Electronic Structure Workshop, Spring 2017

Weine Olovsson

@Linköping University, Wednesday 29th March 2017

National Supercomputer Centre in Linköping Sweden

Introduction

- *Welcome!*
- Presentations from **SNIC** Application Experts
- Free discussion (not lunch, though coffee)
- Future: softwares/topics of interest?

https://www.nsc.liu.se/support/Events/EIstruct_workshop2017

VASP

National Supercomputer Centre in Linköping Sweden

Background

http://vasp.at/

- DFT, post-DFT (HSE06, GW, …), BO-MD
- PAW-method
- widely used in Academia/Industry
- 20-25% of Triolith usage

National Supercomputer Centre at Linköping University

triolith
Software installations

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

apps
abinit
abyss
amber
ansys
arcimboldo_lite
arpack
ase
atk
atompaw
avogadro
bazaar
beagle
blast
boost
caffe
castep
ccp4
cdo
CESM
cmor

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)
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.

The VASP installations are generally maintained by Peter Larsson (pla@nsc.liu.se).

OBS: *you need to have license for using VASP, for how to get access to the NSC installed versions, follow this link.*

Naming scheme for binaries

It is customary to produce several versions of VASP. The following naming scheme is used at NSC:

Name	Description
vasp	Softlink to vasp-half
vasp-half	vasp compiled with -DNGZhalf, "normal" version for bulk system
vasp-gamma	compiled with -DNGZhalf and -DwNGZhalf, gamma-point only (big supercells or clusters)

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VASP 5.4.1 - Feb 05 2016

Directory list:

Version	Description
build01	Optimized version of 5.4.1 05Feb16 with bugfix patch 2.
build02	Change in compiler options due to memory leak problem
build03	VASP with Wannier90

Level of support

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OBS: fix for memory leaks due to compiler settings from `build02` and onwards

The source code for this version was downloaded from the VASP home page on 2016–08–08 (including the bug fix patch #2).

The news in this version is the port for GPU accelerated hardware. At NSC, the GPU version can be found at /software /apps/vasp-gpu.

For full information see the release notes.

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VASP 5.4.1 05Feb16 (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.

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Installed by Weine Olovsson on 2016–09–30.

Description

Fix due to memory leaks problem

Change in the compiler option which enforces data alignment to 256-bit, now setting in makefile.include:

```
FFLAGS     = -assume byterecl -align dcommons -align rec32byte
```

It was found that the option `-align array32byte` leads to large memory leaks. The VASP default is `FFLAGS = -assume byterecl`.

Otherwise similar to previous `build01`.

INCAR parameters

- ENCUT - plane wave energy cutoff
- ALGO - wf optimisation
- 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 - wf optimisation
- 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

Hardware

- **Triolith** (NSC), Intel Xeon E5-2660 2.2GHz

  1 node = 16 cores (32GB RAM)

- **Beskow** (PDC), Cray XC40, Intel Xeon E5v3 2.3GHz

  1 node = 32 cores (64GB RAM), no local disk; use 24 cores/node

- **Kebnekaise** (HPC2N)

  1 node (Intel Xeon E5-2690v4) = 28 cores (128GB RAM)

