## Aldolase results

Relevant jobs are shown in the files flowchart\_\*.pdf

Jobs in red were not in the final workflow, but are included for the timing data.

Compute nodes used are at top of run.err. Then use “sinfo -Nel | grep cn488”

Scarf18,scarf19 are Gold 6126 (Skylake)

Scarf14-17 are Intel E5-2650 (Broadwell, Haswell, Ivy Bridge)

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| --- | --- | --- | --- | --- | --- | --- |
| **Job ID** | **Description** | **Where run** | **MPI/th/GPU** | **Runtime** | **Data produced** | **Notes** |
| job001 | Import | interactive | n/a | negligible | 1 MB | Links to 337 **GB** in Movies |
| job005 | Motion correction | cn488 (scarf15) | 1 / 12 / 0 | Not recorded | 113 **GB** | No GPU for Relion implementation |
| job007 | CtfFind | cn880 (scarf18) | 12 / 0 / 0 | 2m:03s | 3 **GB** | Ctffind not GPU |
| job009 | Select | interactive | n/a | negligible | 2 MB |  |
| job013 | Reference import | interactive | n/a | negligible | 32 MB |  |
| job022 | Autopick | cn793 | 16 / 0 / 0 | 2h:59m:50s | 219 MB |  |
| job024 | Extract 4x | 4xcn778 () + 9xcn833 () + 3xcn884 () | 16 / 0 / 0 | 20m:01s | 58 **GB** | 749k particles extracted |
| job025 | Class2D | 1xcn630 + 4xcn657 + 4xcn658  (scarf17) | 9 / 6 / 0 | 27h:16m:56s | 12 **GB** | 100 2D classes |
| job026 | Select | interactive | n/a | negligible | 262 MB |  |
| job028 | Reference import | interactive | n/a | negligible | 11 MB |  |
| job029 | Refine3D | 3xcn659 + 3xcn663 + 3xcn664  (scarf17) | 9 / 6 / 0 | 2 days (timeout) | 4 **GB** | 12/25 cycles completed (aborted) |
| job030 | Refine3D | cn2g16 | 5 / 1 / 4 | 16h:16m:11s | 7 **GB** | Repeat 29 with GPU |
| job031 | Extract 2x | 12xcn540 + 4xcn648 | 16 / 0 / 0 | 18m:45s | 137 **GB** | 451k particles extracted |
| job032 | Select | interactive | n / a | negligible | 269 MB |  |
| job033 | Reference import | interactive | n /a | negligible | 80 MB |  |
| job034 | Class3D | cn2g19 | 5 / 1 / 4 | 7h:29m:03s | 16 **GB** | Poor result |
| job036 | Class3D | cn2g19 | 5 / 1 / 4 | 7h:28m:54s | 16 **GB** | Poor result |
| job037 | Refine3D | cn2g19 | 5 / 1 / 4 | 22h:55m:54s | 10 **GB** | Not used |
| job038 | MaskCreate | interactive | n / a | negligible | 80 MB |  |
| job039 | Class3D | cn2g19 | 5 / 1 / 4 | 7h:57m:26s | 16 **GB** | 4 3D classes |
| job042 | Select | interactive | n / a | negligible | 131 MB |  |
| job043 | Refine3D | cn2g16 | 5 / 1 / 4 | 13h:32m:01s | 7 **GB** |  |
| job048 | MaskCreate | interactive | n/a | negligible | 80 MB |  |
| job049 | PostProcess | interactive | n/a | negligible | 159 MB |  |
| job050 | CtfRefine | cn497 | 1 / 12 / 0 | 1h:07m:55s | 3 GB |  |
| job051 | Refine3D | cn2g16 | 5 / 1 / 4 | 13h:24m:24s | 8 GB |  |
| job052 | CreateMask | interactive | n/a | negligible | 80 MB |  |
| job053 | PostProcess | interactive | n/a | negligible | 159 MB |  |
| job054 | Extract 1x | cn307 (scarf14) | 16 / 0 / 0 | 1h:06m:49s | 263 **GB** | 219k particles extracted |
| job055 | Reference import | interactive | n/a | negligible | 627 MB |  |
| job056 | Select | interactive | n/a | negligible | 131 MB |  |
| job057 | Refine3D | cn2g28 | 5 / 1 / 4 | 37h:03m:32s | 35 GB |  |
| job058 | CreateMask | interactive | n/a | negligible | 627 MB |  |
| job059 | PostProcess | interactive | n/a | negligible | 1 GB |  |
| job061 | Polish (train) | cn548 | 1 / 12 / 0 | 6h:08m:16s | 736 kB |  |
| job068 | Polish (do) | cn289-291 | 3 / 16 / 0 | 9h:27m:04s | 265 **GB** |  |