4. Electronic structure

Weine Olovsson
National Supercomputer Centre (NSC)
Fridays @IFM Fysikhuset F306

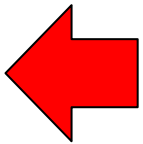
LINKÖPING UNIVERSITY

NSC

Electronic structure software

Different purposes, roughly categories below:

- Density functional theory (DFT), “solid state”
  - VASP
  - Quantum Espresso
- Quantum Chemistry
  - Gaussian
  - NWChem
- Molecular Dynamics (MD)
  - LAMMPS
  - GROMACS



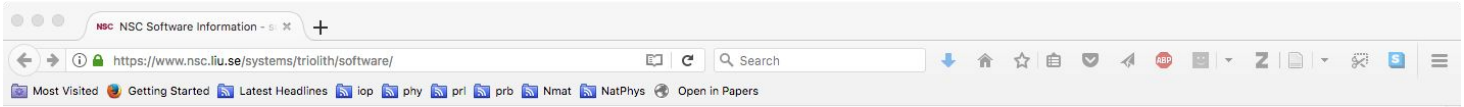
Focus for this session!

- Bulk
- Surfaces, interfaces
- Clusters

Example of DFT software used at NSC:

Software	Basis set	License	Comment
VASP	PAW	cost	popular
Quantum Espresso	pp, PAW	free	many tools
Abinit	pp, PAW	free	
WIEN2k	FPLAPW	cost	XSPEC, TELNES
GPAW	PAW	free	
exciting	FPLAPW	free	BSE, TDDFT
Elk	FPLAPW	free	BSE, TDDFT
Siesta	pp	free	
SPRKKR	KKR	free (register)	spectroscopy
CASTEP	pp	cost	ELNES

https://www.nsc.liu.se/systems/triolith/software/triolith-software-apps.html



NSC

National Supercomputer Centre at Linköping University

NSC / Systems / Triolith / software

triolith

Software installations

devel-tools

allinea-DDT
allinea-MAP
allinea-reports
gcc
intel
openmpi
tau

apps

abinit
abyss
almabte
amber
ansys
arcimboldo_lite
arpack
ase

Basic software documentation at NSC

Directory list:

Version	Description
apps	**installation directory for scientific software and libraries**
devel-tools	**Different compilers, math libraries, mpi etc**

How it works

Software installed by NSC staff for general usage is found in /software/apps/ and its subdirectories. We use an hierarchical scheme like this:

```
/software/apps/[program name]/[version]/[installation name]/
```

It means, for example, that the binary distribution of Gaussian 09 Rev. C01 is installed in:

```
/software/apps/gaussian/G09RevC.01/bdist/
```

In order to provide some minimal documentation, each directory contains a "README.NSC" file with important information about this particular installation and how to run the program. So for the above version of Gaussian, you have three relevant files to read for a quick start:

```
/software/apps/gaussian/README.NSC
/software/apps/gaussian/G09RevC.01/README.NSC
/software/apps/gaussian/G09RevC.01/bdist/README.NSC
```

The first one contains information about Gaussian in general, the second one contains information about G09 Rev. C01 version, and the third one contains notes about that particular installation/compilation.

There is a also a web version based of the content of these files, with much prettier formatting. You may look at it here:

Example of day-to-day tools

- less / vi — reading/editing files
- grace / gnuplot — plotting tools
- Bash — simple scripts
- cif2cell — convert from .cif
- p4vasp — analysis of VASP output
- xcrysden / vesta — view structure
- VNL — create/view structure

Useful for building structures!

Also of interest:

- Python / R — analysis etc. (check out e.g. using jupyter)
- ASE — different tools and Python modules

https://www.nsc.liu.se/systems/triolith/software/triolith-software-apps.html

VASP

Background

- DFT, **post-DFT** (HSE06, GW, …), Born-Oppenheimer MD
- PAW method
- Widely used in academia and industry
- 20-25% of Triolith usage

https://www.vasp.at/ https://www.nsc.liu.se/systems/triolith/software/triolith-software-apps-vasp.html

triolith

Software installations

devel-tools

allinea-DDT
allinea-MAP
allinea-reports
gcc
intel
openmpi
tau

apps

abinit
abyss
almabte
amber
ansys
arcimboldo_lite
arpack
ase

VASP installations at NSC

Directory list:

Version	Description
4.6.36-17Feb09	VASP 4.6.36 (2009-02-17)
5.2.12-11Nov11	VASP 5.2.12 (2011-11-11)
5.3.2-13Sep12	VASP 5.3.2 (2012-09-13)
5.3.3-18Dec12	VASP 5.3.3 (2012-12-18)
5.3.5-01Apr14	VASP 5.3.5 (2014-03-31)
5.4.1-05Feb16	VASP 5.4.1 (2016-08-09)
5.4.1-24Jun15	VASP 5.4.1 (2015-07-24)
5.4.4-18Apr17	VASP 5.4.4 (2017-04-18)
omp-beta-13Mar17	VASP OpenMP Beta (2017-03-13)

Level of support

Tier 1 NSC has at least one application expert on staff with knowledge about this software, and we will try to help you with any problems. We have also ran some internal tests to make sure that the program is working as intended. NSC also commits to installing updates to this program as they become available.

