Engineering Notebook :
VIP High Performance Computing (HPC)

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Team: High Performance Conjugate Gradients (HPCG)

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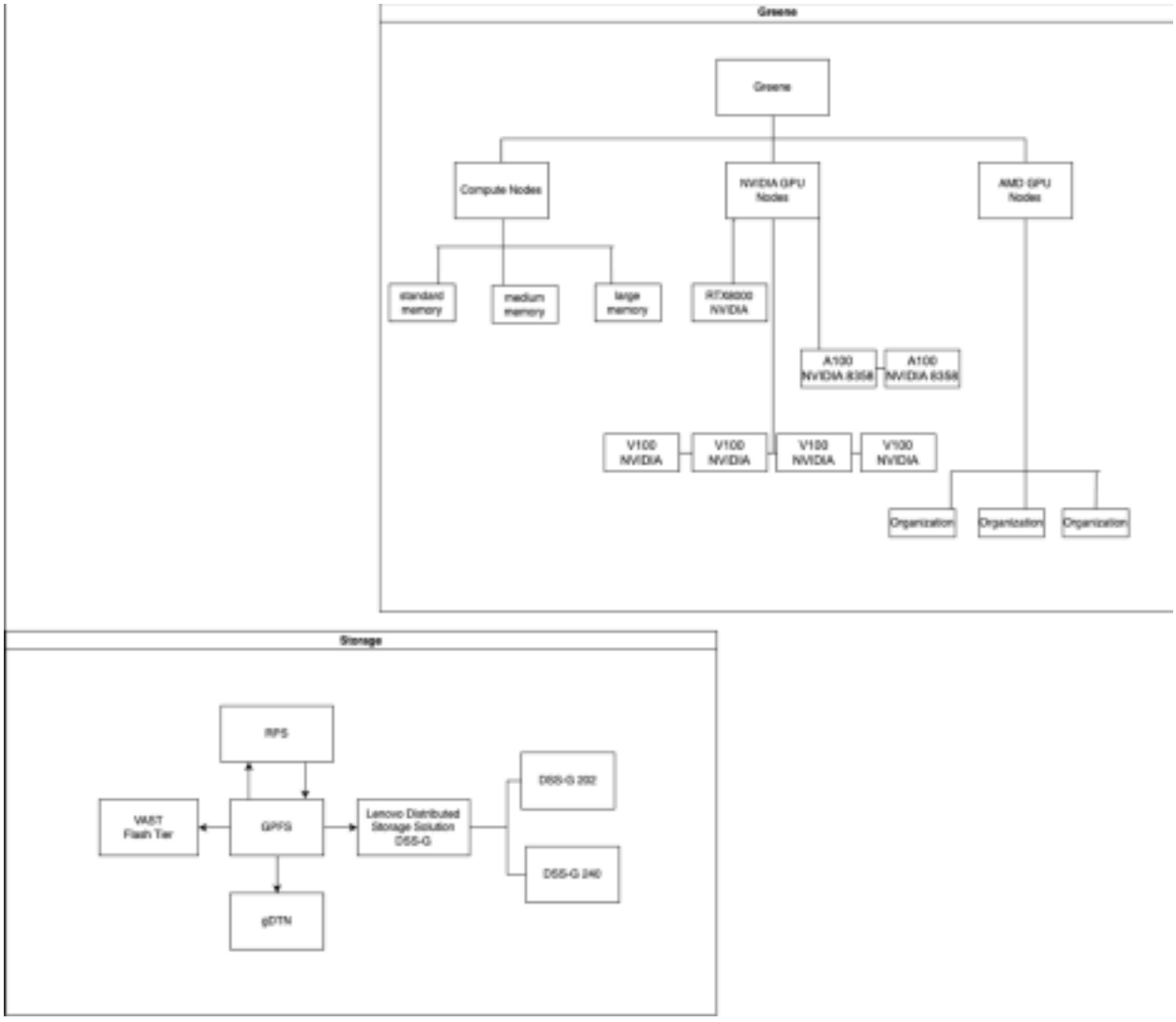
Week 1 (7/17/23)

During the meeting, we covered several key topics. The first part of the discussion focused on a comprehensive review of hardware components. Additionally, an overview of upcoming enhancements to the High-Performance Computing (HPC) operating systems was presented, although the details are still pending finalization. The session also included an introductory segment on Linux, encompassing essential Linux commands and file handling procedures.

