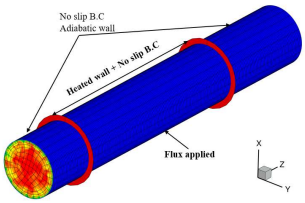
HPC based Introduction to numerical simulations

SGX3 award # 2231406

Revised Course Description

The ET307 Introduction to numerical simulations course provides a comprehensive introduction to numerical simulations with a focus on computational fluid dynamics (CFD).
The students will learn the fundamental component of numerical methods, mesh generation techniques and practical applications of CFD.
The course emphasizes hands on experience through projects using OpenFoam and High-performance computing resources.
Prerequisites:
MA 318. ANALYSIS II
MA 421. ORDINARY AND PARTIAL DIFFERENTIAL EQUATION I
ET307: CAD Applications

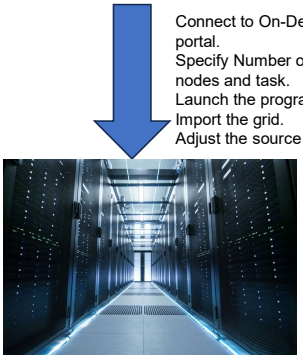


Implementation Schedule

Spring 2025:
- Explore Getaways resources and obtain instructor account.
- Develop test cases and lunch simulation on the server to assess the computational resources.

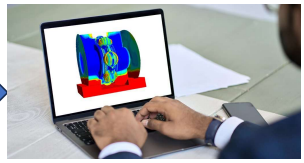
Fall 2025:
- Starting the course following the syllabus and testing the students accounts.

Winter session 2025
- Assess the overall experience and adjustments.



Connect to On-Demand HPC portal.
Specify Number of hours, nodes and task.
Launch the program
Import the grid.
Adjust the source code

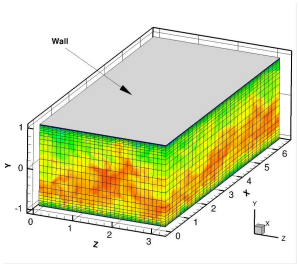
Transfer to the computer



Post-Processing

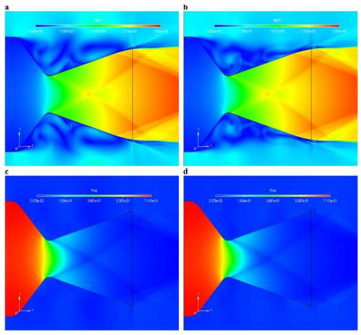
Sample HPC/Gateways Exercise

Problem 1: Access Frontier and Clone repository
Step 1: access your account
Use the user Id and passcode you set up for Frontier to login by typing the following command:
ssh userid@frontier.olcf.ornl.goc
Now access your home account, by typing:
cd /ccs/home/userid.
Step 2: Clone repository
"GitHub is a code-hosting platform for version control and collaboration."
To perform step 2, type the following command:
Git clone https://github/com/olcf/hands-on-with-frontrier.git
You can List the folders in your home directory by typing "ls" and press enter.
You will see the new repository name listed, then type the following to access it by typing: cd hands-on-with-frontier



Resource Needs/List

- On-demand HPC platform that allows instructor and 10 students to transfer the data, check the job status.
- The platform should support OpenFOAM software or other interactive softwares.



Gateway Community Mentor Syllabus Suggestions

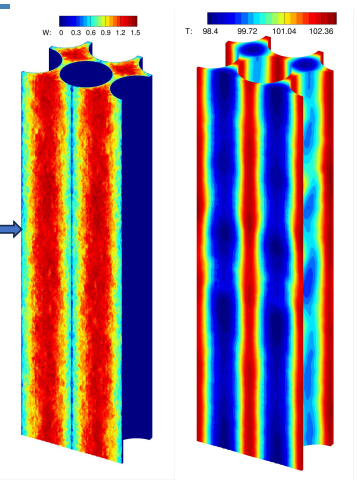
- Content motivating why/when/how HPC is used (e.g., problems too big, complex, dangerous, expensive),
- Content introducing example HPC system use cases (e.g., GE Aerospace, NASA CFD simulations on Frontier),
- Content introducing adaptive mesh refinement frameworks (e.g., AMReX, Parthenon),
- Content introducing real-world CFD codes (e.g., MFIX-Exa, Pele, ECP CFD Codes),
- Content introducing basic HPC system use and typical workflow (e.g., UNIX basics, job schedulers), and
- Guest lectures highlighting how others have used HPC for CFD in the real-world.
- Using different

Datasets

- https://github.com/barbagroup/CFDPythonDataset
- https://github.com/KratosMultiphysics/Kratos
- https://github.com/OpenFOAM/OpenFOAM-dev
- https://github.com/Nek5000/nekRS

Possible Expansions

The class can be expanded to include more complex topics which include multi-physics simulations covering more advanced topics as coupling thermal-fluidics analysis, fluid-structure interactions for graduate level students interested by Computational fluid Dynamics.
Adding deep section on high-performance computing and parallel processing for large-scale simulations .



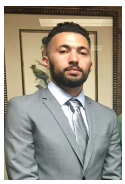
Resources / Science Gateways

- **https://simcenter.designsafe-ci.org/learning-tools/cfd-notebooks/**
- **https://simcenter.designsafe-ci.org/research-tools/cwe-application/**
- **https://theartofhpc.com/**
- **https://access-ci.org/**

Use Cases

- The course is essential for students to bridge the gap between theoretical mathematics and practical problem-solving using computational techniques.
- The course covers fundamental numerical techniques for solving complex mathematical problems that often lack analytical solutions, such as nonlinear equations, differential equations, and large-scale linear systems. By learning these methods, students can tackle real-world engineering and scientific challenges that require approximations and iterative approaches.

Authors



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MORE INFORMATION →
https://hackhpc.github.io/facultyhack-gateways23