Onboarding Users to A64FX via Open OnDemand

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A Brief Glimpse of Research Computing at GT…

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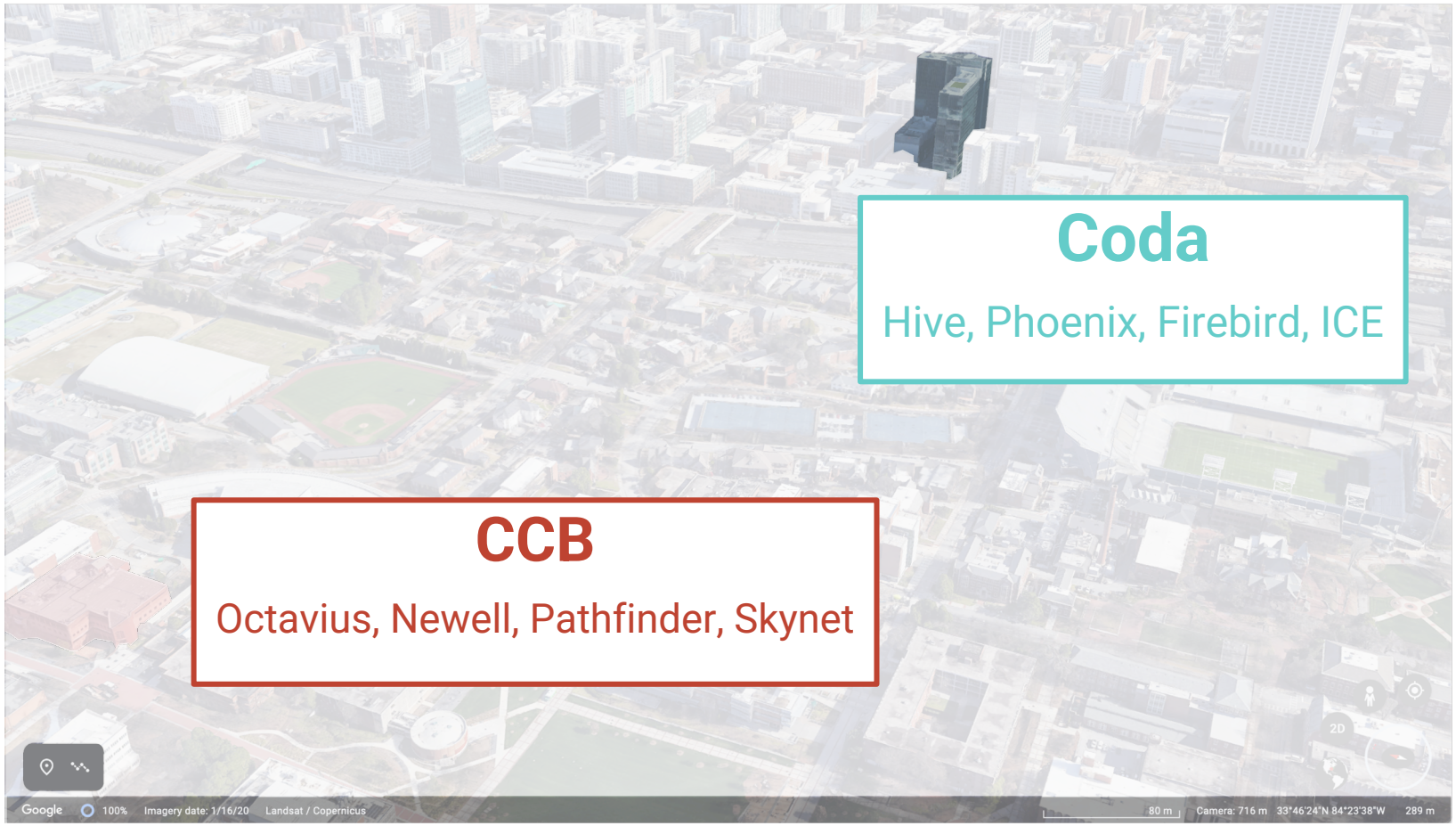
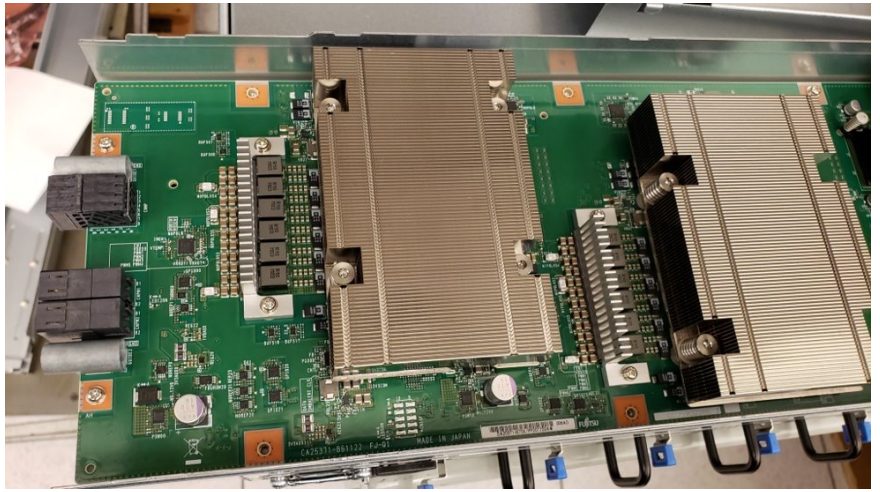
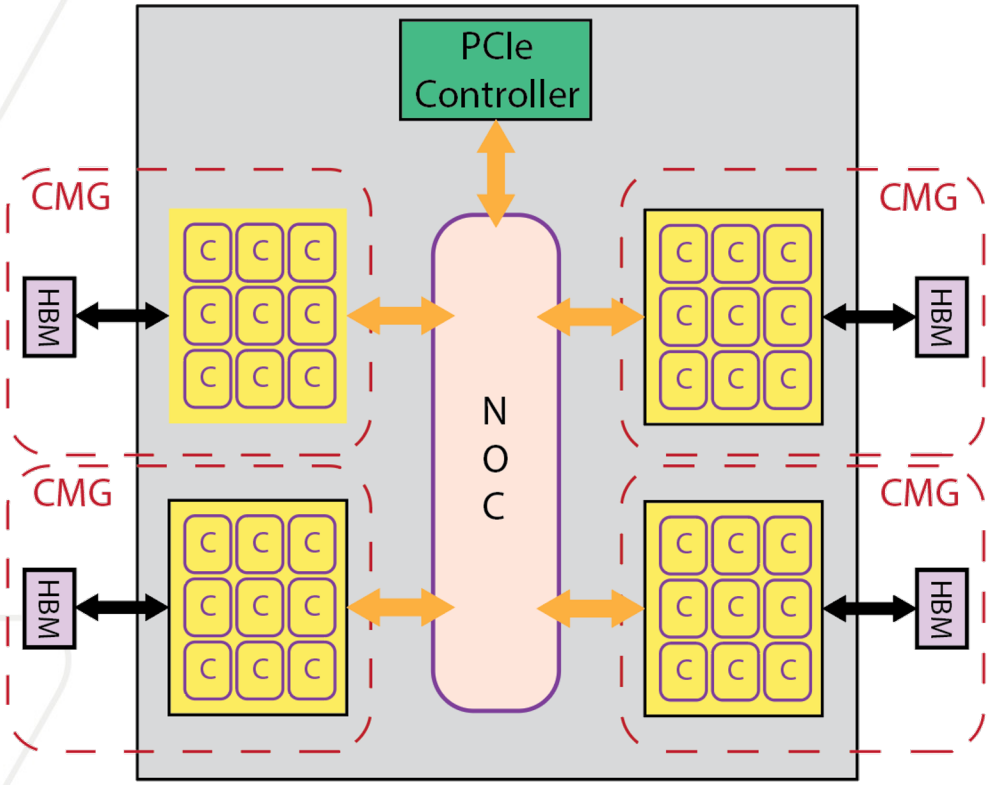


