Jupyter-Based Self-Service Training in OOD for Novel Compute Architectures

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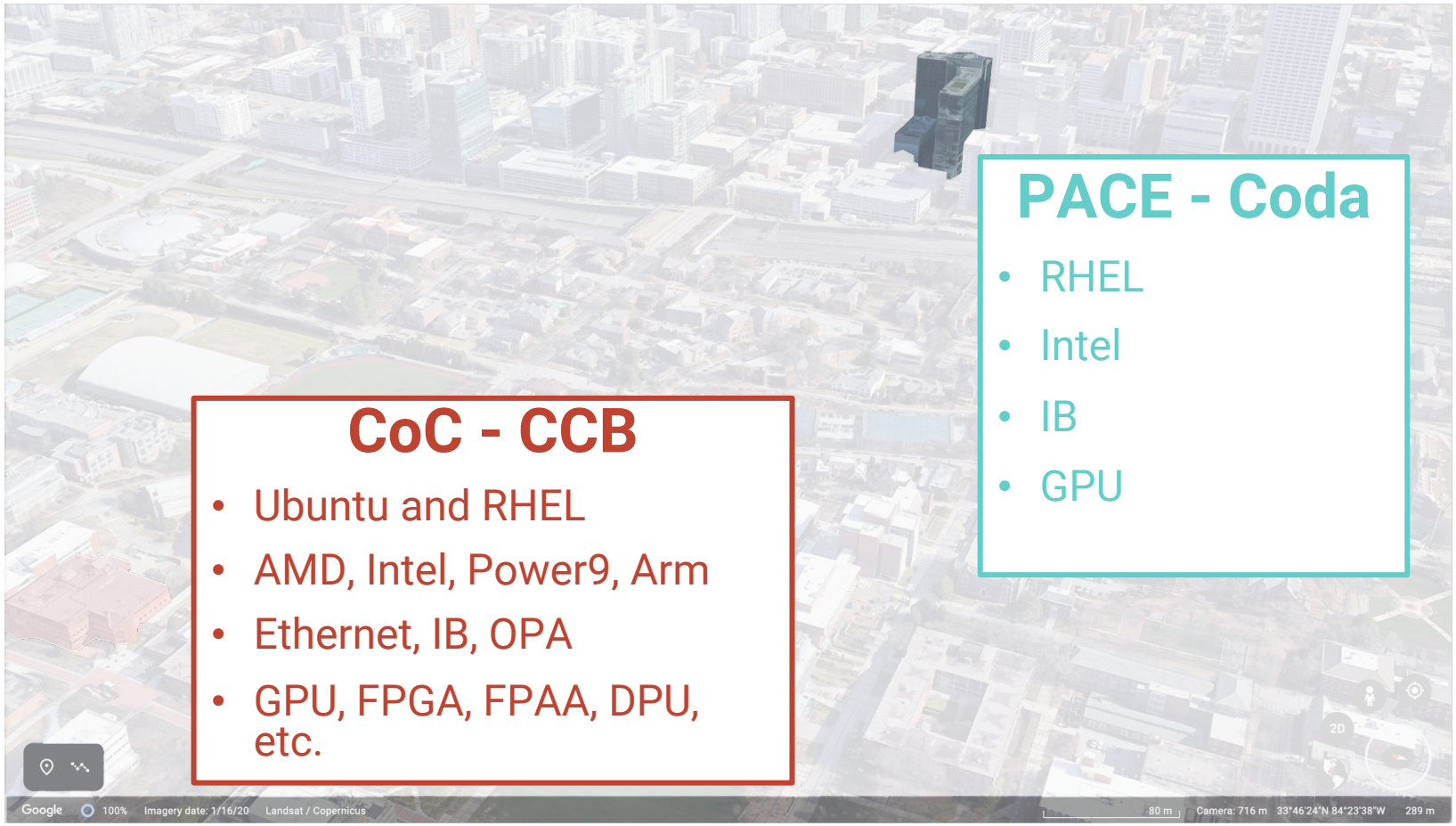
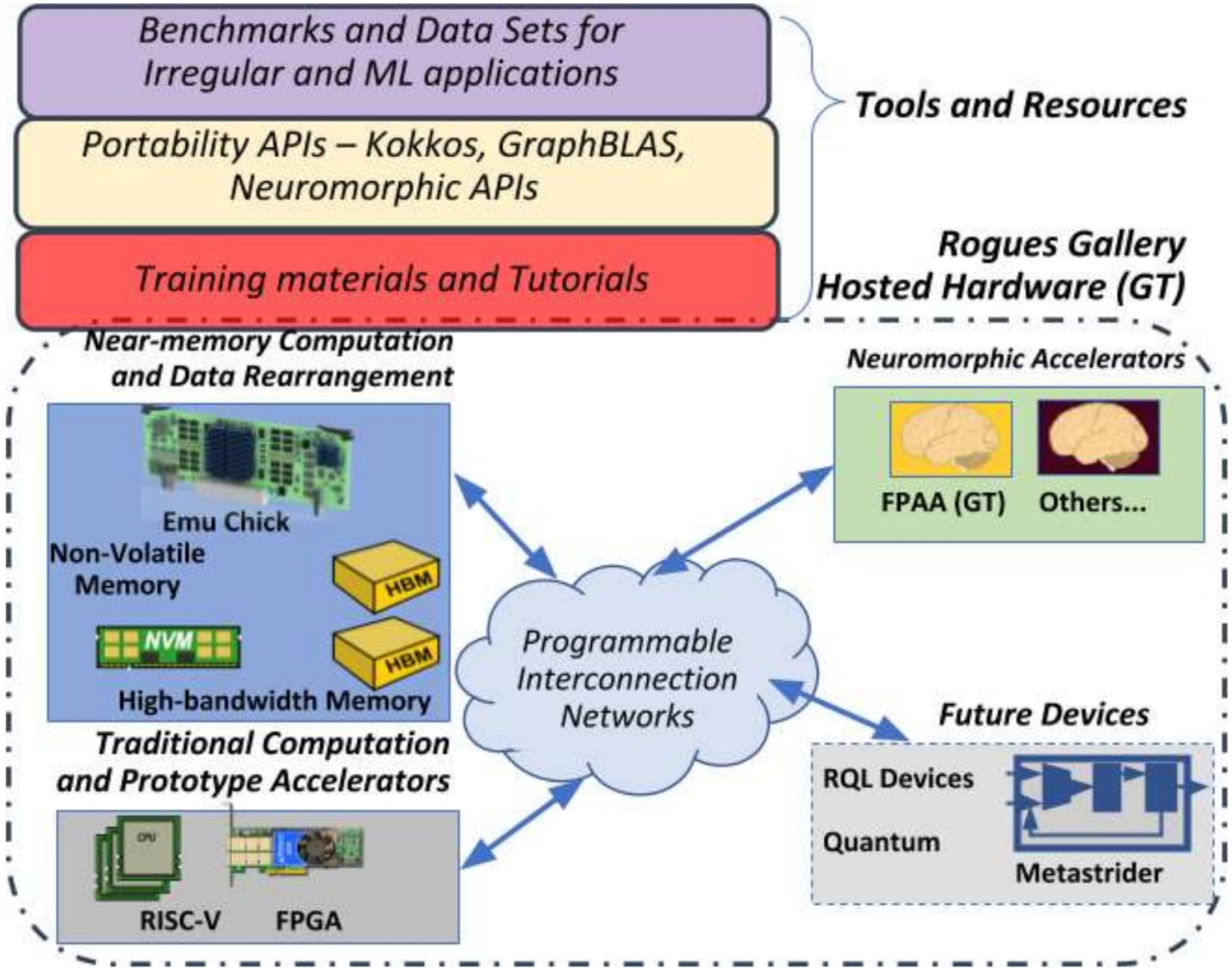