For future reference, the meeting was recorded, and the recording can be accessed at the following link :
(https://nyu.zoom.us/rec/share/5lZs6fK4OQMoHgSJsiKd59CrdsP7QFSUzoQ8epW3RNwrZhQiLs9HJRbWsHQ49_ID.QDiECXCZw01WoXdB).
Key tasks accomplished during the session were the successful setup of NYU HPC accounts and GUI control. Additionally, a hardware structure diagram was created and can be as seen.



Week 2 (7/24/23)

The meeting primarily covered two significant topics. Firstly, an introduction to High-Performance Computing (HPC) operating systems was provided, although the details are yet to be finalized. The discussion included insights into the upcoming enhancements in this domain. Secondly, there was an informative session on Linux, encompassing introductory concepts, Linux commands, and file handling procedures.

For additional resources, participants were directed to a Linux tutorial available at: (https://sites.google.com/nyu.edu/nyu-hpc/training-support/tutorials/linux-tutorial)
Presentation slides from the meeting can be accessed through the following link: (https://drive.google.com/file/d/12VNe1X4Ujvb788hswlbUtQ11OP2tQpyL/view?usp=sharing)

During the meeting, attendees completed tasks that involved experimenting with basic Linux commands, contributing to a hands-on exploration of the operating system's fundamental functionalities.

Week 3 7/31/23

The meeting covered three main topics: Compiler, Tmux, and Slurm. The discussion delved into compiler-related aspects, explored the functionalities of Tmux, and provided insights into the usage of Slurm. Additionally, resources were shared to support further understanding and learning.

For reference, slides from the meeting can be accessed through the following link: [Meeting Slide](https://drive.google.com/drive/u/0/search?q=HPC). Specific information about Slurm, a workload manager, was detailed in the Greene Slurm tutorial, available at: [Greene Slurm Tutorial](https://sites.google.com/nyu.edu/nyu-hpc/training-support/tutorials/slurm-tutorial?authuser=0).

During the meeting, participants successfully completed tasks that involved experimenting with Slurm, and specifically, they submitted a simple job using this resource. This hands-on experience aimed to provide practical insights into the utilization of Slurm for job management within the High-Performance Computing (HPC) context.

Week 4 8/8/23

The meeting with Shenglong on Zoom encompassed several key topics. The discussion began with an exploration of the meaning and significance of SCC (possibly referring to a specific term or entity), followed by an examination of why scientific research necessitates High-Performance Computing (HPC) resources. Additionally, the session covered an introduction to HPCG, shedding light on its relevance and role within the field.

To facilitate further understanding, various resources were shared. The Greene HPC system details and documentation can be found at: [Greene](https://sites.google.com/nyu.edu/nyu-hpc/hpc-systems/greene). A document from Los Alamos National Laboratory titled "Summary_HPCG.pdf" was provided, accessible at: [HPCG Summary](https://www.lanl.gov/projects/crossroads/_assets/docs/ssi/Summary_HPCG.pdf). Furthermore, tutorials from UL HPC were recommended as valuable learning materials.
A task that was successfully completed during the meeting involved reading the UL HPCG tutorial. This task aimed to enhance participants' understanding of the concepts and applications associated with High-Performance Computing through the UL HPCG tutorial materials.

Week 5 8/14/23

The HPCG meeting covered several important topics related to High-Performance Conjugate Gradient (HPCG) computations. The agenda included discussions on how to execute HPCG on the Greene HPC system, the interpretation of HPCG results, and the concept of optimization within this context.

To provide additional resources for participants, a Zoom recording of the HPCG meeting was made available for reference. Furthermore, UL HPC tutorials were recommended to supplement the understanding of HPCG processes and applications.

During the meeting, participants successfully completed tasks associated with the practical implementation of HPCG on the Greene system. These tasks included building a basic version of HPCG on Greene and running it with varying configurations, specifically on a single node, 2 nodes, and 4 nodes. This hands-on experience aimed to familiarize participants with the execution and scalability of HPCG computations on the Greene HPC infrastructure.