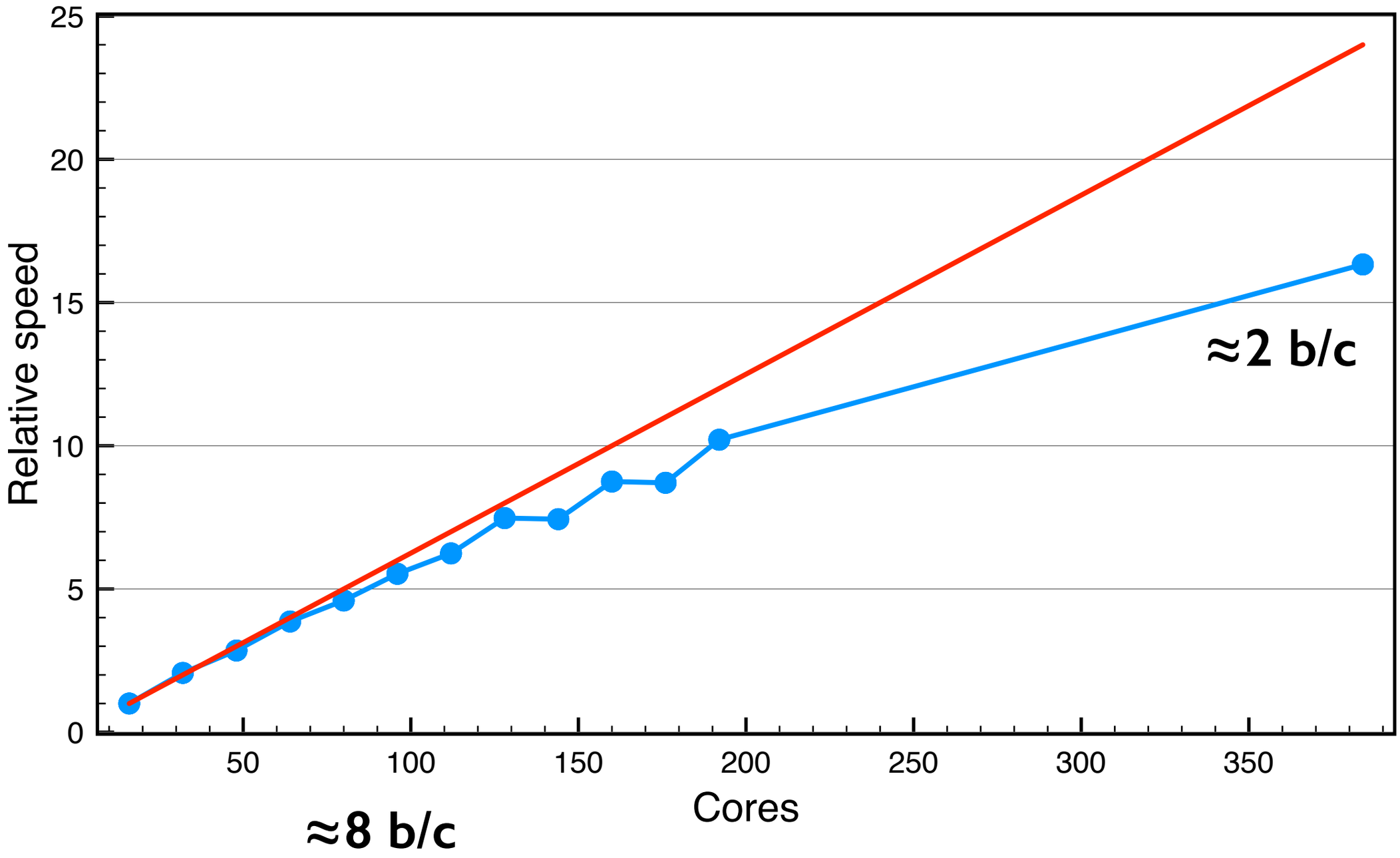
  different best practices → + 2xGPU (NVidia K80) ← **vasp-gpu version**

  1 KNL (Intel Xeon Phi 7250) node = 68 cores (192GB RAM)

How many cores?
- Efficient and/or fast?

- Start from # of bands, NBANDS
- 1 band/core: usually doesn't work
- 2 bands/core: ~50% parallel efficiency
- 8 bands/core: good starting point
  - try e.g. **cores ≈ NBANDS / 8**