Please see the page describing our software support categories for more information.
You can also contact support@nsc.liu.se for further information.

triolith

Software installations

devel-tools

allinea-DDT
allinea-MAP
allinea-reports
gcc
intel
openmpi
tau

apps

abinit
abyss
almabte
amber
ansys
arcimboldo_lite
arpack
ase

VASP 5.4.4 - Apr 18 2017

Directory list:

Version	Description
build02	Optimized version of 5.4.4.

Level of support

Tier 1 NSC has at least one application expert on staff with knowledge about this software, and we will try to help you with any problems. We have also ran some internal tests to make sure that the program is working as intended. NSC also commits to installing updates to this program as they become available.

Please see the page describing our software support categories for more information.
You can also contact support@nsc.liu.se for further information.

The source code for this version was downloaded from the VASP home page on 2017–04–24.

The release notes can be found at this link.

Changes in this version:

- Bugfixes and stability enhancements.
- SCAN metaGGA functional, SCAN+rVV10.
- Improvements for GPU port.

triolith

Software installations

devel-tools

allinea-DDT
allinea-MAP
allinea-reports
gcc
intel
openmpi
tau

apps

abinit
abyss
almabte
amber
ansys
arcimboldo_lite
arpack
ase

VASP 5.4.4 (Build 02)

Level of support

Tier 1 NSC has at least one application expert on staff with knowledge about this software, and we will try to help you with any problems. We have also ran some internal tests to make sure that the program is working as intended. NSC also commits to installing updates to this program as they become available.

Please see the page describing our software support categories for more information.
You can also contact support@nsc.liu.se for further information.

Installed by Weine Olovsson on 2017–04–27.

Description

This is VASP for Triolith, built with the Intel 2017 suite of Fortran compiler, MKL, and MPI ("buildenv-intel/2017"). It mostly follows previous recipe for NSC VASP installations by Peter Larsson. Changes compared to the original settings are:

- Enabling of the LONGCHAR option, which lets you specify INCAR tag values longer than 255 characters, e.g. indidvidual magnetic moments for all atoms in a cell.
- Set MPI_BLOCK to 64k (it improvements MPI performance).
- Hard-coded path to the vdw_kernel.bindat file. It is read from /software/apps/vasp/5.3.5–01Apr14 /vdw_kernal.bindat automatically, so that you don't need to have the file in the working directory.
- Compiled with -DnoSTOPCAR, so you cannot stop calculations inside an SCF loop using STOPCAR. This reduces the load on the parallel file system, and you can always stop a calculation using the SLURM `scancel` command.

INCAR parameters

- ENCUT - plane wave energy cutoff
- ALGO - wavefunction optimization
- NBANDS - if not set, auto-determined
- NSIM - for RMM-DIIS algorithm (ALGO)
- NCORE or NPAR - bands treated in parallel
- KPAR - k-point parallel

INCAR parameters

- ENCUT - plane wave energy cutoff **Recommended to set!**
- ALGO - wavefunction optimization
- NBANDS - if not set, auto-determined **Must be the same for Etot comparison!**
- NSIM - for RMM-DIIS algorithm (ALGO)
- NCORE or NPAR - bands treated in parallel
- KPAR - k-point parallel

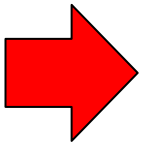
Consider hardware...

- **Triolith** (NSC), Intel Xeon E5-2660 2.2GHz
  - 1 node = 16 cores (32 GB RAM)
- Beskow (PDC), Cray XC40, Intel Xeon E5v3 2.3GHz
  - 1 node = 32 cores (64 GB RAM), no local disk; use 24 cores/node
- Kebnekaise (HPC2N)
  - 1 node (Intel Xeon E5-2690v4) = 28 cores (128 GB RAM)
  - + 2xGPU (NVidia K80) ⟸ **vasp-gpu version**
  - 1 KNL (Intel Xeon Phi 7250) node = 68 cores (192 GB RAM)