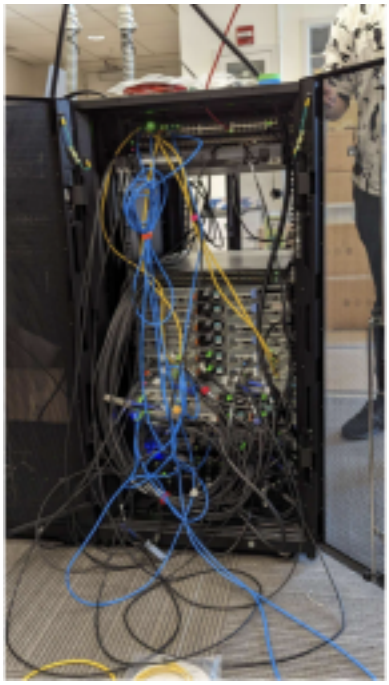
Week 6 9/11/23

The week covered several important topics, starting with a webinar on the SCC23 Reproducibility Challenge. The agenda included discussions and insights into the challenges and strategies involved in ensuring the reproducibility of research.

In addition, there was a practical demonstration on how to connect cables on a cluster, providing valuable information on the physical setup and maintenance of hardware components within a cluster environment. A subgroup meeting was also held to discuss matters related to a notebook and website, focusing on collaborative efforts and updates in these areas.

To support these discussions, a hardware sheet was shared as a resource, offering detailed information on the cluster's hardware components. The sheet can be accessed at: [Hardware Sheet](https://docs.google.com/presentation/d/1TUGOQVo6AXgrEHkmPxv2LjHa3cmIvMdLE0-m_d8aDvY/edit#slide=id.g1e4794a6e06_0_43).

The meeting notes indicate that specific tasks were completed; however, the details of these tasks are not provided. If you have specific information about the tasks completed during the meeting, feel free to share, and I can provide more detailed information based on that input.



Week 7 9/18/23

The meeting focused on several key topics related to High-Performance Computing (HPC) Lab activities. The first item on the agenda involved the installation of the system, specifically Rocky Linux, within the HPC Lab environment. This installation is a foundational step for setting up the HPC infrastructure.

Additionally, there was a discussion and hands-on session on optimizing HPCG (High-Performance Conjugate Gradient) computations. Optimization is crucial for enhancing the efficiency and performance of HPC applications.

A subgroup meeting was also held to address matters related to the development and maintenance of the lab's website, emphasizing collaborative efforts within the subgroup.

To support participants, resources from UL HPC Tutorials were provided. These tutorials likely offer valuable insights and guidance on various aspects of high-performance computing.

The meeting notes indicate that specific tasks were completed during the session. Participants tested various configurations using the 'srun' command with different parameters for nodes, tasks per node, CPUs per task, and memory. The tasks included testing configurations with different combinations of these parameters using the xhpcg application:

1. `srun --nodes=1 --tasks-per-node=12 --cpus-per-task=4 --mem=180GB xhpcg` 2. `srun --nodes=4 --tasks-per-node=48 --mem=180GB xhpcg`
3. `srun --nodes=4 --tasks-per-node=12 --cpus-per-task=4 --mem=180GB xhpcg`
4. `srun --nodes=4 --tasks-per-node=24 --cpus-per-task=2 --mem=180GB xhpcg`

These tests likely aimed to assess the performance and scalability of the xhpcg application under different computing configurations.

Week 8 9/25/23

The meeting for the HPC Lab covered two main topics: the installation of the system, specifically Rocky Linux, and the creation of a subgroup website and presentation slides.

Regarding the system installation, the focus was on deploying Rocky Linux within the HPC Lab environment. Rocky Linux is a community-driven enterprise operating system designed to be compatible with Red Hat Enterprise Linux. Participants likely discussed and possibly executed the steps required for this installation to ensure a stable and reliable system for high-performance computing tasks.

In addition to the system installation, there was an emphasis on subgroup collaboration, with the creation of a website and presentation slides. These resources serve as platforms for sharing information, updates, and collaborative efforts within the subgroup.

