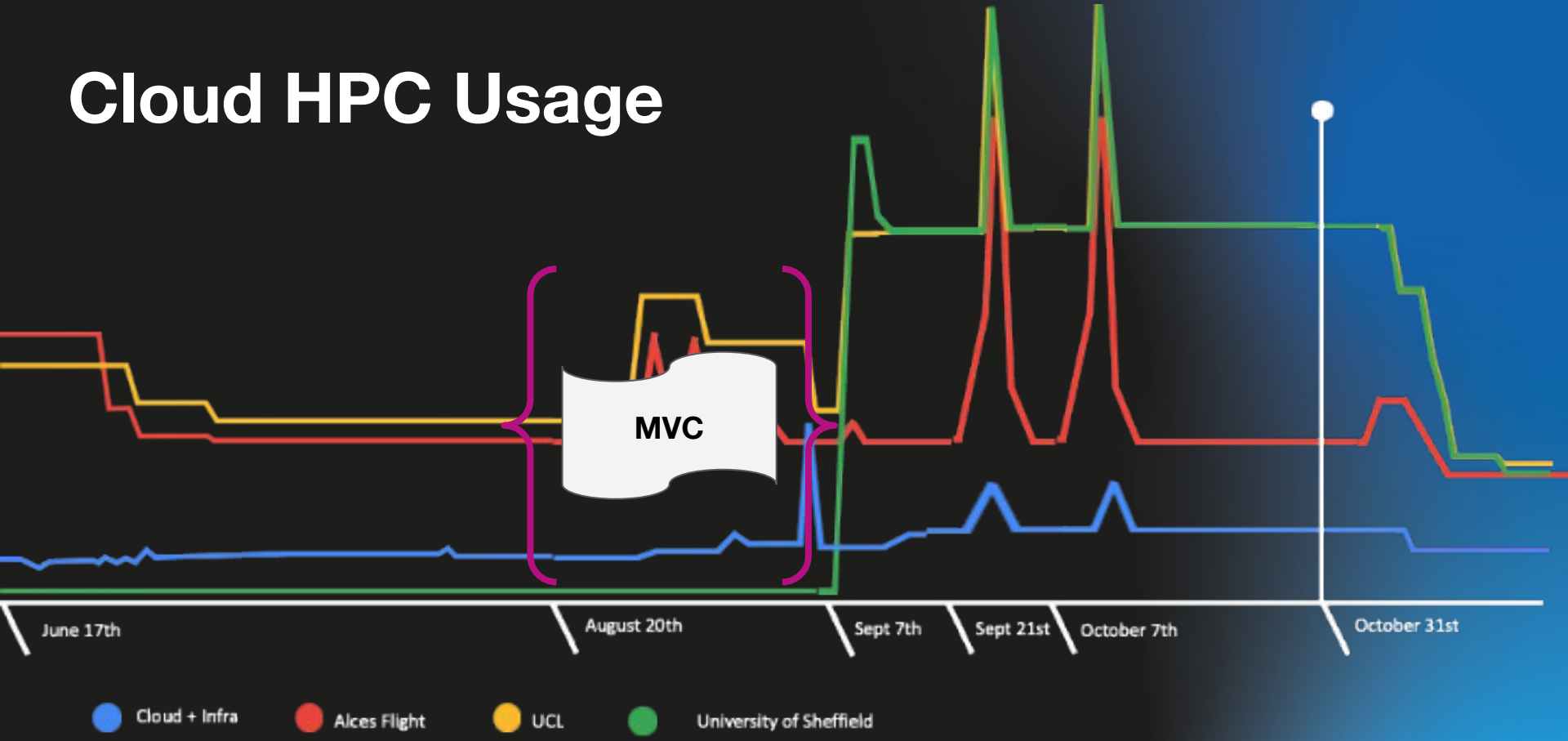

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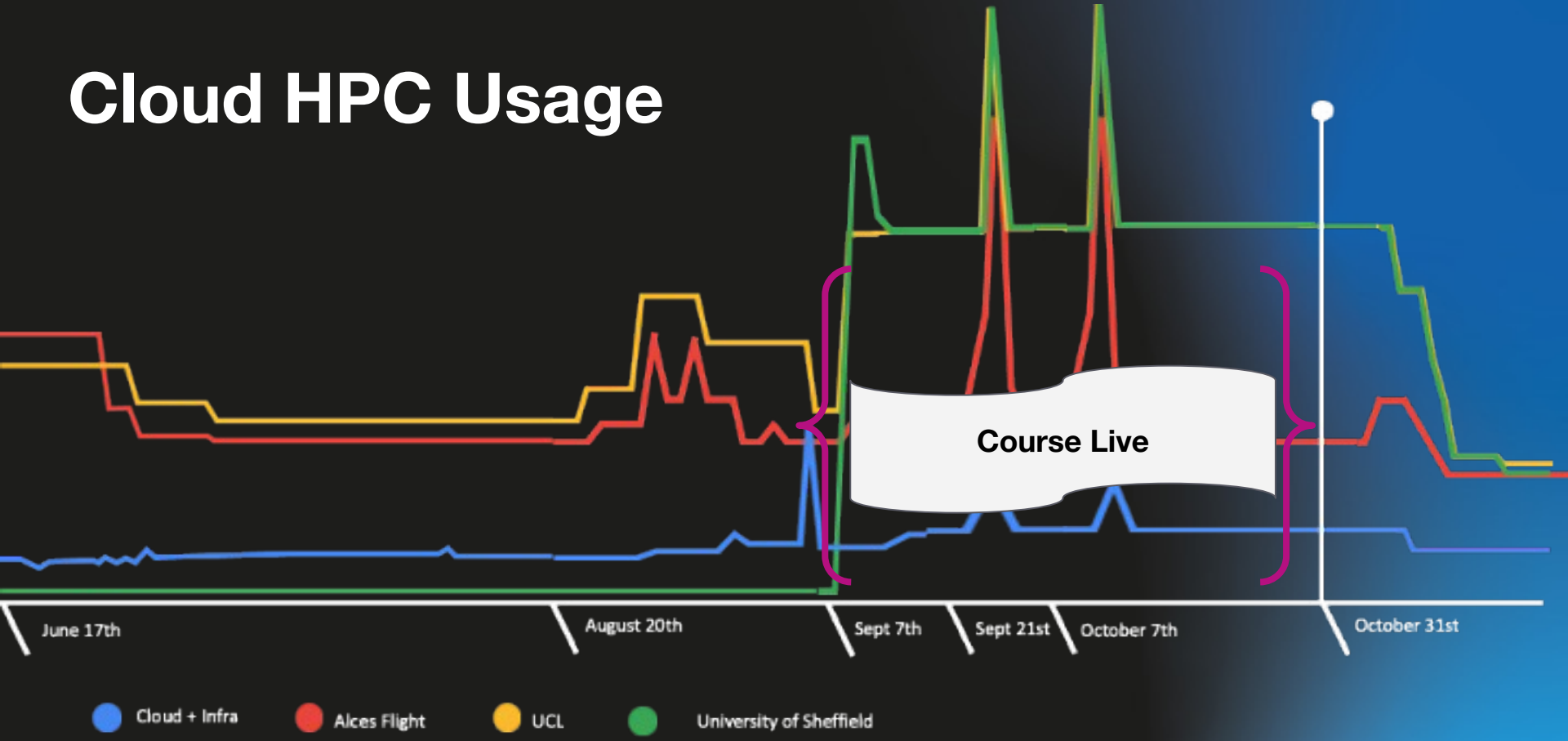