} ***different best practices!***

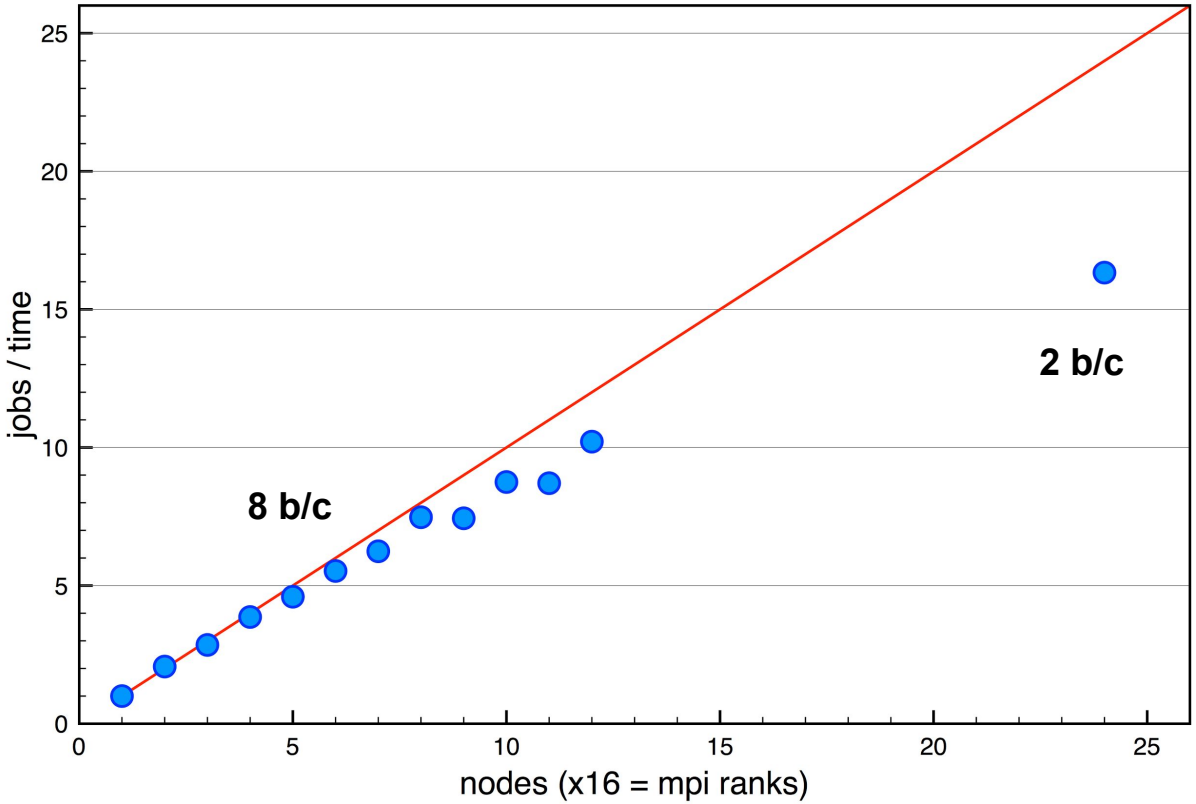
How many cores? Efficient and/or fast?

- Start from number of bands, **NBANDS**
- 1 band/core: usually doesn't work well
- 2 bands/core: ~50% parallel efficiency
- 8 bands/core: good starting point