Octavius: Hive's Rogue Little Brother

- Octavius is supported by the National Science Foundation
  - 16 A64FX nodes are part of NSF MRI award #1828187 to allow exploration of Arm+SVE as an alternative to AVX512
  - Hosted within the Center for Research into Novel Computing Hierarchies (CRNCH) Rogues Gallery testbed, funded by NSR award #2016701
- Timeframe and architecture mirror Stonybrook's Ookami (but at a smaller scale)
  - Deployed in Fall 2020
  - 2x HPE Apollo80 chassis, each with 8 nodes



Octavius: NUMA (and Name)



- >2.7 TFLOPS
- Supports Scalable Vector Extension (SVE)
  - Enables Vector Length Agnostic (VLA) programming, which contributes to portability, scalability, and optimization
- 4 Core Memory Groups (CMGs)
  - 12 cores
  - 64KB L1$ per core
    - 256b cache line
  - 8MB L2 shared between all cores
    - 256b cache line
  - 0 L3$
  - 8GB HBM at 256GB/s

http://www.jicfus.jp/jp/wp-content/uploads/2018/11/msato-190109.pdf

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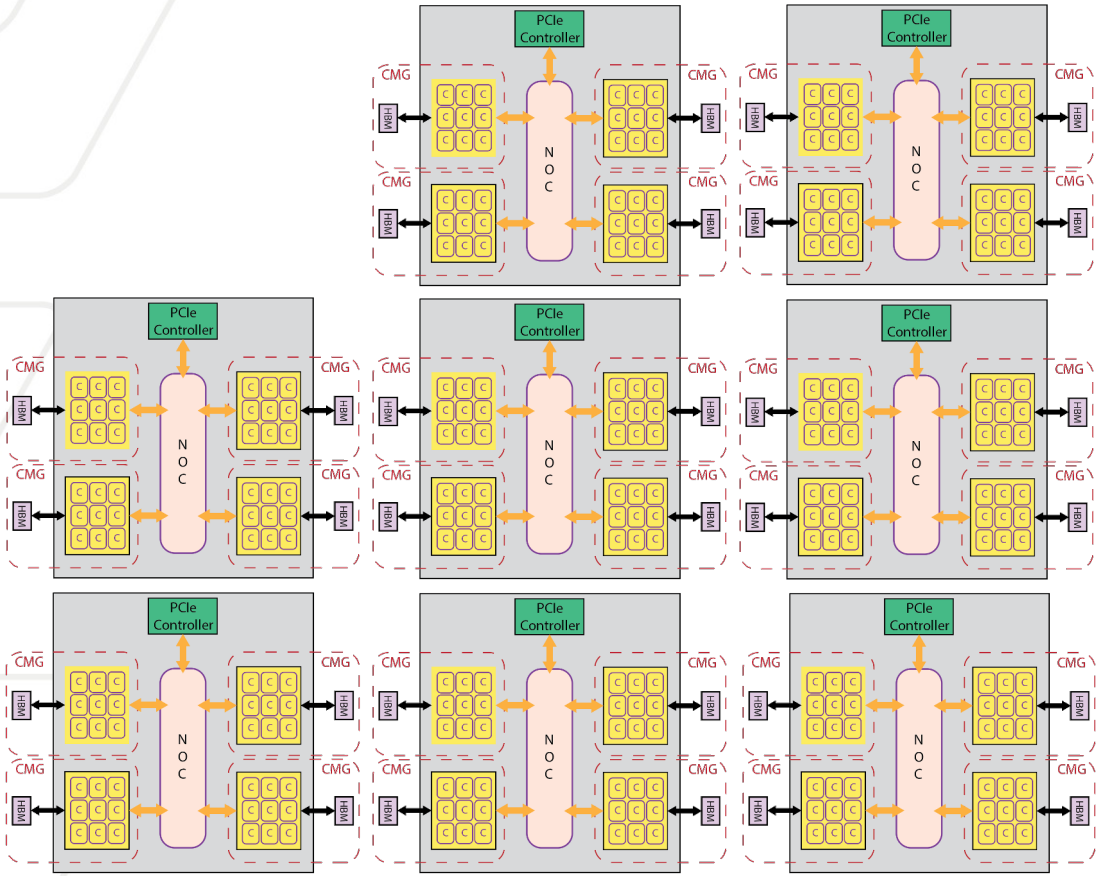