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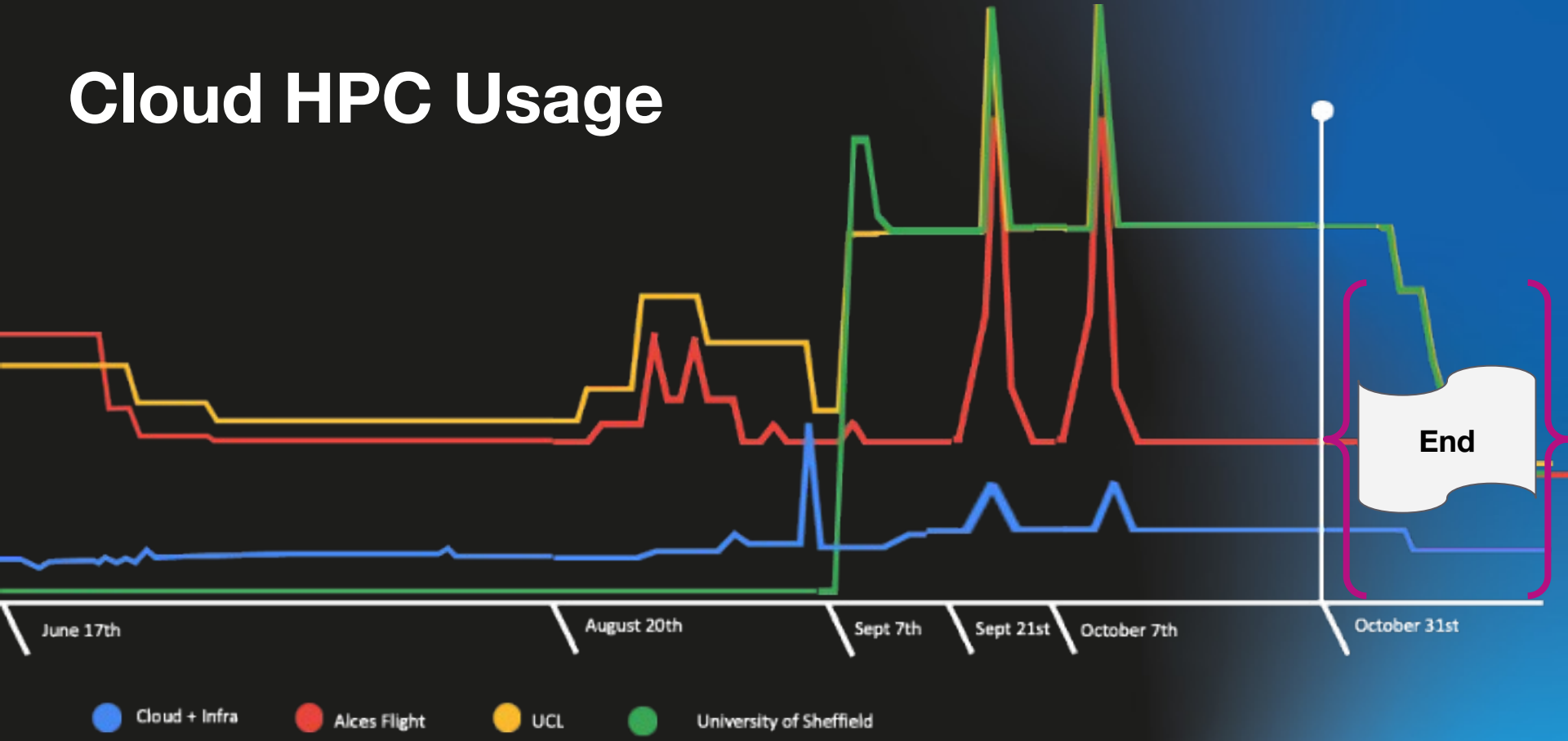

