

Condor: a cheap HPC

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30 September 2020

Condor: what is it

- A **batch** processing system
- Use **idle time** on desktop computers

Advantages

- Cheap , we all need desktops
- No extra hardware needed
- No large server rooms needed
- Restart jobs when they fail
- Development environment is identical to desktop.
- Output files directly available on desktop.

What it is not good for

- **Fast interconnect** .
- Processes that needs to be **distributed** over several servers
- Jobs requiring a **huge amount of RAM** .

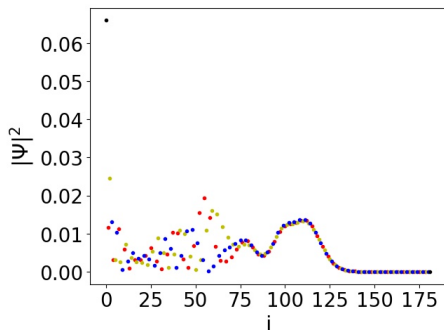
Condor clusters are **complementary** to HPCs like **Hamilton** .

Requirements

- A fully managed environment.
- All desktops to have identical software and libraries.

Example 1: Polaron Transfer

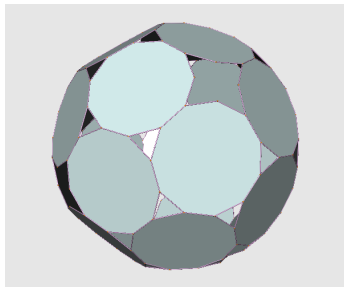
- Energy transfer across a cell membrane protein (alpha-helix)
- Scan 9 unknown model parameters
- Submit **5 millions** jobs over a few weeks



Polaron Transfer

Example 2: Impossible Geometries

- Protein cage: 24 regular hendecagon (11-edges polygon)
- Known to be **impossible mathematically**
- Possible if one deforms some edges and corner by up to 0.5%
- [Nature 569 \(2019\) 438-442](#) : *An ultra-stable gold-coordinated protein cage displaying reversible assembly.*



Question : Find other similar cages

Method : Scan a very large number of geometries.

Conclusions

Condor

- is a **powerful** tool
- is **cheap**
- **easy** to use