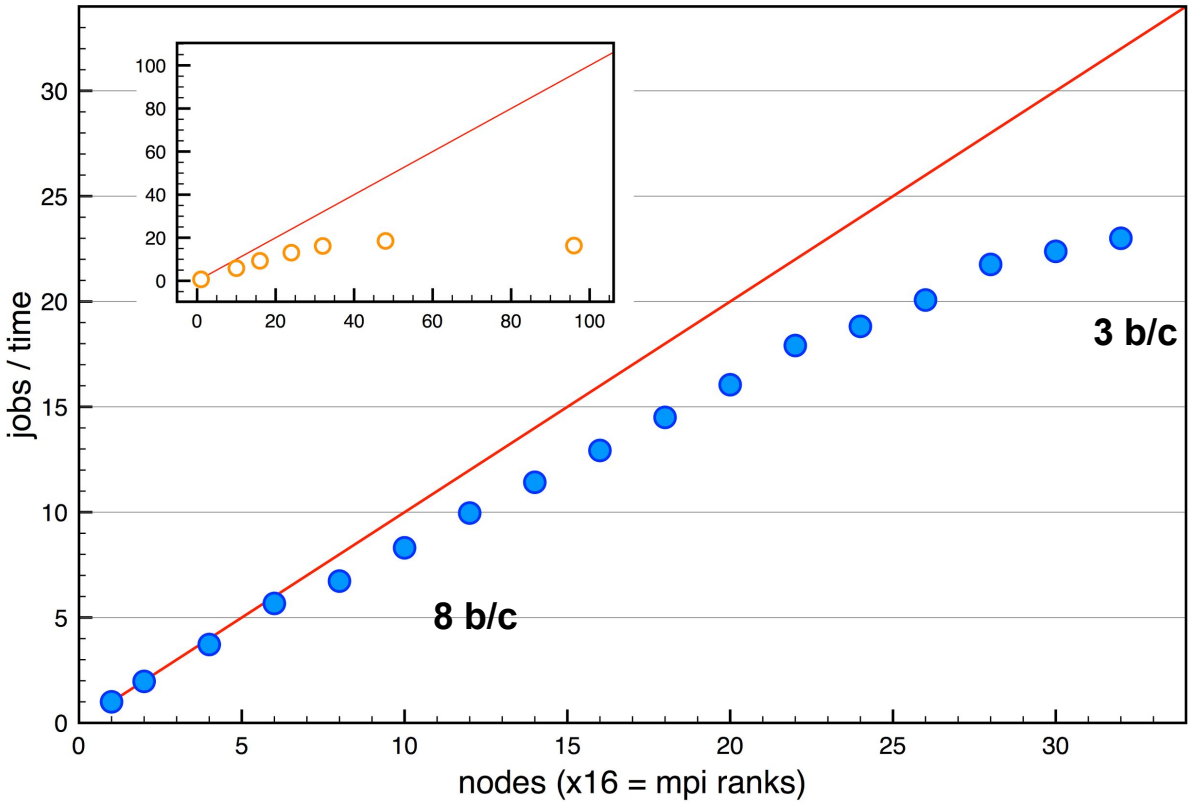
Test with **cores ≈ NBANDS / 8**

Si-H/Ag(111) 129 atoms, VASP PBE



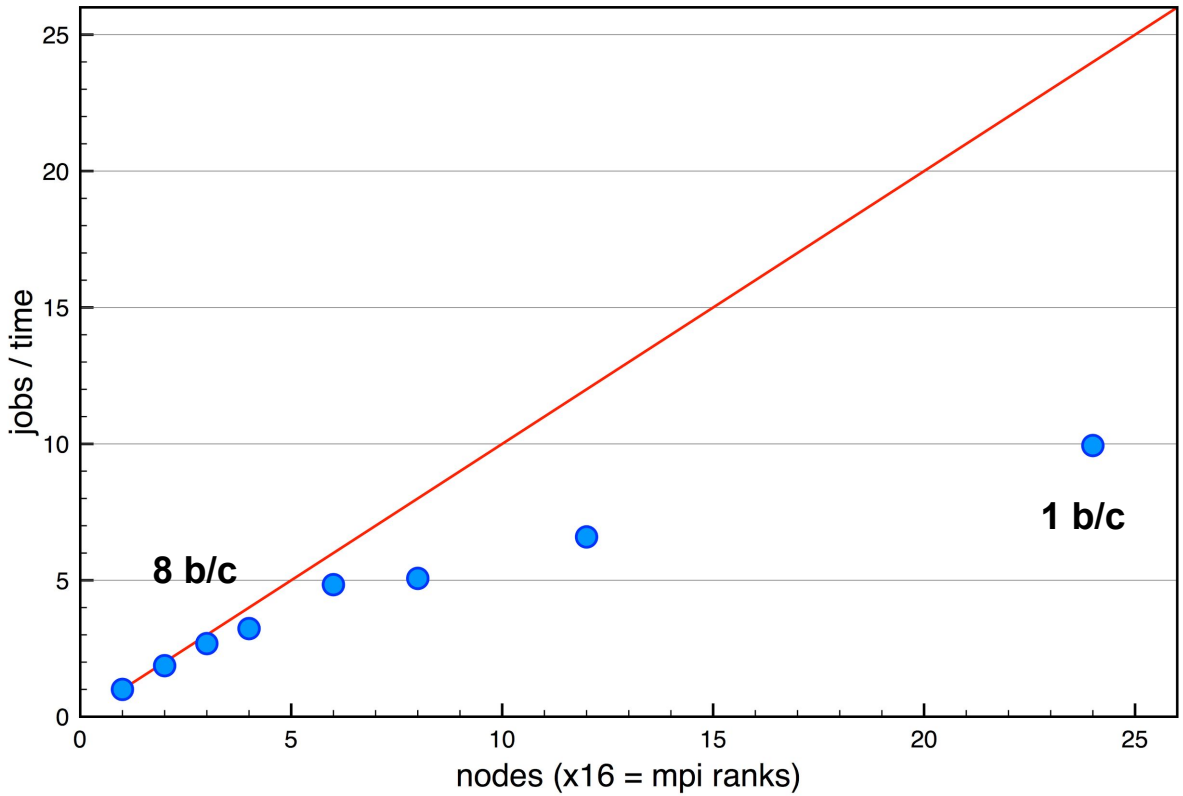
NBANDS = 750
4 k-points

GaAsBi 512 atoms, VASP PBE



NBANDS = 1536
4 k-points

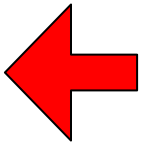
GaAsBi 128 atoms, VASP HSE06



NBANDS = 384
12 k-points

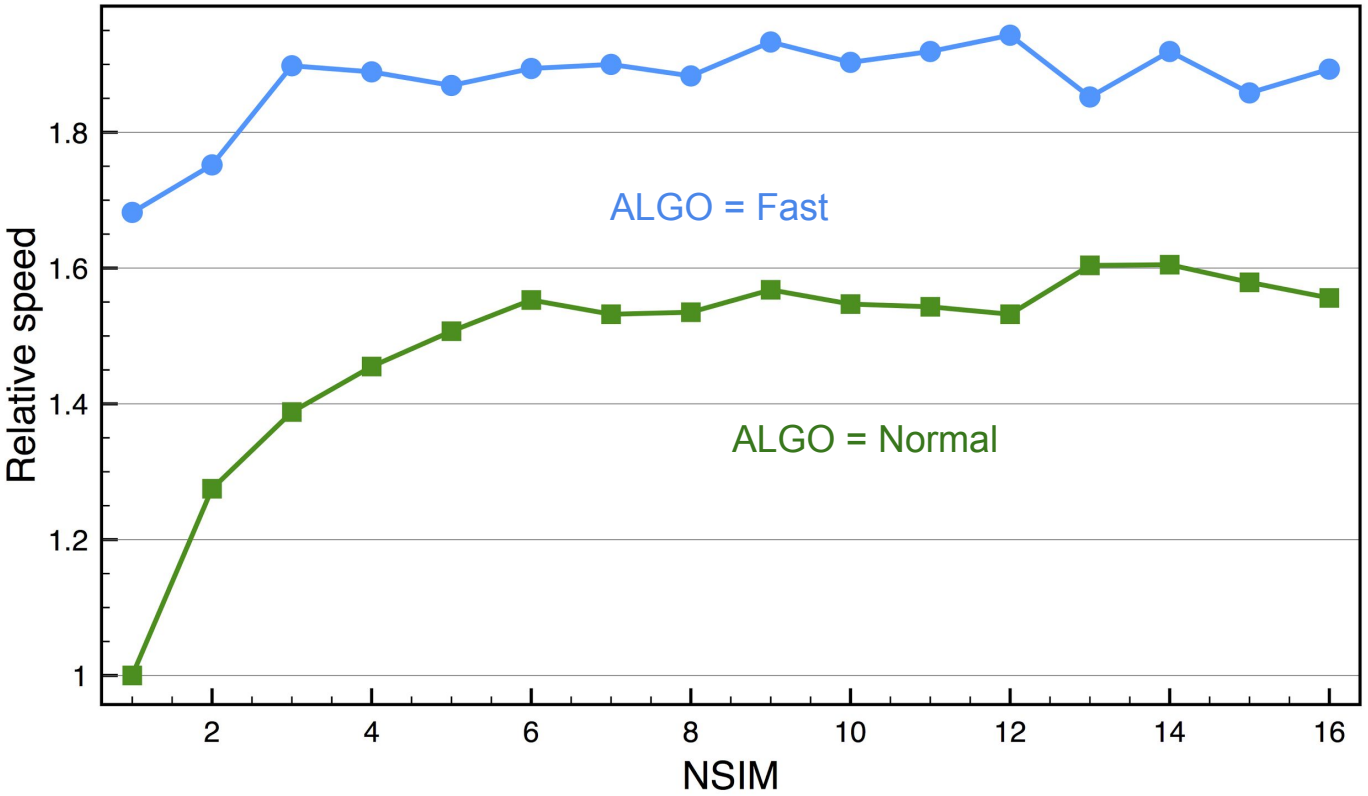
NSIM

- Blocking mode for RMM-DIIS algorithm
- ALGO = Fast / VeryFast