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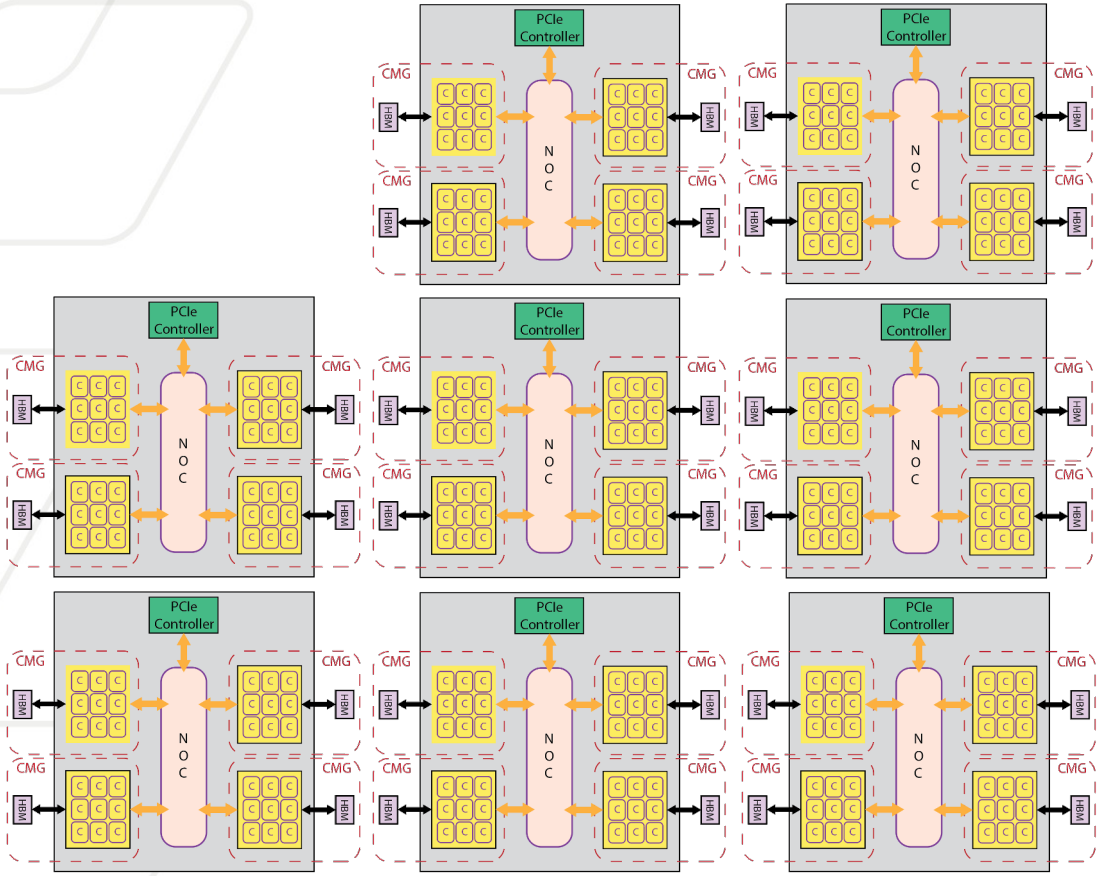

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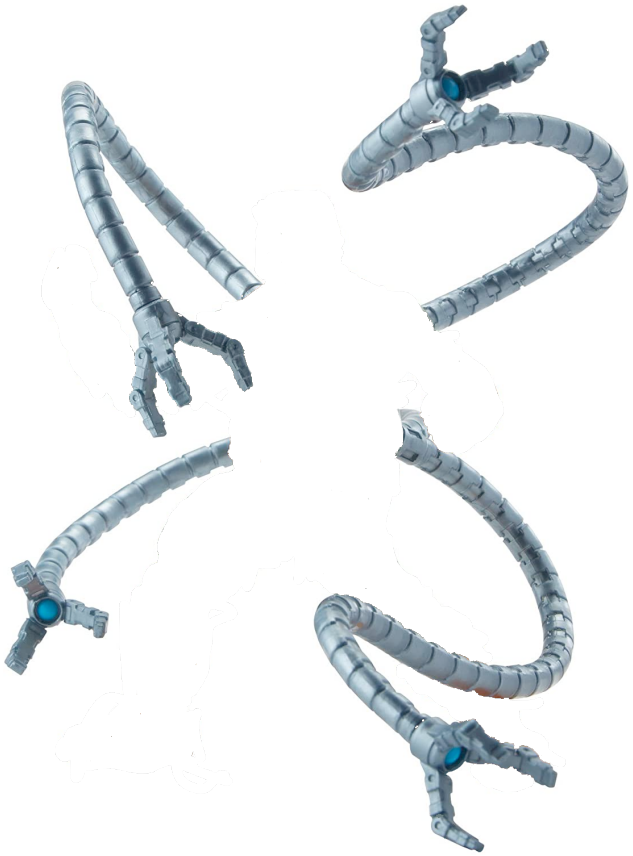

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Octavius: Environment and Software

- x86 VM login node
- Slurm 21.08 manages Octavius access (and other RG compute)
  - Debug queue to test/compile code before running at scale
- Cray, Arm, and Gnu compiler/library modules
  - Expect insights to also be applicable to larger clusters like Ookami
- Shared home and NVMe-backed scratch storage