The Rogues Gallery

***NSF MRI award #1828187**: "MRI: Acquisition of an HPC System for Data-Driven Discovery in Computational Astrophysics, Biology, Chemistry, and Materials Science."*

***NSF award #2016701**: "CCRI: Medium: Rogues Gallery: A Community Research Infrastructure for Post-Moore Computing"*



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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)

Configuring Compute Nodes for OOD

- Not surprisingly, it worked out of the box
  - (since our OOD VM is x86)
- Followed OSC templates that leverage xfce + TurboVNC
  - Aarch64 xfce is available from EPEL, but libturbojpeg needs to be manually built with the appropriate flag
- Everything else pretty much out of the box
  - Given the nature of the user community, the only modular software we've provided at the moment are compilers, math libraries, and MPI

How We Leverage Jupyter

- Apps directory set up by architecture
  - E.g. all Octavius-related apps prefixed with a64fx_*
  - Access to apps controlled via POSIX group, e.g. rg-arm-users
- We provide a dropdown that auto-populates available templates
  - E.g., containerized versions of TF and PyTorch
- Tutorials are merely a port of the standard Jupyter notebook
  - Resource request fixed to match the needs of the tutorial
    - 8 cores on fixed queue and fixed time
  - Job script copies a template notebook to session directory
  - Key with tutorial design is to keep code execution native to mimic typical workflow while leveraging the ipython capabilities for enhancement

Launching Containerized Notebooks

form.yml.erb

```
<%-
  require "csv"
  output= File.read('/net/netscratch/ondemand-jupyter/templates.txt')
  templates = CSV.parse(output)
-%>
# Batch Connect app configuration file
#
# @note Used to define the submitted cluster, title, description, and
#   hard-coded/user-defined attributes that make up this Batch Connect app.
---
title: "Jupyter"
cluster: "crnch"
attributes:
  modules: ""
  extra_jupyter_args: ""
  bc_num_cores:
    help: 'Number of CPUs/Cores.'
    id: bc_num_cores
    label: CPUs/Cores Per Node
    max: 48
    min: 1
    step: 1
    value: 1
    widget: number_field
    cacheable: false
```

```
  custom_template:
    label: "Starting Interface/Template"
    widget: select
    options:
      - [ "None - use Jupyter to select file to work on", ""]
      - [ "This isn't real, because why not", ""]
    <%- templates.each do |a| -%>
      - [ "<%= a[0] %>", "<%= a[1] %>" ]
    <%- end -%>
  custom_queue:
    widget: select
    id: bc_queue
    label: "Octavius Partition"
    cacheable: false
    options:
      - [ "Debug: up to 4 nodes and 1 hour", "rg-arm-debug"]
      - [ "Short: up to 16 nodes and 2 hours", "rg-arm-short"]
      - [ "Long: up to 16 nodes and 6 hours", "rg-arm-long"]
form:
  - extra_jupyter_args
  - modules
  - custom_queue
  - bc_num_hours
  - bc_num_slots
  - bc_num_cores
  #- bc_email_on_started
  - custom_template
```