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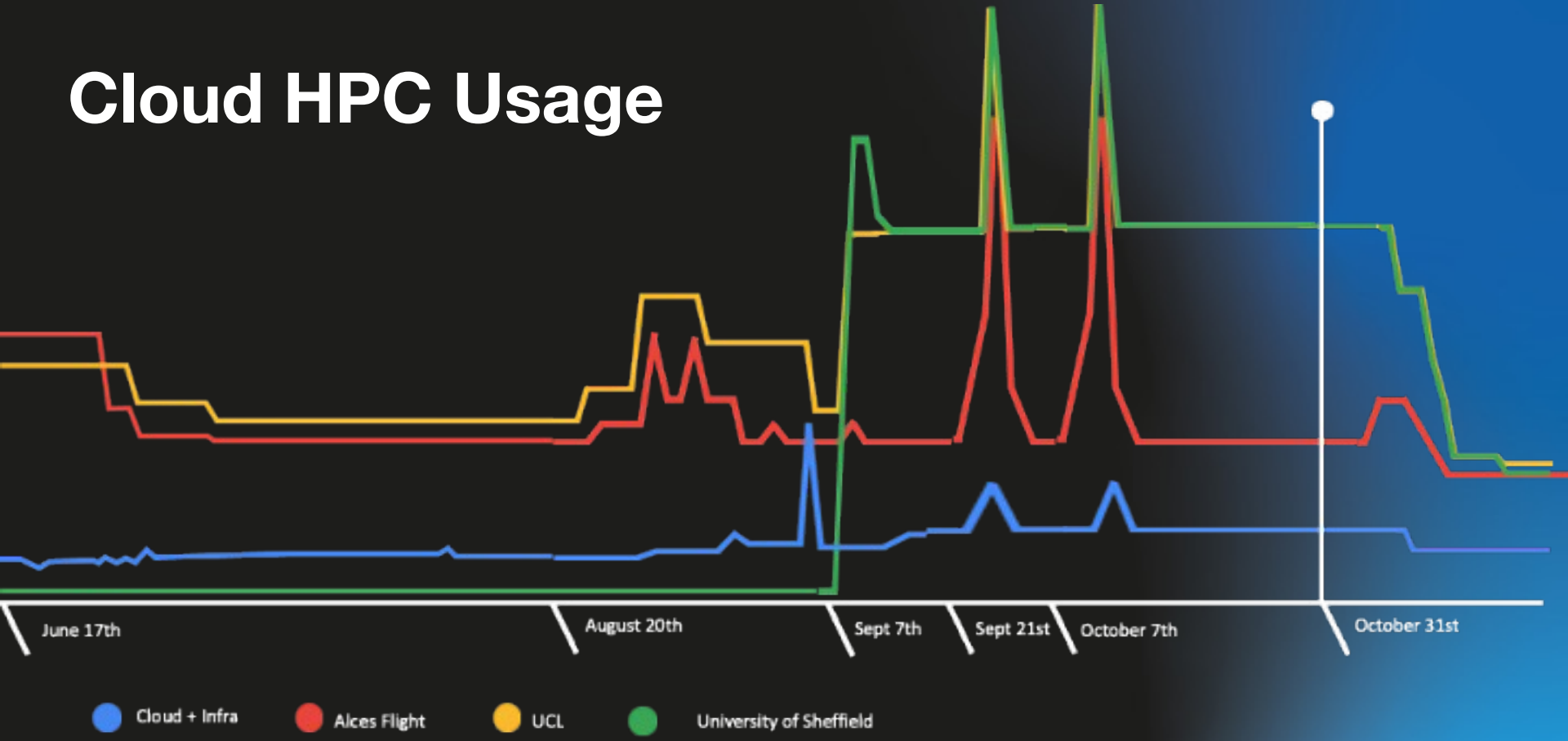

