SOFTWARE AND SUSTAINABILITY
S2 RESEARCH GROUP

Dmitrijs Regular Meeting 16-11-2023

Vincenzo Stoico @ GreenLab
PostDoctoral Researcher
v.stoico@vu.nl

VU VRIJE UNIVERSITEIT AMSTERDAM

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**: ½ - ⅓ 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
Treatments: 2 * 5	**Trials: 100 - 300**	

Compare with GL2; HW Improvement: CORES Impact

CORES impact

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?

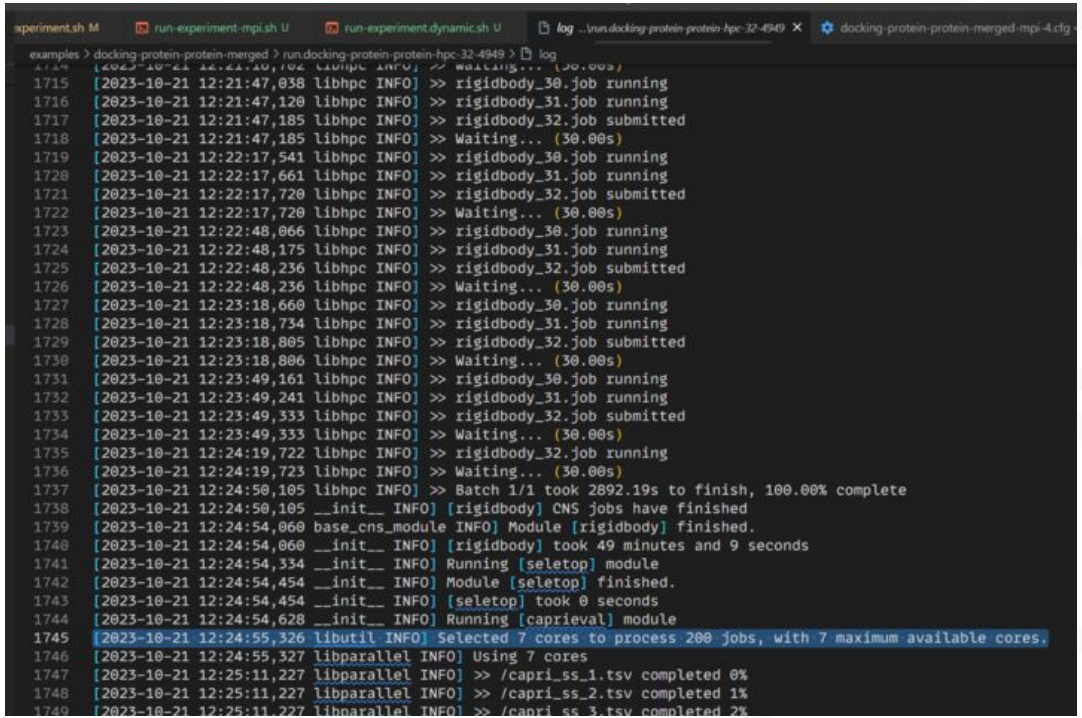
- Research Design? [Vincenzo]
  - Motivation
  - Related Work
  - Novelty
- Start Experiment
- Start Defining the Template of the Repository
- Other

ToDos

- ~~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]

ToDos

- Check how SLURM assigns jobs to cores



ToDos

- Check ncores MPI

Thanks!

Any Questions?

SOFTWARE AND SUSTAINABILITY
S2 RESEARCH GROUP

VU VRIJE UNIVERSITEIT AMSTERDAM