- ALGO = Normal (Davidson algorithm)
- Not for hybrid-DFT (Damped, All, Normal)
- NSIM = 4 (default)



“Usually good”

Si-H/Ag(111) 129 atoms VASP PBE



NBANDS = 750
4 k-points

NCORE / NPAR

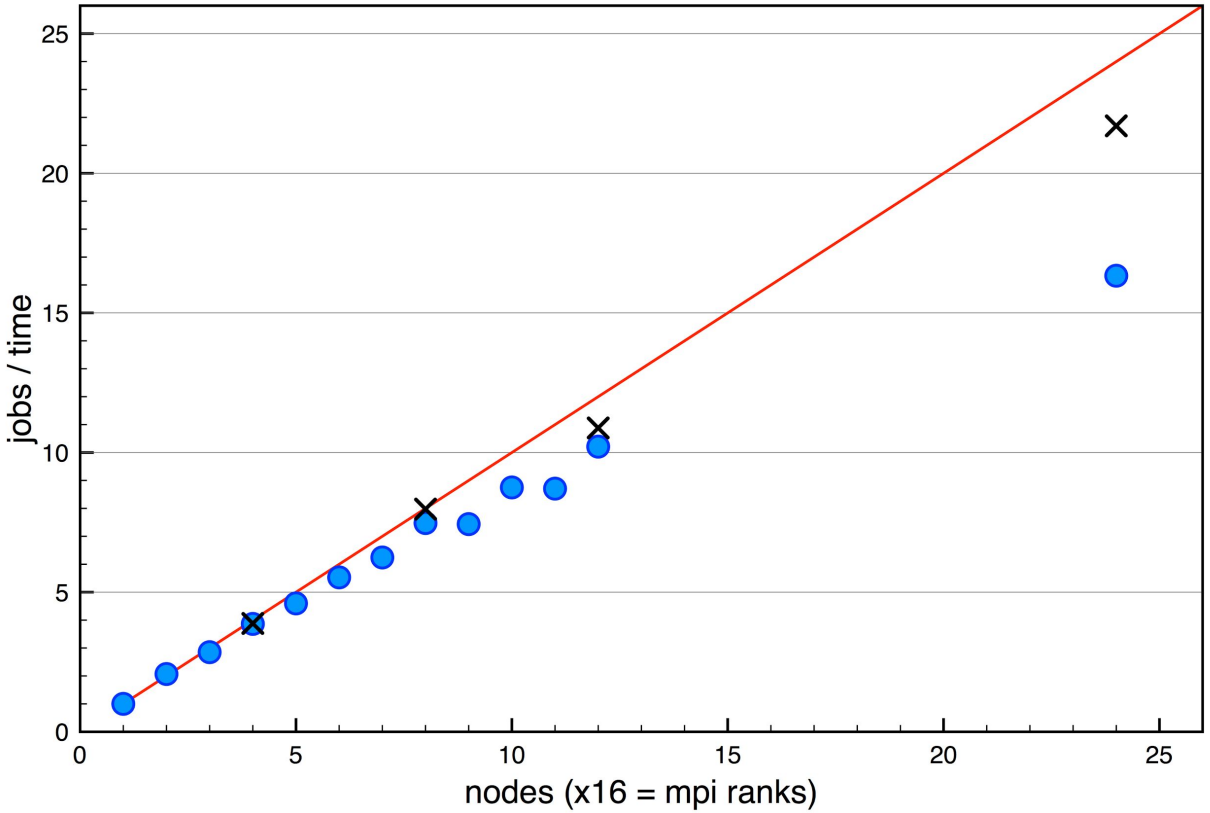
- Cores per orbital / bands treated in parallel
- Davidson & RMM-DIIS algorithm
- ALGO = Normal, Fast, VeryFast
- NPAR = 1, saves memory
- NPAR = number of compute nodes (x2)
- NCORE = cores per compute node (or socket)