The Hurdles of New Technologies and Users

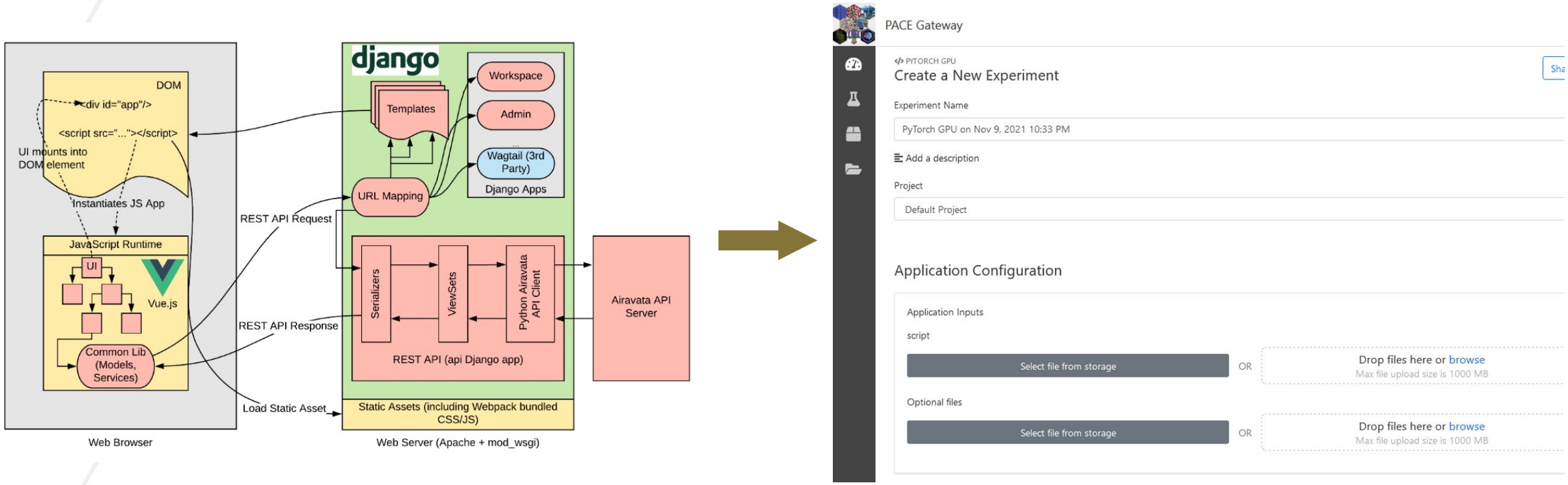
- As exciting as algorithm exploration and software porting might be for veteran users…
  - The “tried-and-true” tools often take several cycles to adapt
    - This happens with updates to traditional architectures too
    - Vendors contribute heavily to upstream, but it can still take time to trickle down
  - Vendor-provided tools are great to use!
    - …but even as a port of something familiar, there’s still a learning curve
    - And these tools may be proprietary!
- Meanwhile, new users are constantly inbound
  - Remote command line access can be intimidating (and feel prohibitive)
  - Even for experienced users, interactive server workflows can be problematic

These Aren't New Issues! But...

- Knowledge transfer can be a difficult process
  - Documentation relies on the "Goldilocks principle"...on a user-by-user basis.
  - Trainings are great but might not be convenient for the users.
  - Command-line self-service tutorials may not include the instructive element available in other forms.
- Many solutions are less than elegant
  - Performance problems (X11 forwarding)
  - Scalability issues (FastX licensing, X2Go resource needs)
  - Less-than intuitive interfaces (SSH tunneling)
  - Client application requirements (e.g. VNC)
  - Local security rules can be an impediment (Port blocking)

Gateways Expand the Impact of Clusters…

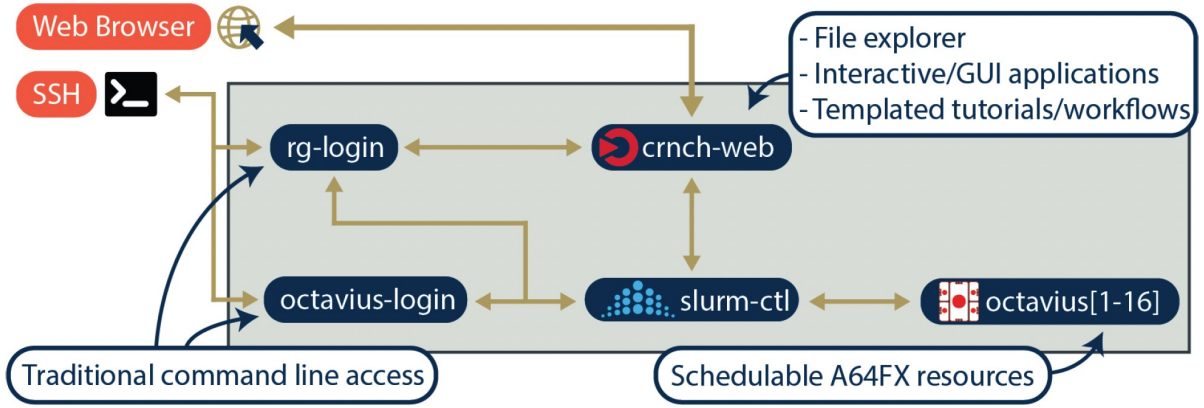
For example, Software as a Service via Django + Apache Airavata:



https://dl.acm.org/doi/pdf/10.1145/3311790.3396650

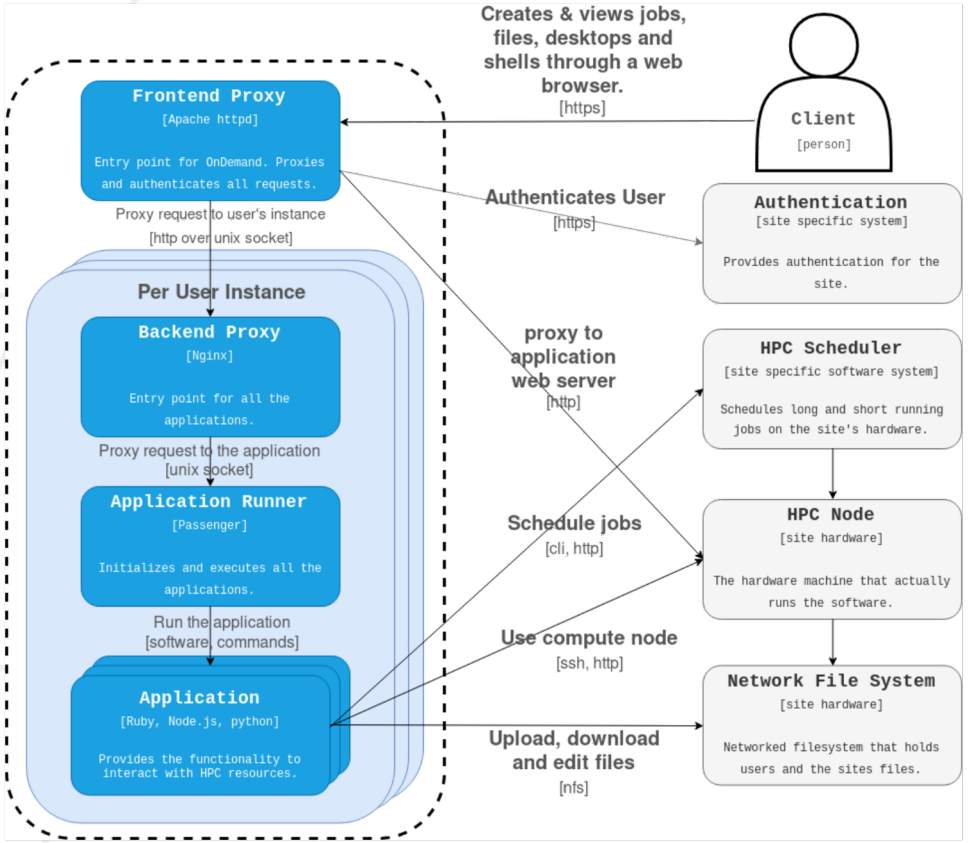
…But Emerging Technologies Demand Flexibility

- Before software can be available as a service, the software needs to exist
  - Optimizing existing software for new architectures is a time-intensive process
  - New architectures can tackle new problems, which may or may not be identified
- Enter Open OnDemand (OOD)
  - Developed and maintained by OSC
  - Complements traditional CLI workflow
  - Reduced time to compute



Hudak, D., et al., 2018. Open OnDemand: a web-based client portal for HPC centers. *Journal of Open Source Software*, *3*(25), p.622.

How Does OOD Work?



- Users connect to the Apache frontend
  - Shibboleth, CAS, OpenID, SAML, PAM, etc. supported for authentication
- Backend Nginx spawned per user (PUN) to interface with the cluster
  - Proxy request to various passenger applications, e.g. execute an interactive compute job or engage the filesystem
- **FULL HPC ACCESS VIA BROWSER**

Installing and Configuring OOD

- Most of the heavy lifting is on the OOD server (x86) itself, which can be a basic
  - Available as RPMs for CentOS/RHEL 7/8 (this is what we did)
  - Documentation fully details installation
    - Manual build of mod_auth_cas on CentOS/RHEL 8, not included in documentation
  - 3 main YAML configuration files
    - /etc/ood/config/ood_portal.yml
    - /etc/ood/config/nginx_stage.yml
    - /etc/ood/config/clusters.d/<cluster>.yml
  - *ood-portal-generator* utility to update actual web server configurations with OOD default values and custom definitions from the YAML files

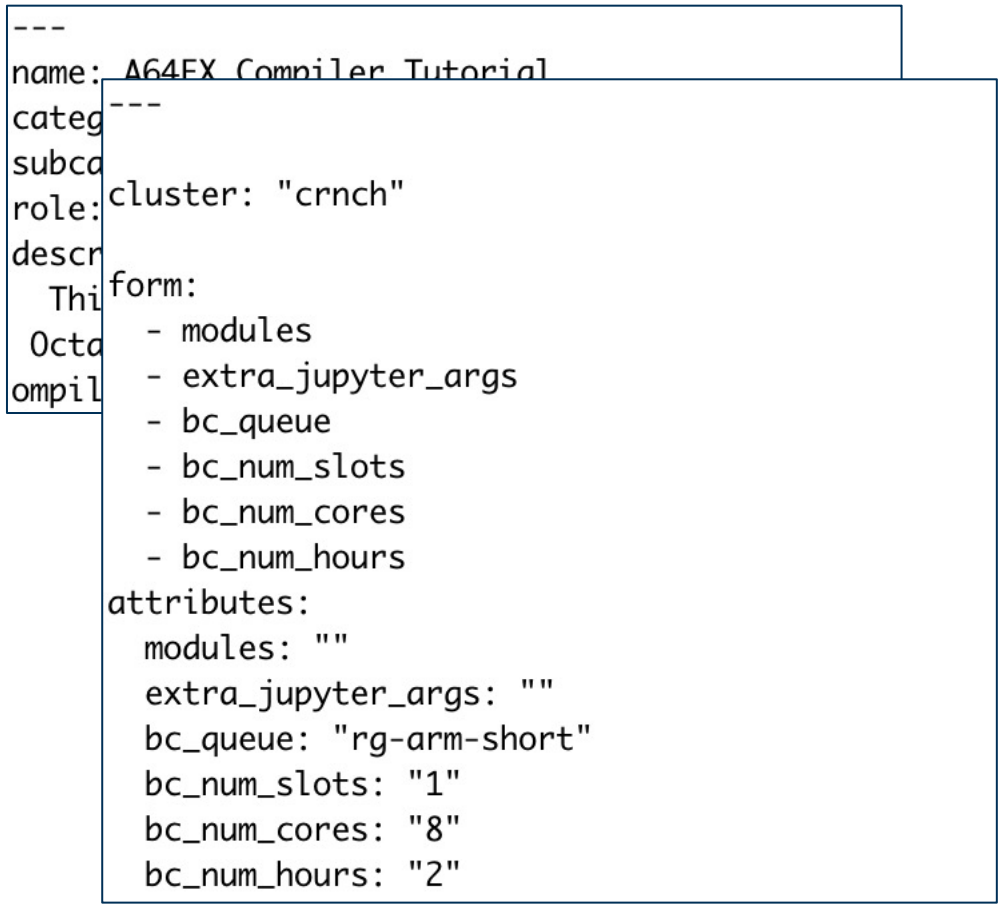
Installing and Configuring OOD (cont'd)