> “We all had our roles and responsibilities. Had we not gone in with clear intentions this would not have worked.
>
> - Andrea Townsend-Nicholson

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3.

October, 2020 - Today

Taking HPC to Medical School.

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After the initial investment:

- Ran a second, “hands-off” cohort.
- Cohort proved successful! Environment was good to travel.
- Class runs approximately 2x per year, 30 students/course.
- Has lived on public cloud (AWS, Azure) and on-premises.

4.

Build + Benefit from our Experience!

Portable HPC is possible - here's what you need to do.

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DO:

- Start with a single application
- Get everything into one place
- Establish your team and job roles early

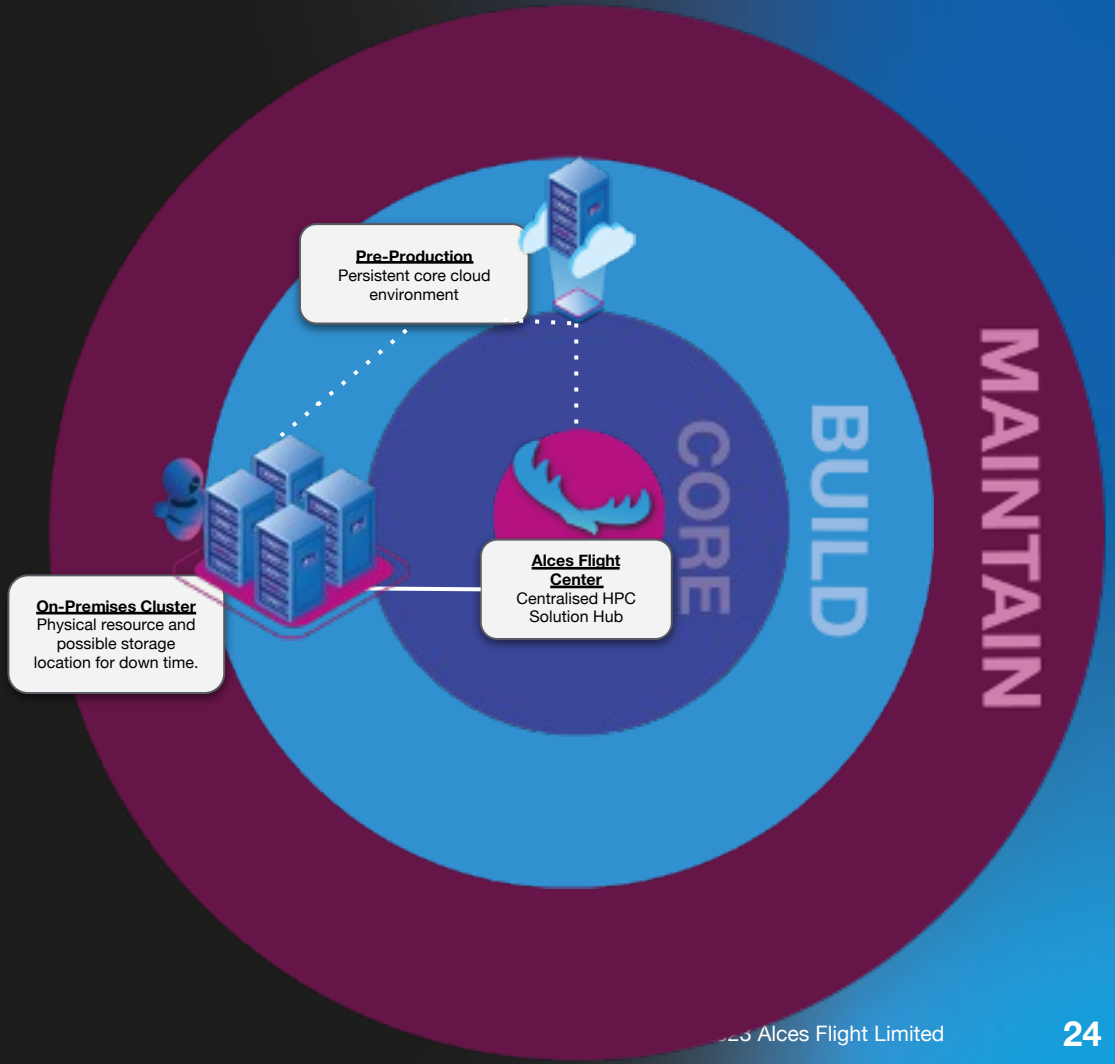
If people know what their job is and when to accomplish it then you're 75% of the way there.