I find it easier to stick with NCORE, e.g. on Triolith,
NCORE = 16

KPAR

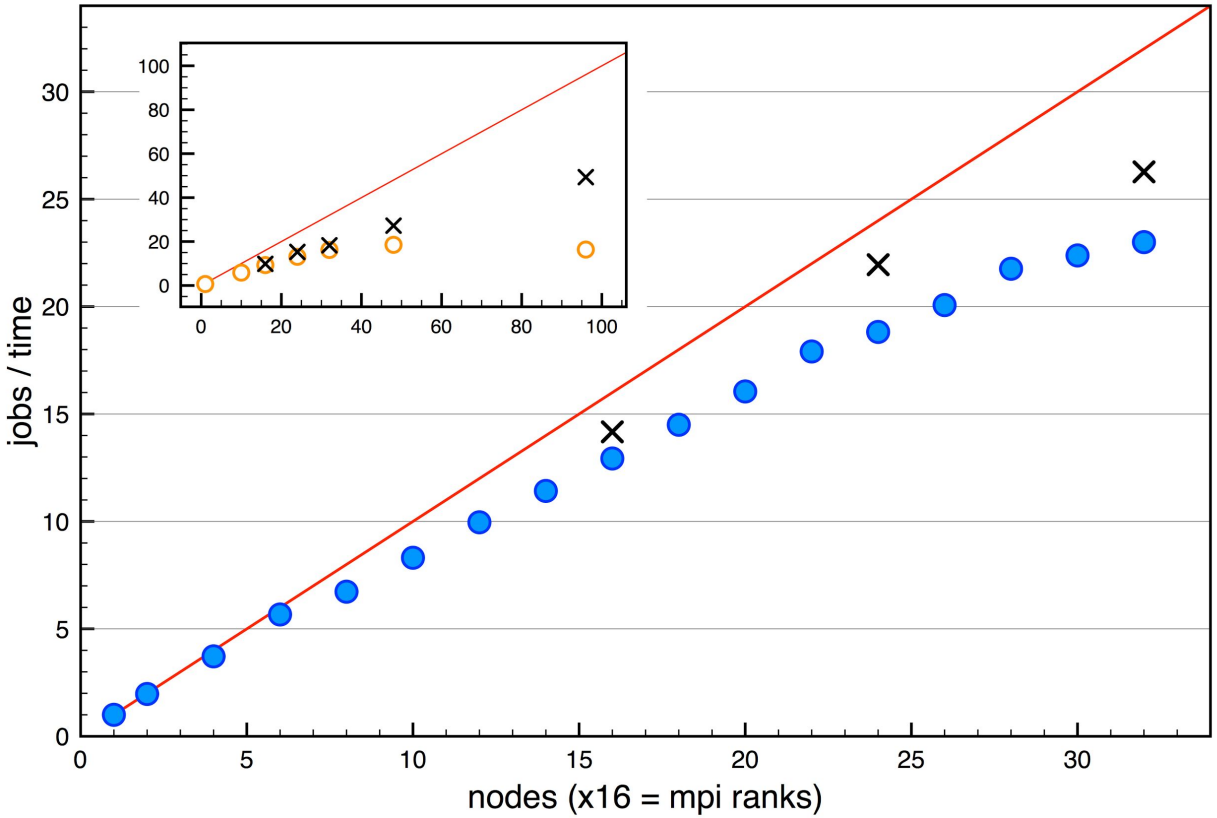
- KPAR = number of k-points treated in parallel
- Good for **hybrid-DFT** runs
- Increase cores at least x2
- Try **KPAR = min (nodes, k-points)**

