

# Dmitrijs Regular Meeting 16-11-2023

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# ToDoS

- Design of the Experiment [Vincenzo]
- Parameters Domain, a range [Dmitrijs]
  - Check batch file parameters:
    - tasks-per-node
    - nodes
- Check the behavior of the parameters [Dmitrijs]
- Normal Distribution for Treatment
- Energy Consumption of sacct [Dmitrijs]
- Setting the Overleaf [Dmitrijs]
- List the resource that we can profile using SLURM [Dmitrijs]



# Experiment Definition

**Type:** Single-Object Study

**Objects:** Haddock

**Three Experiments:** one for each mode

**Dependent Variables:**

- Energy Consumption (J)
- Performance (Utilization)
  - Memory,
  - Network\*,
  - Disk
  - CPU

\*if applicable



# A lot of Independent Variables, less factors

- **SLURM** - #Nodes, #Task-per-node, Topology (**Fixed** following a criteria - Max Available?) \* Only HPC Mode
- **Factors:**
  - Mode: HPC, Local, MPI
    - Local: ncores
  - HPC:
    - queue\_limit
    - concat (Parameter Specific to Haddock)
    - scheduling algorithm
  - MPI: ncores - Does Ncores have the same meaning as local mode?



# Experiment Execution

## Before the Experiment

1. Warm-up run
2. Execute a set of **trials** per treatment
3. **Sleep time:**  $\frac{1}{2}$  -  $\frac{1}{3}$  of the execution time
4. **Treatment Params:** check feasibility
5. Ensure **normality** of the measurements

## Experiment Execution (Auto)

1. 10 - 30 **trials** per **Treatment**
2. Cool Down - Repeat

## Data Analysis

1. Normality Test
2. Comparing among independent/dependent groups

Discussion



# Local/MPI

Workflows	Node	Cores
	GL2	2
Protein-Protein		4
Antibody-Antigen		8
Treatments: 2 * 3	Trials: 60 - 180	



# Local/MPI

Workflows	Node	Cores
	GL6	2
Protein-Protein		4
Antibody-Antigen		8
		16
		32
		<b>Compare with GL2; HW Improvement: CORES Impact</b>
		<b>CORES impact</b>
<b>Treatments: 2 * 5</b>	<b>Trials: 100 - 300</b>	



# HPC Mode

Subject	Scheduling	Queue Limit - Parallelism
		Low
Protein-Protein	Fixed Priority	Medium
Antibody-Antigen	Backfill	
		High
Treatments: 12	Trials: 120 - 360	





# Timeline

- **Deadline** Local Mode: 7th of December



# What's Next?

- Research Design? [Vincenzo]
  - Motivation
  - Related Work
  - Novelty
- Start Experiment
- Start Defining the Template of the Repository
- Other

- ~~Design of the Experiment [Vincenzo]~~
- Parameters Domain, a range [Dmitrijs]
  - Value/Max Value for
    - Tasks-Per- node
    - Nodes = 3/4
    - Topology
- Check the behavior of the parameters [Dmitrijs]
- Energy Consumption of sacct [Dmitrijs] when the computation is distributed
- Setting the Overleaf [Dmitrijs]
- Check if network can be profile with SLURM [Dmitrijs]

- Check how SLURM assigns jobs to cores

```

examples > docking-protein-protein-merged > run.docking-protein-protein-hpc-32-4949 > log
1715 [2023-10-21 12:21:47,038 libhpc INFO] >> rigidbody_30.job running
1716 [2023-10-21 12:21:47,120 libhpc INFO] >> rigidbody_31.job running
1717 [2023-10-21 12:21:47,185 libhpc INFO] >> rigidbody_32.job submitted
1718 [2023-10-21 12:21:47,185 libhpc INFO] >> Waiting... (30.00s)
1719 [2023-10-21 12:22:17,541 libhpc INFO] >> rigidbody_30.job running
1720 [2023-10-21 12:22:17,661 libhpc INFO] >> rigidbody_31.job running
1721 [2023-10-21 12:22:17,720 libhpc INFO] >> rigidbody_32.job submitted
1722 [2023-10-21 12:22:17,720 libhpc INFO] >> Waiting... (30.00s)
1723 [2023-10-21 12:22:48,066 libhpc INFO] >> rigidbody_30.job running
1724 [2023-10-21 12:22:48,175 libhpc INFO] >> rigidbody_31.job running
1725 [2023-10-21 12:22:48,236 libhpc INFO] >> rigidbody_32.job submitted
1726 [2023-10-21 12:22:48,236 libhpc INFO] >> Waiting... (30.00s)
1727 [2023-10-21 12:23:18,660 libhpc INFO] >> rigidbody_30.job running
1728 [2023-10-21 12:23:18,734 libhpc INFO] >> rigidbody_31.job running
1729 [2023-10-21 12:23:18,805 libhpc INFO] >> rigidbody_32.job submitted
1730 [2023-10-21 12:23:18,806 libhpc INFO] >> Waiting... (30.00s)
1731 [2023-10-21 12:23:49,161 libhpc INFO] >> rigidbody_30.job running
1732 [2023-10-21 12:23:49,241 libhpc INFO] >> rigidbody_31.job running
1733 [2023-10-21 12:23:49,333 libhpc INFO] >> rigidbody_32.job submitted
1734 [2023-10-21 12:23:49,333 libhpc INFO] >> Waiting... (30.00s)
1735 [2023-10-21 12:24:19,722 libhpc INFO] >> rigidbody_32.job running
1736 [2023-10-21 12:24:19,723 libhpc INFO] >> Waiting... (30.00s)
1737 [2023-10-21 12:24:50,105 libhpc INFO] >> Batch 1/1 took 2892.19s to finish, 100.00% complete
1738 [2023-10-21 12:24:50,105 __init__ INFO] [rigidbody] CNS jobs have finished
1739 [2023-10-21 12:24:54,060 base_cns_module INFO] Module [rigidbody] finished.
1740 [2023-10-21 12:24:54,060 __init__ INFO] [rigidbody] took 49 minutes and 9 seconds
1741 [2023-10-21 12:24:54,334 __init__ INFO] Running [seletop] module
1742 [2023-10-21 12:24:54,454 __init__ INFO] Module [seletop] finished.
1743 [2023-10-21 12:24:54,454 __init__ INFO] [seletop] took 0 seconds
1744 [2023-10-21 12:24:54,628 __init__ INFO] Running [caprieval] module
1745 [2023-10-21 12:24:55,326 libutil INFO] Selected 7 cores to process 200 jobs, with 7 maximum available cores.
1746 [2023-10-21 12:24:55,327 libparallel INFO] Using 7 cores
1747 [2023-10-21 12:25:11,227 libparallel INFO] >> /capri_ss.1.tsv completed 0%
1748 [2023-10-21 12:25:11,227 libparallel INFO] >> /capri_ss.2.tsv completed 1%
1749 [2023-10-21 12:25:11,227 libparallel INFO] >> /capri_ss.3.tsv completed 2%
  
```



# ToDoS

- Check ncores MPI



# Thanks!

Any Questions?