- Passenger applications written as a combination of YAML configurations, embedded ruby, javascript, and python. Each application includes:
  - manifest.yml

```
---
name: A64FX Compiler Tutorial
category: A64FX
subcategory: Tutorials
role: batch_connect
description: |
  This app will launch a Jupyter Notebook on an
 Octavius A64FX node to explore the available c
ompiler and performance library stack.
```

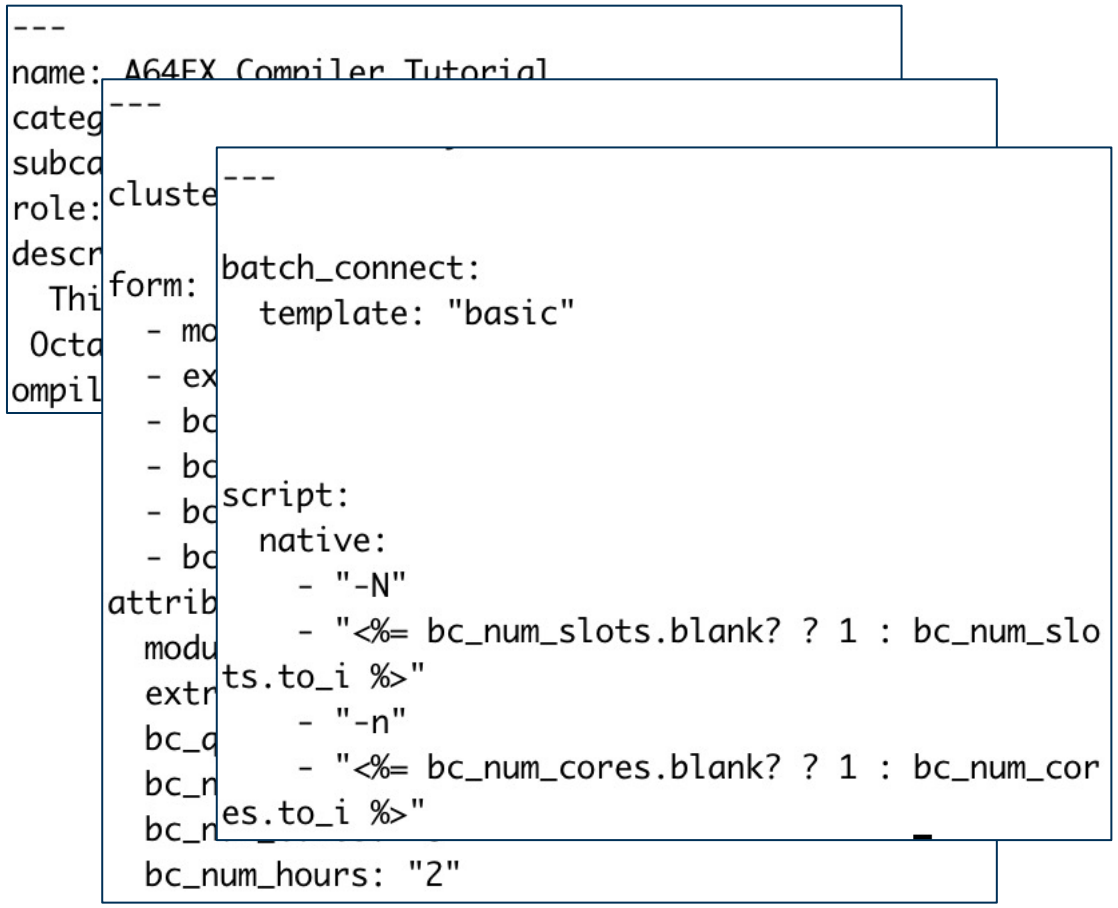
Installing and Configuring OOD (cont'd)

- Passenger applications written as a combination of YAML configurations, embedded ruby, javascript, and python. Each application includes:
  - manifest.yml
  - form.yml(.erb)



Installing and Configuring OOD (cont'd)

- Passenger applications written as a combination of YAML configurations, embedded ruby, javascript, and python. Each application includes:
  - manifest.yml
  - form.yml(.erb)
  - submit.yml(.erb)
- Passive user workflow orchestration
  - Guide them to the right resources per workflow/hardware/policy