Consider Investment

What time and costs do you want to put in to making an HPC project portable?

Base Solution

How we built the nUCLeus environment.



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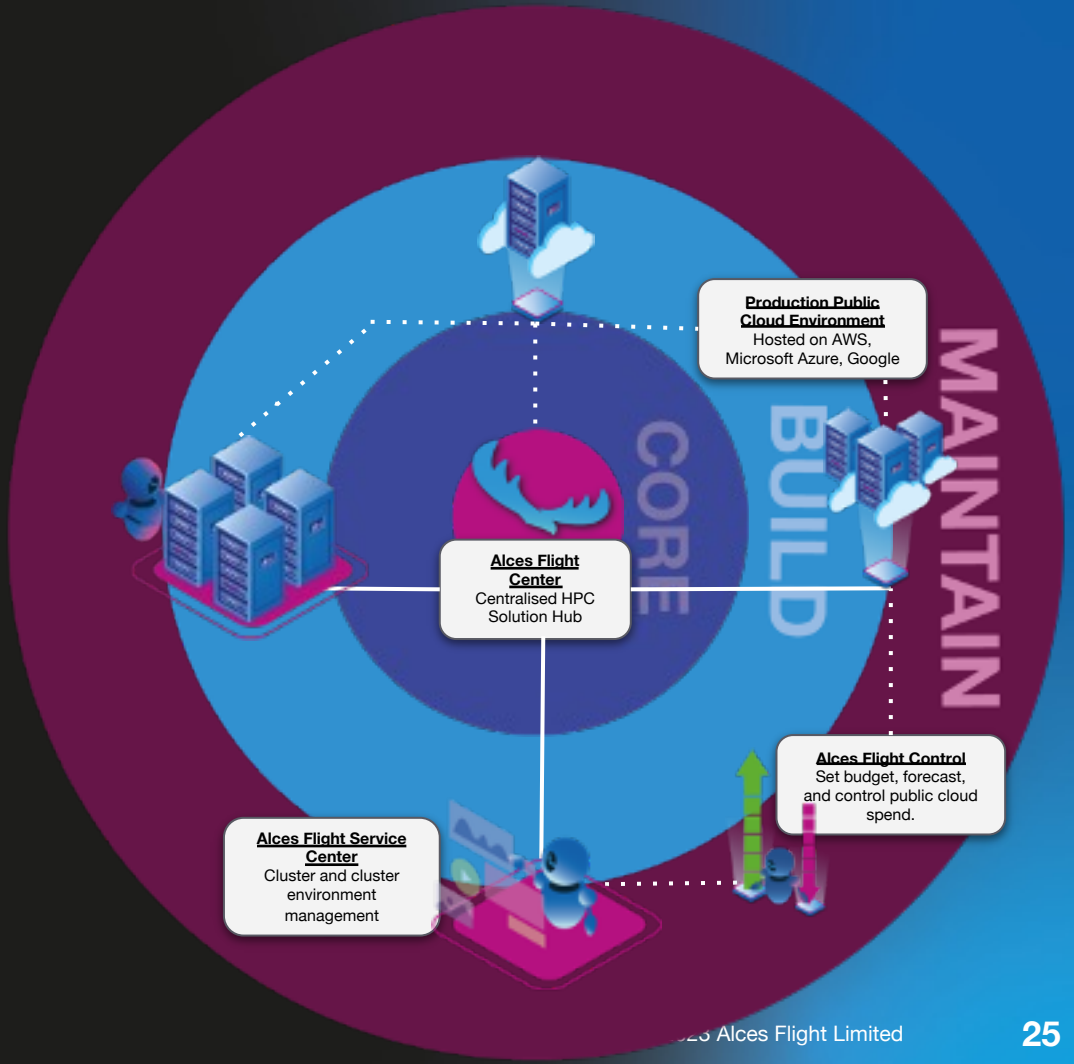
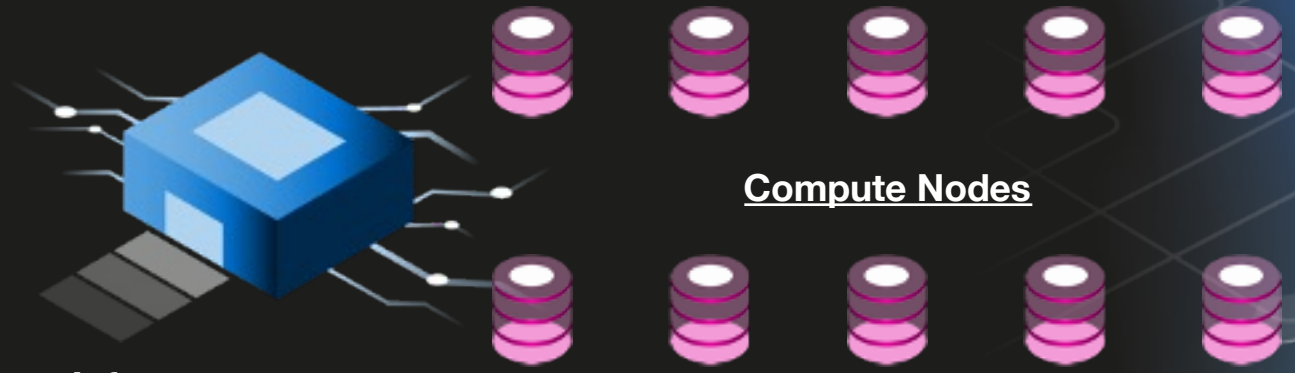