To support these activities, participants were provided with external resources, including the official Rocky Linux website (https://rockylinux.org/) and the HPCG Benchmark website (https://www.hpcg-benchmark.org/). These resources likely offer valuable information, documentation, and tools for the Rocky Linux installation process and high-performance computing benchmarks.

A task that was completed during the meeting involved progress on a subgroup website and presentation slides. The link provided (https://sites.google.com/d/1aXTbq9BK20z72rGCVjYlYXp4uA2zsm0y/p/1cI3EIP38jmZhdt7RTVt 1hOHhu4-eygcV/edit) likely directs to a collaborative platform where participants contributed to the development of the subgroup's online presence and presentation materials.

Week 9 10/2/23

The meeting focused on running Intel-optimized HPCG (High-Performance Conjugate Gradient) and utilized various resources for this purpose.

To optimize HPCG using Intel tools, participants referred to the official Intel documentation for getting started with Intel-optimized HPCG, which can be found at: [Intel Optimized HPCG Guide](https://www.intel.com/content/www/us/en/docs/onemkl/developer-guide-linux/2023-1/getting-started-with-intel-optimized-hpcg.html)
To access the necessary Intel tools, participants likely downloaded the Intel OneAPI Base Toolkit and HPC Toolkit. The download links for these toolkits can be found at: - [Intel OneAPI Base

Toolkit](https://www.intel.com/content/www/us/en/developer/tools/oneapi/base-toolkit-download.html)
- [Intel HPC Toolkit](https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit.html#gs.741iim)

Tasks completed during the meeting included copying the Intel benchmark onto the Greene system, which is likely the HPC infrastructure being used for the experiments. Subsequently, participants successfully ran Intel HPCG using a single node, indicating progress in the implementation and testing of Intel-optimized HPCG on the Greene HPC system.

This meeting aimed to leverage Intel's optimization tools for improved performance in HPCG computations, and the completed tasks suggest successful initial steps in this optimization process.

Week 10 10/9/23

The meeting was focused on building the Intel-optimized version of HPCG (High-Performance Conjugate Gradient) from source code, utilizing various Intel tools.

Resources Used:
- [Getting Started with Intel-Optimized HPCG](https://www.intel.com/content/www/us/en/docs/onemkl/developer-guide-linux/2023-1/get ting-started-with-intel-optimized-hpcg.html)
- [Intel OneAPI Base Toolkit](https://www.intel.com/content/www/us/en/developer/tools/oneapi/base-toolkit-download.html)
- [Intel HPC Toolkit](https://www.intel.com/content/www/us/en/developer/tools/oneapi/hpc-toolkit.html#gs.741iim)

Tasks Completed:
1. Building Intel-Optimized HPCG:
   Participants successfully built the Intel-optimized version of HPCG from its source code. This process involved using Intel tools such as Intel Math Kernel Library (MKL), Intel C++ Compiler (ICC), and Open MPI. The goal was to leverage these tools for optimizing the performance of HPCG on the selected system.

2. Running Intel HPCG:
   Following the successful build, participants executed Intel HPCG on the Greene system. The testing included running HPCG with a single node as well as with 4 nodes. This step aimed to assess the performance and scalability of the Intel-optimized HPCG implementation in a distributed computing environment.

These tasks signify significant progress in integrating Intel's optimization tools into the HPCG application, ultimately enabling the execution and evaluation of HPCG on the chosen high-performance computing infrastructure. The meeting's focus on optimization and testing aligns with best practices in ensuring efficient performance in HPC applications.

Week 11 10/16/23

The meeting covered various topics, including notes on Intel HPCG, researching the GPU version of HPCG, and discussions related to a competition strategy table for SCC23.

Resources Used:
- [NVIDIA GPU Containers for HPC Benchmarks](https://catalog.ngc.nvidia.com/orgs/nvidia/containers/hpc-benchmarks)
- [Optimizing High-Performance Conjugate Gradient Benchmark for GPUs](https://developer.nvidia.com/blog/optimizing-high-performance-conjugate-gradient-benchmark-gpus/)

Tasks Completed:
1. Intel HPCG Notes:
   Participants compiled notes on Intel HPCG, likely covering details about the Intel-optimized version, including building and running processes. These notes could encompass information on optimization strategies, performance considerations, and best practices for running HPCG with Intel tools.