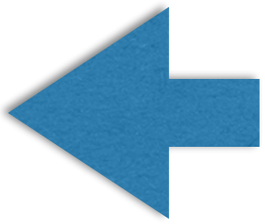
Si-H/Ag(111) 129 atoms @triolith



NBANDS=750, 4 k-points

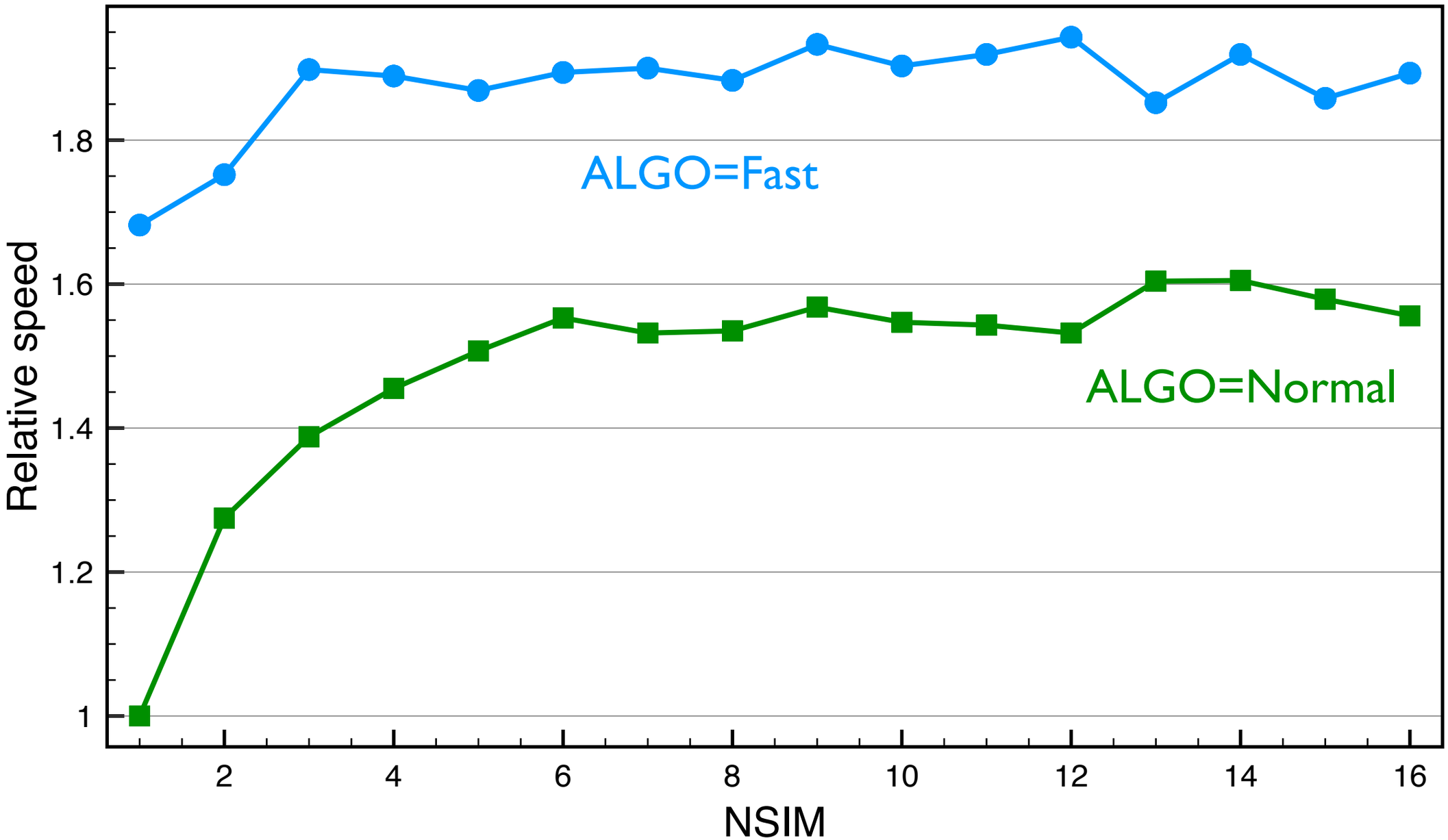
NSIM

- 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 @triolith



NBANDS=750, 4 k-points

NCORE / NPAR

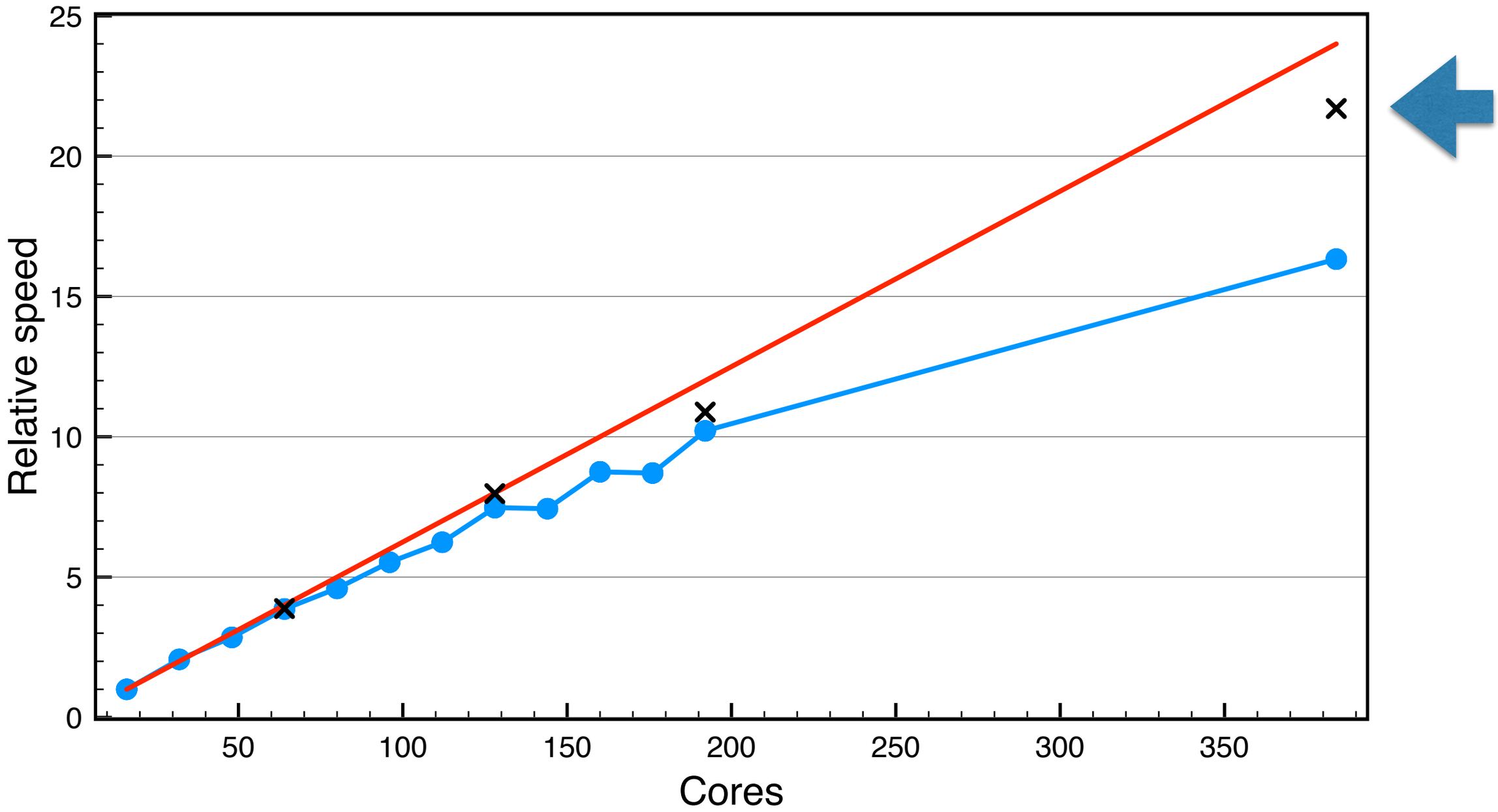
- cores per orbital / bands treated in parallel
- Davidson & RMM-DIIS algorithm