Launching Containerized Notebooks

submit.sh.erb

```
# Launch the Jupyter Notebook Server
<%- if context.custom_template == "TensorFlow.ipynb" -%>
  set -x
  export ONDEMAND_FILE="${odir}/<%=context.custom_template%>"
  export TEMPLATE_FILE="${sdir}/<%= context.custom_template %>"
  # Launch the Jupyter Notebook Server
  cp $ONDEMAND_FILE $TEMPLATE_FILE
  TEMPLATE_FILE=${TEMPLATE_FILE#*ondemand/}
  singularity run "${odir}"/tensorflow-arm.sif jupyter notebook --debug --
config="${CONFIG_FILE}" <%= context.extra_jupyter_args %> \
    --NotebookApp.default_url="/tree/ondemand/$TEMPLATE_FILE"
<%- elsif context.custom_template == "PyTorch.ipynb" -%>
  set -x
  export ONDEMAND_FILE="${odir}/<%=context.custom_template%>"
  export TEMPLATE_FILE="${sdir}/<%= context.custom_template %>"
  # Launch the Jupyter Notebook Server
  cp $ONDEMAND_FILE $TEMPLATE_FILE
  TEMPLATE_FILE=${TEMPLATE_FILE#*ondemand/}
  singularity run "${odir}"/pytorch-arm-neoverse-n1_r21.10-torch-1.9.0-openblas-jupyter.sif
jupyter notebook --debug --config="${CONFIG_FILE}" <%= context.extra_jupyter_args %> \
    --NotebookApp.default_url="/tree/ondemand/$TEMPLATE_FILE"
]
<%- else -%>
  set -x
  jupyter notebook --config="${CONFIG_FILE}" <%= context.extra_jupyter_args %>
<%- end -%>
```

Arm Compiler Tutorial

script.sh.erb

```
#!/usr/bin/env bash

# Benchmark info
echo "TIMING - Starting main script at: $(date)"

# Get Running Script Directory
get_script_dir () {
   SOURCE="${BASH_SOURCE[0]}"
   while [ -h "$SOURCE" ]; do
      DIR="$( cd -P "$( dirname "$SOURCE" )" && pwd )"
      SOURCE="$( readlink "$SOURCE" )"
      [[ $SOURCE != /* ]] && SOURCE="$DIR/$SOURCE"
   done
   $( cd -P "$( dirname "$SOURCE" )" )
   pwd
}
sdir="$(get_script_dir)"
export SDIR=$sdir
odir="/net/projects/notebook/ondemand-jupyter/"

# Set working directory to home directory
cd "${HOME}”

#
# Start Jupyter Notebook Server
#

<%- unless context.modules.blank? -%>
# Purge the module environment to avoid conflicts
module purge

# Load the require modules
module load <%= context.modules %>

# List loaded modules
module list
<%- end -%>

# Benchmark info
echo "TIMING - Starting jupyter at: $(date)"

# Launch the Jupyter Notebook Server
set -x
export ONDEMAND_FILE="${odir}/arm_compilers_evaluation.ipynb"
export TEMPLATE_FILE="${sdir}/arm_compilers_evaluation.ipynb"
cp $ONDEMAND_FILE $TEMPLATE_FILE
TEMPLATE_FILE=${TEMPLATE_FILE#*ondemand/}
jupyter notebook --config="${CONFIG_FILE}" <%= context.extra_jupyter_args %> \
  --NotebookApp.default_url="/tree/ondemand/$TEMPLATE_FILE"
```

Arm Compiler Tutorial

jupyter arm_compilers_evaluation (autosaved) Logout

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3 (ipykernel)

Run Code

In [5]:
```
%%bash --err naive

ml arm21
cd arm-sve-tools/01_Compiler/01_Naive
for compiler in {arm,cray,gnu}
do
    make clean >/dev/null
    make run COMPILER=${compiler} 2>&1
done | tee /dev/stderr 2> >(sed -n 's&.*multiply took: \([0-9.]*\).*&\1&p' >&2)
```

```
------------------------------------------------------
armclang --version
Arm C/C++/Fortran Compiler version 21.1 (build number 1069) (based on LLVM 12.0.1)
Target: aarch64-unknown-linux-gnu
Thread model: posix
InstalledDir: /net/projects/tools/aarch64/rhel-8/arm-allinea/21.1/arm-linux-compiler-21.1_Generic-AArch64_RHEL-8_aarch64-linux/bin
armclang++ -Rpass=\(loop-vectorize\) -Rpass-missed=\(loop-vectorize\) -o mm_arm_def.exe mm.cpp
------------------------------------------------------
------------------------------------------------------
armclang --version
Arm C/C++/Fortran Compiler version 21.1 (build number 1069) (based on LLVM 12.0.1)
Target: aarch64-unknown-linux-gnu
Thread model: posix
InstalledDir: /net/projects/tools/aarch64/rhel-8/arm-allinea/21.1/arm-linux-compiler-21.1_Generic-AArch64_RHEL-8_aarch64-linux/bin
armclang++ -Rpass=\(loop-vectorize\) -Rpass-missed=\(loop-vectorize\) -Ofast -mcpu=native -o mm_arm_opt.exe mm.cpp
mm.cpp:42:13: remark: loop not vectorized [-Rpass-missed=sve-loop-vectorize]
            for (k= 0; k < m; ++k){
```