2. Research on GPU Version of HPCG:
   Attendees conducted research on the GPU version of HPCG, exploring resources such as NVIDIA GPU Containers for HPC Benchmarks. The focus was likely on understanding how HPCG can be optimized and executed efficiently on GPU architectures.

Learned about Singularity:
   Participants completed the task of learning about Singularity, which is a containerization solution commonly used in high-performance computing environments. Understanding Singularity is beneficial for managing software environments and dependencies in a reproducible and portable manner.

Overall, the meeting covered a range of topics, reflecting a comprehensive exploration of HPCG on both CPU and GPU architectures, as well as strategic considerations for an upcoming competition.

Week 12 10/23/23

The meeting for the HPC Lab included several key activities related to Ansible, Nvidia HPCG with Singularity, and subgroup discussions.

Tasks Completed:

1. Install Ansible and Write Playbook:
   The HPC Lab progressed by installing Ansible, a configuration management tool, and participants wrote a playbook. Ansible playbooks are scripts that define a set of tasks to be executed on remote machines. These tasks likely pertain to the configuration and setup of the lab environment.

2. Run Nvidia HPCG with Singularity:
   The lab successfully executed Nvidia HPCG using Singularity. This involves running the HPCG benchmark within a Singularity container, providing an isolated and reproducible environment for the application. The resource link provided (https://catalog.ngc.nvidia.com/orgs/nvidia/containers/hpc-benchmarks) may have been used to obtain the Singularity container for Nvidia HPCG.

3. Subgroup Meeting to Discuss Progress and HPCG:
   A subgroup meeting was held to discuss progress and likely focused on the implementation and results of running Nvidia HPCG. The discussion might have included sharing insights, challenges, and plans for further optimization or experimentation with HPCG.

Resources Used:
- [NVIDIA GPU Containers for HPC Benchmarks](https://catalog.ngc.nvidia.com/orgs/nvidia/containers/hpc-benchmarks)

Completed HPCG Runs:
   The lab successfully ran Nvidia HPCG on both 4 GPU nodes and 1 GPU node. These tasks likely involved assessing the performance and scalability of HPCG on the lab's hardware infrastructure.

These completed tasks indicate progress in setting up the lab environment, leveraging Ansible for automation, and successfully running and evaluating Nvidia HPCG with Singularity on GPU nodes. The subgroup meeting likely provided a platform for collaborative discussions and strategic planning based on the achieved results.

Week 13 10/30/23

The subgroup meeting focused on updating members on progress and challenges related to HPCG. Participants shared insights from running HPCG on designated hardware, discussed

challenges faced, and proposed solutions. The meeting also included planning for future tasks, optimizations, and strategies for collaborative efforts. Emphasis was placed on effective documentation to track progress and facilitate knowledge sharing. Overall, the meeting aimed to coordinate efforts and ensure alignment towards achieving the subgroup's objectives.

Week 14 12/4/23

The final subgroup meeting served as a concluding session with three main agenda items:

1. Final Website Changes:
   Participants made the last adjustments to the subgroup's website. This likely involved ensuring that all relevant information, updates, and resources were accurately reflected on the site for future reference.

2. Final Presentation and Work Discussion:
   The group finalized the presentation summarizing all the work accomplished throughout the semester. This involved highlighting key achievements, challenges overcome, and insights gained. The presentation likely covered aspects such as HPCG implementations, optimization efforts, and any noteworthy outcomes from the project.

3. Farewell and Best Wishes:
   The meeting concluded with a farewell segment. Team members expressed gratitude for the collaboration and teamwork, acknowledging the efforts put into the project. Farewell messages were shared, and the team extended best wishes for success in future endeavors, particularly in the upcoming semester.

Overall, the final subgroup meeting provided an opportunity to wrap up the project, ensure the completion of outstanding tasks, and bid farewell to team members, expressing appreciation and optimism for their future endeavors.