Si-H/Ag(111) 129 atoms, VASP PBE



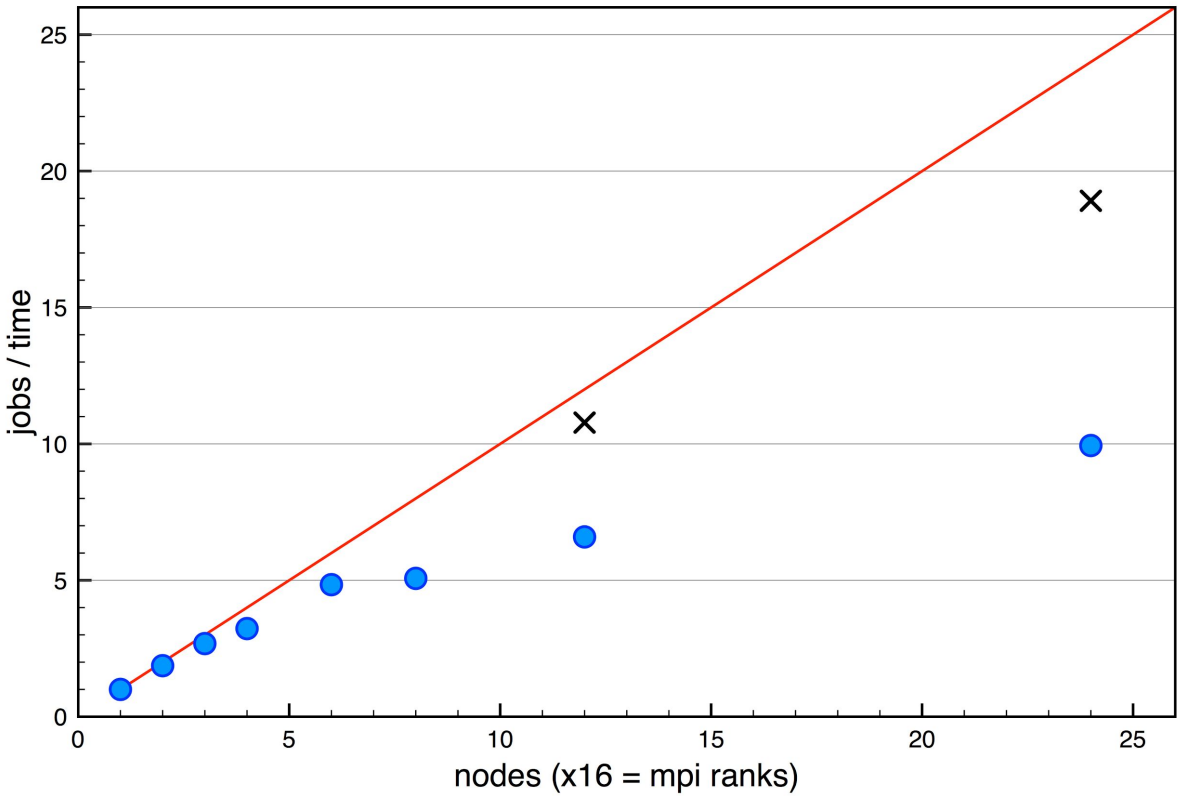
NBANDS = 750
4 k-points

GaAsBi 512 atoms, VASP PBE



NBANDS = 1536
4 k-points

GaAsBi 128 atoms, VASP HSE06



NBANDS = 384
12 k-points

Summary, “rules of thumb”

- Job size (max): total cores ≈ NBANDS / 8
- NSIM = 4 (default), typically OK
- NCORE = cores/node (16 on Triolith)
- KPAR = min (nodes, k-points)
    - In particular useful for **hybrid-DFT**
- In general, INCAR default settings are OK
- GPU: important to increase NSIM

VASP6: beta release

- Binaries soon available to license holders at NSC!
- General release in future
- OpenMP and MPI
  - General improvement of speed
  - Better scaling over many nodes

https://cug.org/proceedings/cug2017_proceedings/includes/files/pap134s2-file2.pdf

Resources

- Manual
  Read all (really)!
- Wiki
  Examples, tutorials
- Forum
  Check for your question
- Peter Larsson's NSC blog
  - Discussion on running VASP etc.

Find the links at:

https://www.vasp.at/

https://www.nsc.liu.se/~pla/ https://www.nsc.liu.se/systems/triolith/software/triolith-software-apps-vasp.html

Typical questions to support@nsc.liu.se

- Complicated INCAR…
- Structure (POSCAR)
- k-mesh (KPOINTS)
- NCORE/NPAR, KPAR
- VASP version
- Cores
- Memory

https://www.nsc.liu.se/support/

Typical questions to support@nsc.liu.se

- Complicated INCAR… simplify & try again
- Structure (POSCAR) reasonable/correct?
- k-mesh (KPOINTS) Gamma-centered?
- **NCORE**/~~NPAR~~, KPAR simplify!
- VASP version try latest! `$module add vasp/5.4.4-18Apr17`
- Cores too few/many?
- Memory larger memory nodes: reduce cores/node:
  - ENCUT, k-mesh `#SBATCH -C fat` `#SBATCH --ntasks-per-node=8`

https://www.nsc.liu.se/support/

Quantum Espresso

triolith

Software installations

devel-tools

allinea-DDT
allinea-MAP
allinea-reports
gcc
intel
openmpi
tau

apps

abinit
abyss
almabte
amber
ansys
arcimboldo_lite
arpack
ase

Quantum Espresso installations at NSC

Directory list:

Version	Description
4.3.2	Quantum Espresso 4.3.2
5.0	Quantum Espresso 5.0
5.0.1	Quantum Espresso 5.0.1
5.0.2	Quantum Espresso 5.0.2
5.0.3	Quantum Espresso 5.0.3
5.1	Quantum Espresso 5.1
5.2.0	Quantum Espresso 5.2.0
5.2.1	Quantum Espresso 5.2.1
5.3.0	Quantum Espresso 5.3.0
5.4.0	Quantum Espresso 5.4.0
6.0	Quantum Espresso 6.0
6.1	Quantum Espresso 6.1

Level of support

Tier 2 NSC has only limited experience with this software, but we will try to help as much as possible. We have ran

triolith

Software installations

devel-tools

allinea-DDT
allinea-MAP
allinea-reports
gcc
intel
openmpi
tau

apps

abinit
abyss
almabte
amber
ansys
arcimboldo_lite
arpack
ase

Quantum Espresso 6.1

Directory list:

Version	Description
build01	Intel compilers, no OpenMP, including EPW, WEST, Yambo
build02	Intel compilers, no OpenMP, including EPW, WEST, Yambo

Level of support

Tier 2 NSC has only limited experience with this software, but we will try to help as much as possible. We have ran some tests, for example, if the program comes with a test suite, but they may be far from exhaustive. We will try to install and test new versions, as soon as we can.

Please see the page describing our software support categories for more information.
You can also contact support@nsc.liu.se for further information.

Note that the Quantum Espresso installation includes the EPW (Electron-Phonon Wannier) code.

Also provided are WEST (Without Empty STates) for GW calculations and Yambo for Bethe-Salpeter equation calculations.

The source code was downloaded from the QE home page in March 2017.

Here below are release notes for QE 6.1 as listed:

New in 6.1 version:

- Hybrid functionals: Band parallelization over pair of bands, contributed by Taylor Barnes et al, http://dx.doi.org/10.1016/j.cpc.2017.01.008

triolith

Software installations

devel-tools

allinea-DDT
allinea-MAP
allinea-reports
gcc
intel
openmpi
tau

apps

abinit
abyss
almabte
amber
ansys
arcimboldo_lite
arpack
ase

Quantum Espresso 6.1 with EPW, WEST and Yambo build01

Level of support

Tier 2 NSC has only limited experience with this software, but we will try to help as much as possible. We have ran some tests, for example, if the program comes with a test suite, but they may be far from exhaustive. We will try to install and test new versions, as soon as we can.

Please see the page describing our software support categories for more information.
You can also contact support@nsc.liu.se for further information.

This is a first installation of Quantum Espresso 6.1 using Intel compiler, MKL, and Intel MPI, essentially following the same recipe as earlier installations. No OpenMP support. The maximum number of allowed k-points was increased to 150,000 in `Modules/parameters.f90`.

Several other software packages are optional to install together with QE. In this build, EPW, WEST, Yambo, qe-gipaw and wannier90 are made available.

How to run

Launch your desired QE binary with mpprun, for example to run `pw.x`:

```
mpprun /software/apps/espresso/6.1/build01/bin/pw.x -input file.in
```

Installation

The following modules was used:

Quantum Espresso

- DFT, Car-Parinello MD
- pseudopotentials (different choices)
- Popular for e.g. phonon calculations
- Open source, frequently updated
- Interface with Schrödinger suite
  - Workshop in Linköping 16th Nov 2017

License for our Academic users!

SCHRÖDINGER MATERIALS

http://www.quantum-espresso.org/ https://www.nsc.liu.se/systems/triolith/software/triolith-software-apps-espresso.html

Caveats

- Common issue:

```
mpprun pw.x < job.in > job.out
```

crash?!

```
mpprun pw.x -inp job.in > job.out
```

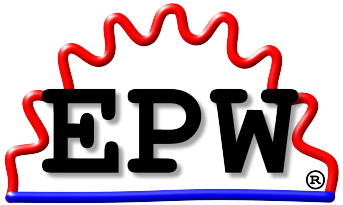
use instead!

- **Be careful with I/O!**
  - `pw.x` - use default settings
  - `ph.x` - phonons, use **local** scratch disks

See NSC website for setting things up!
Beskow: no local scratch disks!

https://www.nsc.liu.se/systems/triolith/software/triolith-software-apps-espresso-6.1.html

QE installed together with:



EPW: electron-phonon interaction using Wannier functions

WEST: large scale GW calculations

Yambo: optics from BSE

https://www.nsc.liu.se/systems/triolith/software/triolith-software-apps-espresso.html

Virtual NanoLab (VNL)

Building structures with VNL

- Build supercells, surfaces, interfaces, …
  - Examples and tutorials available
- 2 concurrent licenses at NSC
  - VASP functionality with the paid license
  - Free academic free license win/linux/(mac)
- Easier to use via remote desktop, **ThinLinc**

recommended

```
$ module add vnl/2017.0
$ vnl &
```

https://quantumwise.com/products/vnl