- ALGO = Normal & Fast, VeryFast
- NPAR = 1, saves memory
- NPAR = number of compute nodes (x2)
- NCORE = cores per compute node (or socket)

I find it easier to use NCORE, e.g. on triolith:
NCORE=16

KPAR

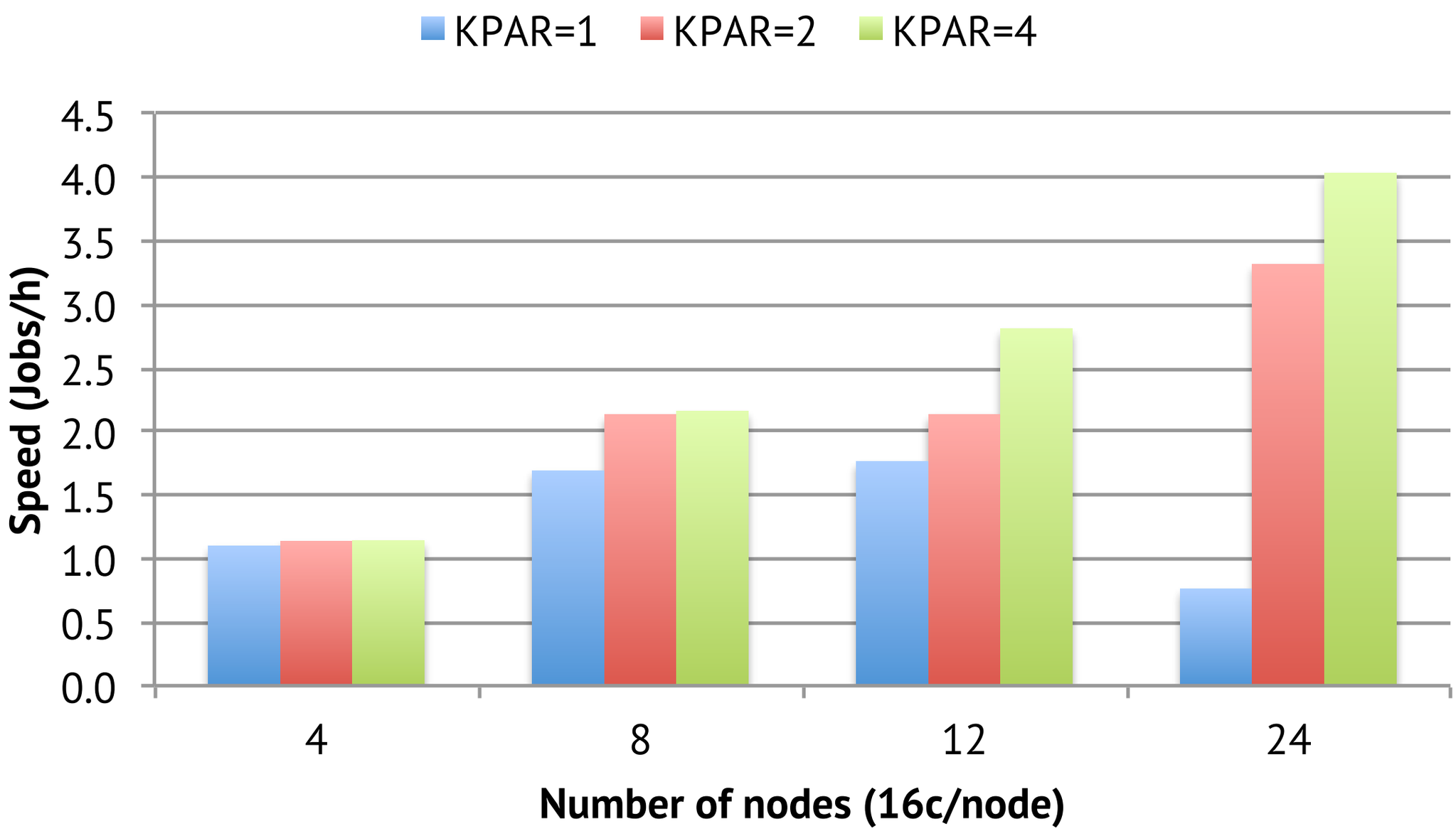
- KPAR = number of k-points treated in parallel
- good for **hybrid-DFT** jobs
- increase cores at least 2x
- try **KPAR = min (nodes, k-points)**

