Condensed matter physics

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Need

Our group has ~ 4 people doing electronic structure
  calculations

- Parallelized using MPI

- Infiniband network (low latency c.f. Gigabit Ethernet)

- Memory >= 2 GB / core

- Disk >= 200 GB/user

Typical jobs: 8-32 cores for 24 h.

Bionano Linux cluster in Kalmar

- Funded by Sparbanksstiftelsen (Carlo, Alf)
- 4x 8 core intel Xeon, 2GB/core, gigabit ethernet
- 1TB disk (backed up nightly)
- Installed 2009 , downtime a few days due to power loss
- 50 % use (Physics, Biology, Chemistry)
- Good
  - Local cluster for testing, Cheap
  - Ability to run tests outside que system
  - Still competitive cores
- Bad
  - Old software (can be upgraded)
  - Disks will not survive forever (50000 h, no errors)

Lunarc (Lund)

For production runs:

- >2000 cores, >= 2GB/core, infiniband

- Medium application 80000 core hours/month for our group

- Good

  - Easy to get allocation

  - Access to large amounts of cores

- Bad

  - No access to local nodes for debuging

  - Que time larger than bionano

Our needs

Small local cluster for testing / development

Large resources but infrequently served well by Lunarc