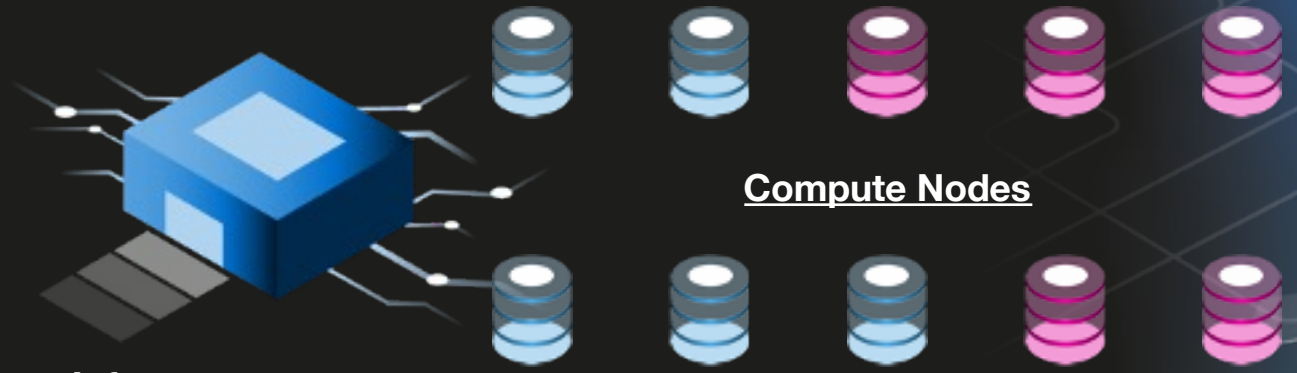
nUCLeus Environment:



Core Infrastructure

- Gateway
- Head Node
- Admin

nUCLeus Environment:



Core Infrastructure

- Gateway
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Making HPC Portable:

- Alces methodology is platform agnostic
- Team worked to containerise the workload

After two cohorts, the workload was free and ready to live for another 2-3 years.

Investment Options

Three potential ways to approach your project.

Investment Options: Time + Money Poor

- Pursue public cloud grant monies
- Utilise OpenFlightHPC for environment build
- Consider RSE team in your institution or pursue potential graduate projects.

OpenFlightHPC

All tools used to build the environment are open-source!

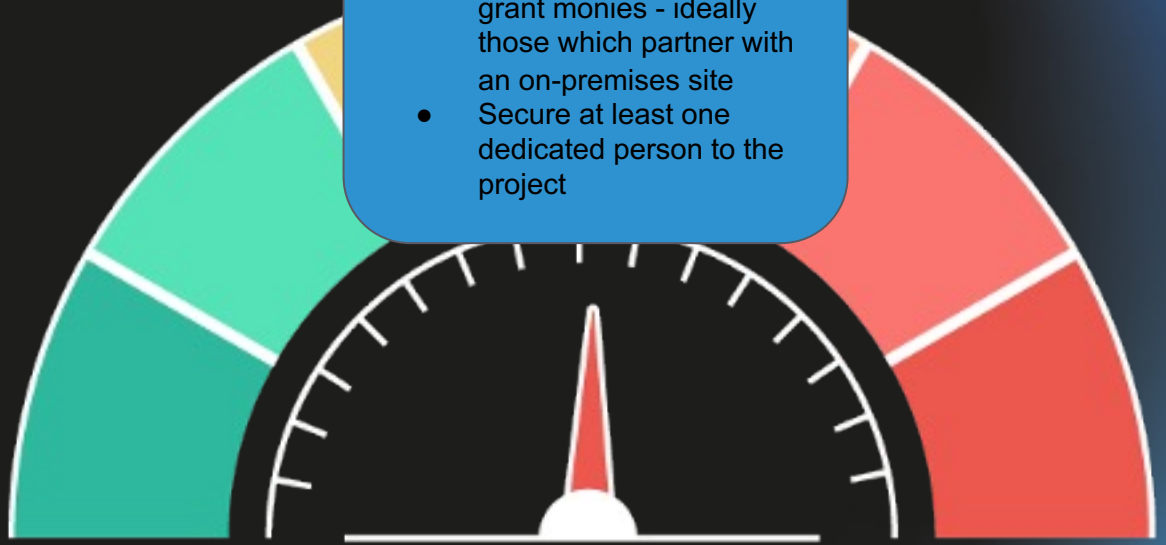
https://www.openflighthpc.org/

Alces Flight Solo

- Personal research environment for HPC.
- Pre-Packaged content and toolsets included.
- Fully configurable.
- Can be made part of Alces' managed service offering or kept as-is.