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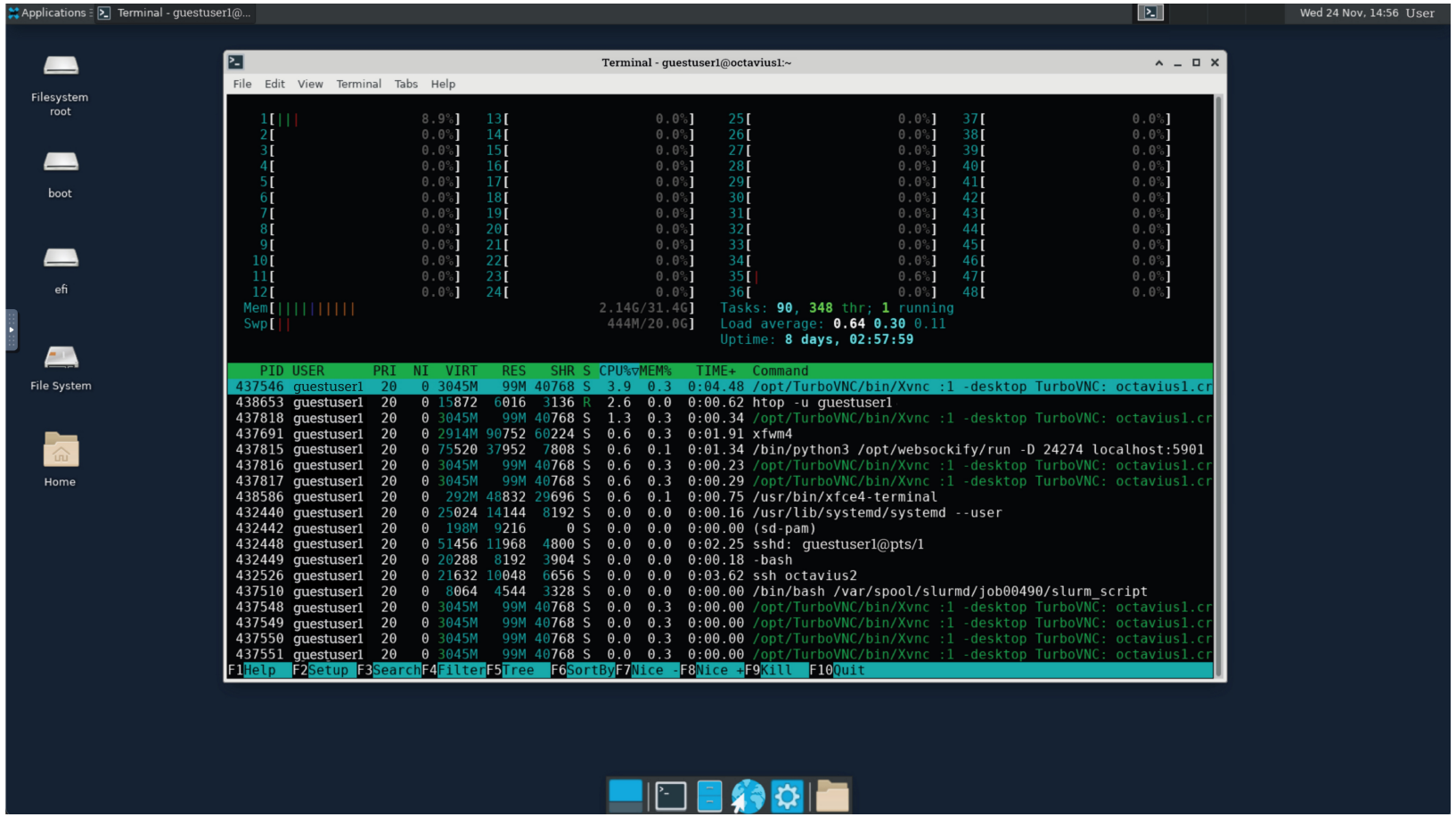
Configuring Compute Nodes for OOD

- Most OSC apps that leverage VNC expect xfce + TurboVNC
  - Aarch64 xfce is available from EPEL, but libturbojpeg needs to be manually built with the appropriate flag
- Additionally, need websockify
  - Easily installed via system pip
- Beyond these basic dependencies, any software called by the apps needs to be present on the compute node
  - Each application is customized with an associated batch script to load modules, set environment, feed content through socket, etc.

Scaling Concerns?

- Applications spawn on compute nodes, but PUN does have overhead
  - The need to reconnect to existing PUNs introduces some challenges for traditional load balancing
  - OSC reports supporting 600 unique users/month, 60 concurrent
  - PACE recently explored OOD VM capacity with WebLOAD
    - Initial tests of 12c/12GB VM indicated max ~50 concurrent users
    - At 16c/64GB VM, performance appeared stable in excess of 100 users