Read the results into a dataframe

The values we stored in 'naive' are stored as a new-line delimited string, so we will use numpy.fromstring to read them into an array, reshape into a 3x3 2D array, transpose, and then create a dataframe with appropriate index and column labels. The restructuring of the data is so that we can take advantage of the "simpler" plotting calls in pandas versus matplotlib.

In [6]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

naive_df = pd.DataFrame(np.transpose(np.fromstring(naive,dtype=float,sep='\n').reshape(3,3)),
                        index=['Def','Opt','NoVec'],columns=['Arm','Cray','Gnu'])
print(naive_df)
```

```
         Arm   Cray    Gnu
Def    2.582  0.710  3.758
Opt    1.224  0.708  1.268
NoVec  1.225  0.710  1.269
```

jupyter arm_compilers_evaluation (autosaved) Logout

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3 (ipykernel)

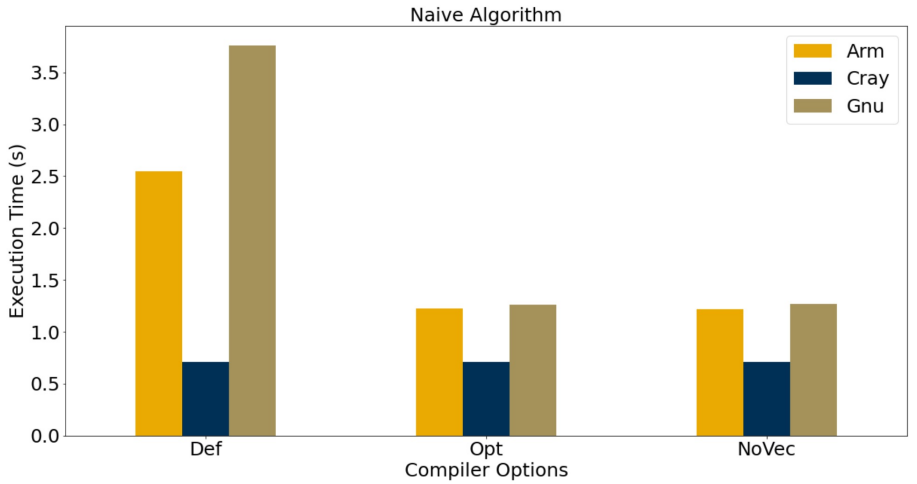
Run Markdown

```
         Arm   Cray    Gnu
Def    2.544  0.710  3.758
Opt    1.224  0.708  1.265
NoVec  1.215  0.710  1.268
```

Make a bar plot with the results

Given the nature of the data, we can summarize the results of the different compilers and options using a bar plot. Given a pandas dataframe, we can run the plot.bar function to handle each of our different combinations (and set the plot size and labels using pyplot calls).

In [4]:
```
naive_df.plot.bar(rot=0,figsize=(20,10),color=['#EAAA00','#003057','#A4925A'])
plt.title('Naive Algorithm',fontsize=25)
plt.legend(prop={'size': 25})
plt.ylabel('Execution Time (s)',fontsize=25)
plt.yticks(fontsize=25)
plt.xlabel('Compiler Options',fontsize=25)
plt.xticks(fontsize=25)
plt.show()
```



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

Bored today/tomorrow? Check out the CRNCH Summit 2022 videos