Investment Options: Some Time + Money

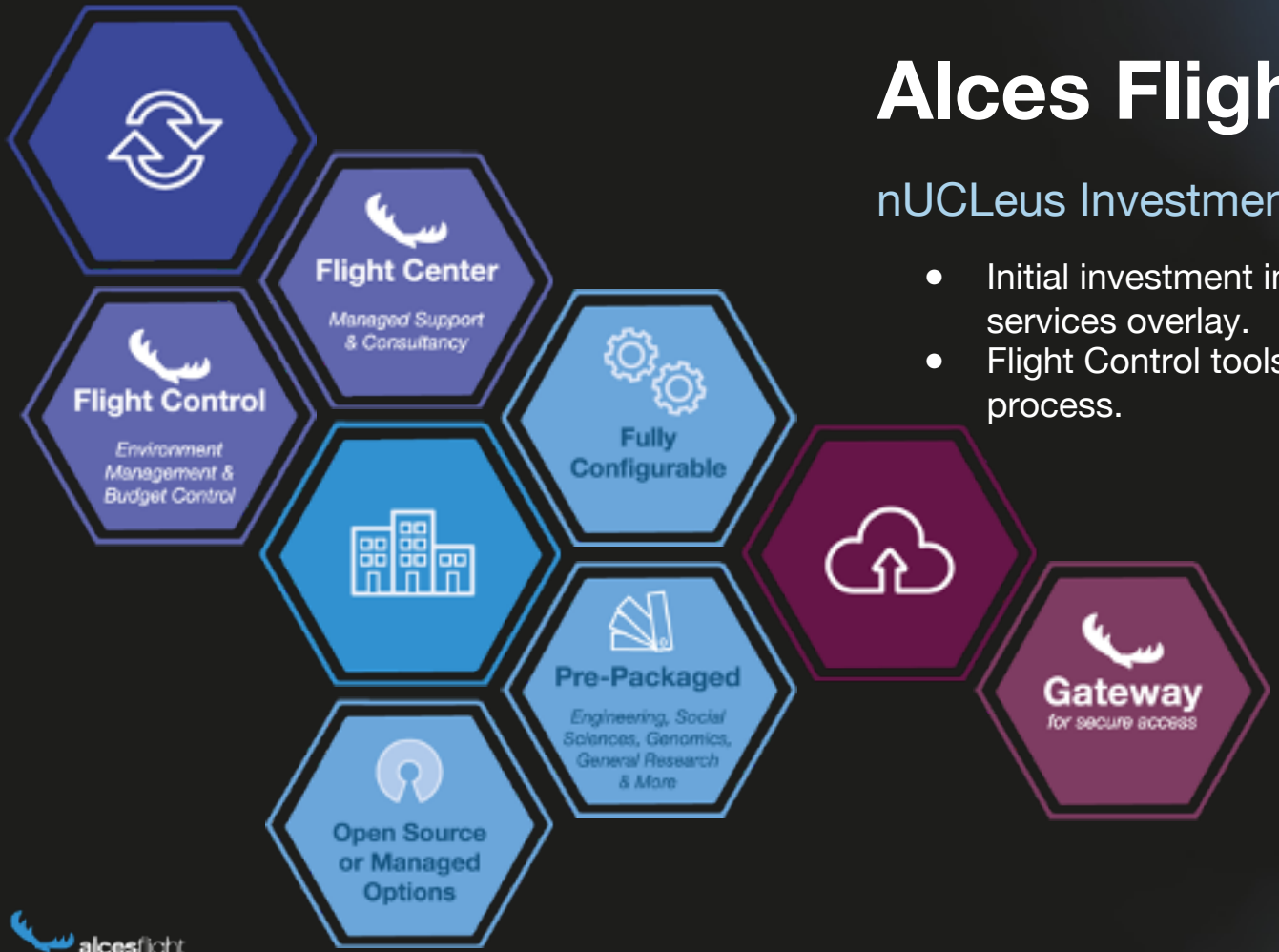
- Consider Alces Flight project build
- Pursue public cloud grant monies - ideally those which partner with an on-premises site
- Secure at least one dedicated person to the project



Alces Flight Products

nUCLeus Investment - Year One

- Initial investment included managed services overlay.
- Flight Control toolset built during process.