Virtual Desktop



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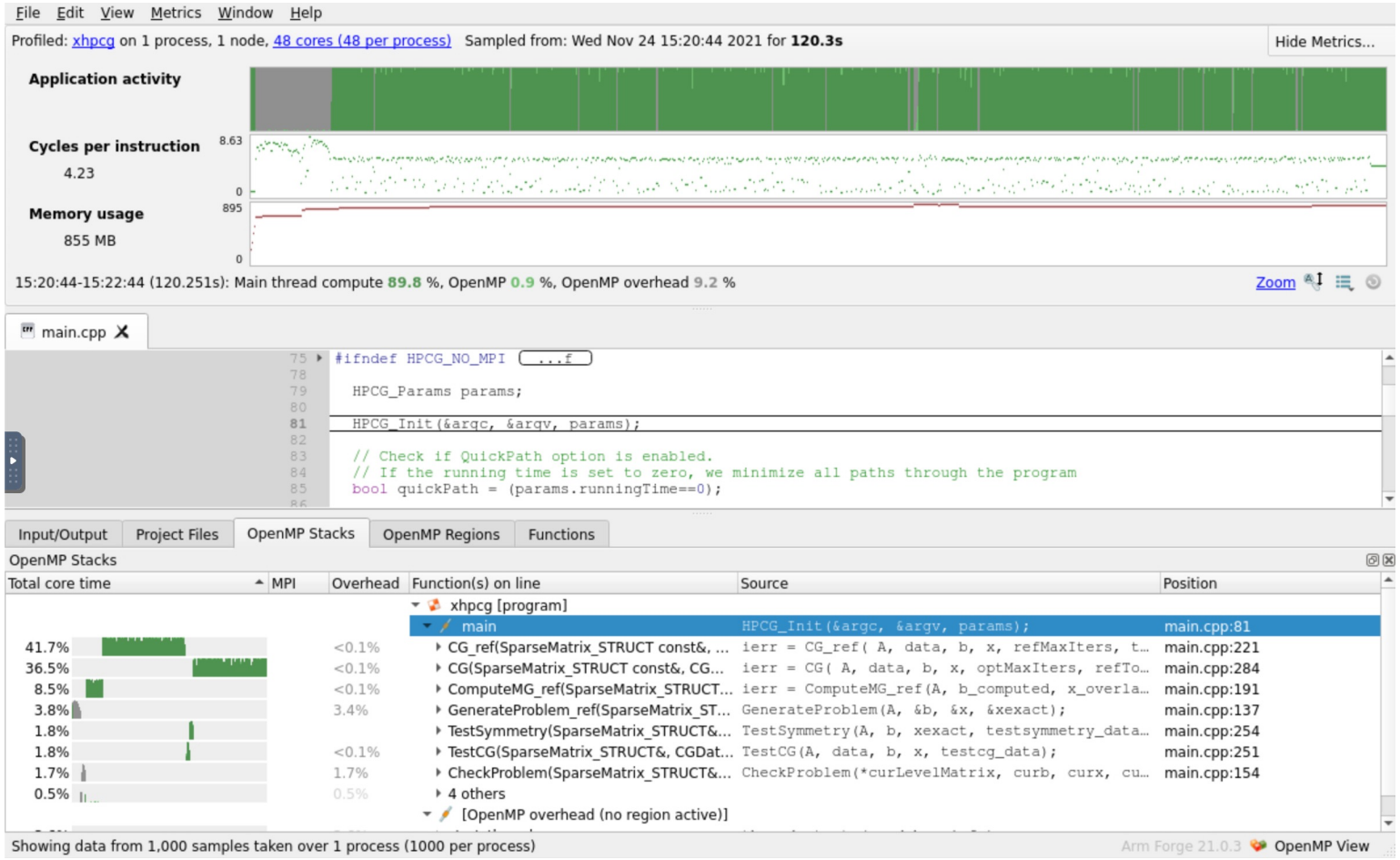
Arm Forge Suite



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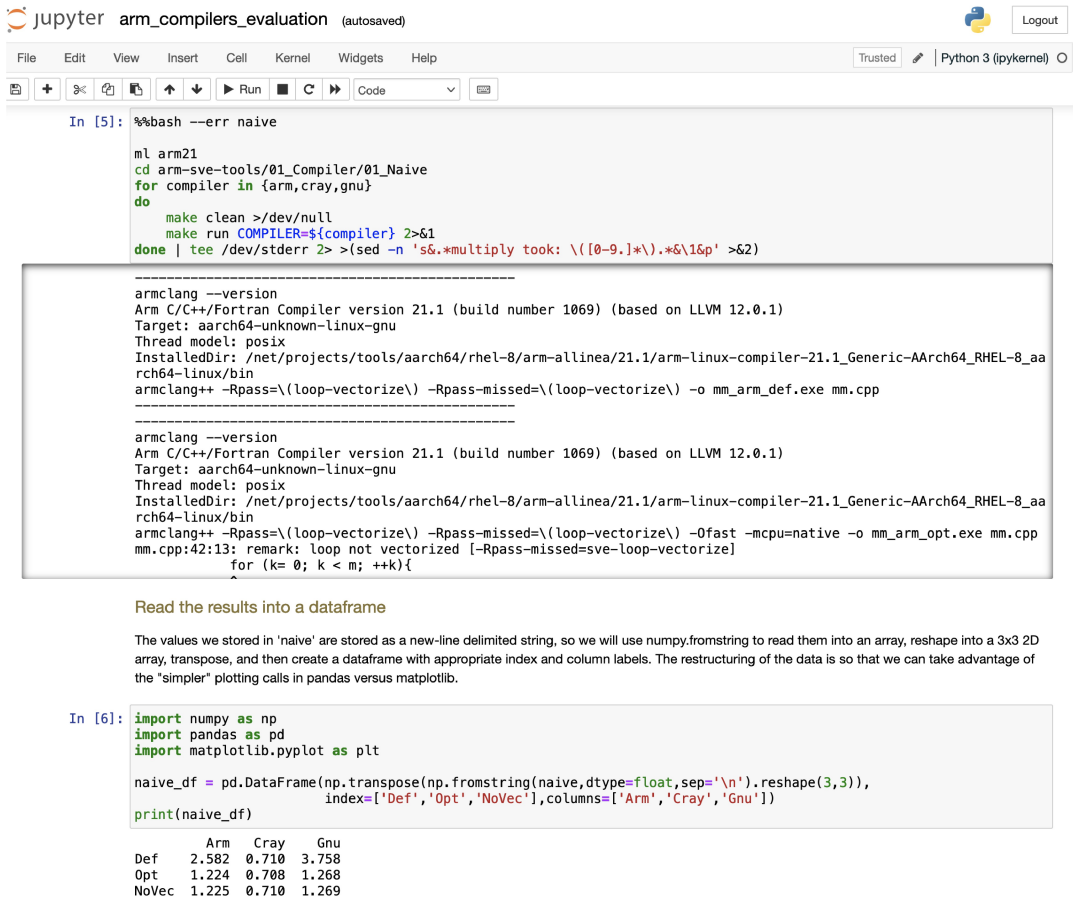
Arm Compiler Tutorial



Conclusion

- Onboarding new users can be a challenge
- OOD is a powerful platform to lower the barrier to entry
  - Provides full cluster access while improving GUI/interactive experiences
- Can leverage applications and example code to produce self-service tutorials
- Similarly, can leverage the dynamic content capabilities to abstract complex workflows (such as containerized solutions)
- Expanding Rogues Gallery OOD capabilities and looking to grow the community
  - Encourage innovative contributions to A64FX using Octavius

Acknowledgements

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