Alces Flight Products

nUCLeus Investment - Year Two

- Utilised Alces Flight Open Source
- Kept connections in place in case new or bigger project comes along.

Approximate Costs

	Year One	Year Two	Year Three
Alces Flight Managed Service	£5,000	£2,000	£0
Cloud Cost	£2,000	£2,000	£0
	£7,000	**£4,000**	**£0**

Notes:

- nUCLeus environment agreement included grants from both Alces and AWS/Azure.
- List price investment closer to £15,000 - 20,000, decreasing to £10,000 - 15,000 in second year. Assumption of 12-month subscription.

Additional Value

- Environment creation expertise.
- Help with optimisation / containerisation.
- Controlled forecasting and testing.

Investment Options: Time + Money Rich

- Consider Alces Flight project build
- Look at public cloud as well as environmental datacenter sandboxes (cloud-native and green)
- Place two dedicate persons on the team

Portable AND Green

- Green HPC conversation is now happening more often than not.
- Green HPC will likely be just as important, if not more, than making your workload portable.
- Consider optimisation of workload and cloud/on-premises green credentials.

DON'T:

- Try to do it all yourself
- Think short term
- Make your solution bespoke

Investment in portability is time consuming up front, but costs can drop significantly if you commit to following best practice.

RESOURCES:

- nUCLeus for HPC Education
- nUCLeus Success Story
- Complete Project Video

Available Soon in CompBioMed e-Seminar #30

Thanks!

Cristin Merritt

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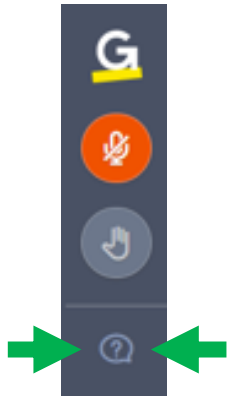
Questions

Thank you for your time.

Q&A

To pose a question, please click on the symbol and send your question via the 'Ask the staff a question' panel



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Thank you for participating!

…don't forget to fill in our feedback questionnaire…

Visit the CompBioMed website (www.compbiomed.eu/training)
for a full recording of this and other e-Seminars,
to download the slides
and to keep updated on our upcoming trainings

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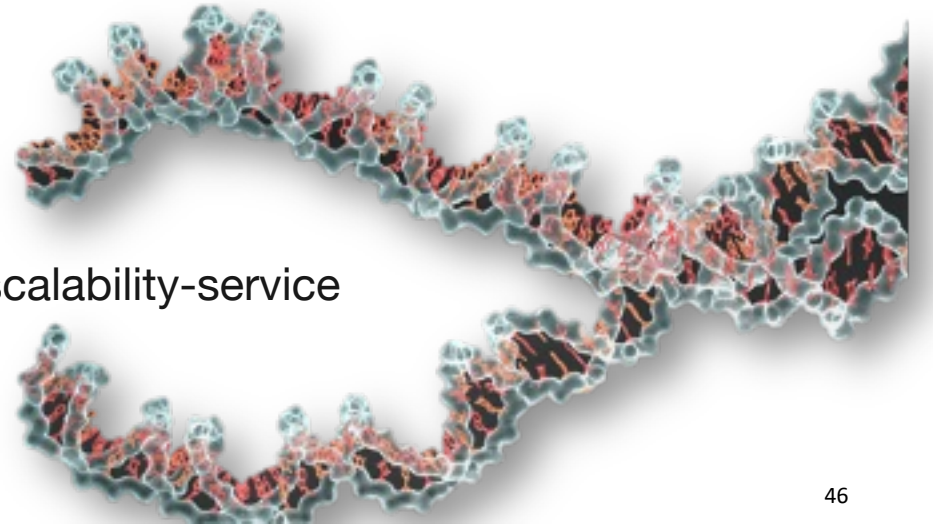
CompBioMed's *Free* Scalability Service

- Improves performance of your biomedicine applications on high performance computers
  - Experts in both biomedical applications and high performance computers
  - Make your biomedicine applications run in parallel
  - Improving the scalability of those already parallelised



- www.compbiomed.eu/compbiomed-scalability-service

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  - General technical questions
    - Slack: #scalability channel of ***the InSilicoWorld Community of Practice***
    - Email: compbiomed-support@ucl.ac.uk
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      - Formal collaborative relationship with CompBioMed Centre of Excellence

- Application and Data Security
  - Great care when adapting your applications and managing your data
    - Our Data Policies cover Data Privacy, Data Security and Research

InSilicoWorld Community of Practice

The first community entirely on *in silico* medicine on Slack

www.insilico.world/community

Expertise	• The community is invitation only: in this way we ensure only interested experts have access
Collaboration	• Join teams and collaboratively work on shared goals, projects, concerns, problems or topics
Safe space	• A pre-competitive space where experts from academia, industry, and regulatory agencies can ask for and exchange advices

More than 500 experts have already joined the community and its channels

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