Si-H/Ag(111) 129 atoms @triolith



KPAR=4

NBANDS=750, 4 k-points



- from Peter Larsson, NSC

support@nsc.liu.se

- complicated INCAR…
- structure (POSCAR)
- k-mesh (KPOINTS)
- NCORE/NPAR, KPAR
- VASP version
- cores
- memory

support@nsc.liu.se

ALGO=N

- complicated INCAR… simplify & try again!
- structure (POSCAR) reasonable/correct?
- k-mesh (KPOINTS) Γ-centered?
- **NCORE**/~~NPAR~~, KPAR simplify!
- VASP version try latest!

```
$ module add vasp/5.4.1-05Feb16
```

- cores too few/many?
- memory larger memory nodes:

```
#SBATCH -C fat
```

  - ENCUT
  - k-mesh

reduce cores/node:

```
#SBATCH --ntasks-per-node=8
```

```
INCAR: NCORE=8
```

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VASP OpenMP Beta - Mar 13 2017

Directory list:

Version	Description
build01	Initial installation

Level of support

Tier 3 NSC will not be able to help you much with this program, either because we lack the in-house experience, or because it is a test installation. In general, these types of installations are untested, and will not be updated unless you send a request to NSC.

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 beta test version of VASP with OpenMP/MPI hybrid implementation, provided by the VASP developers. It can be used for **testing** purposes, not for publication, by VASP license holders at NSC. Observe that problems might arise, feedback on using this beta version is welcome.

Before using, read the additional instructions and information in:

```
/software/apps/vasp/omp-beta-13Mar17/notes.txt
```

Resources

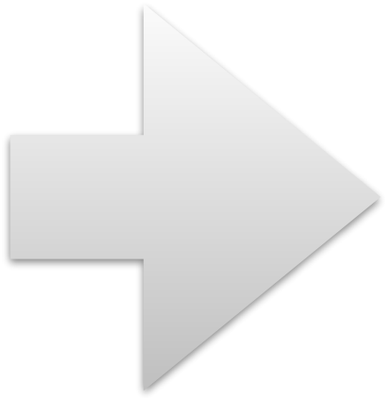
- Manual

Read all (really)!

- Wiki

examples, presentations

- Forum



Find the links:

http://vasp.at/

- Peter Larsson's blog at NSC:

https://www.nsc.liu.se/~pla/

info & discussion

Quantum Espresso

National Supercomputer Centre in Linköping Sweden

Introduction

- DFT, CP-MD
- pseudopotentials (different choices)
- popular for phonon calculations
- open source, frequently updated

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castep
ccp4
cdo
CESM
cmor

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 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.

The Quantum Espresso installations are generally maintained by Weine Olovsson (weiol@nsc.liu.se).

How to run

Launch the desired QE binary with "mpprun":

triolith

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Quantum Espresso 6.1

Directory list:

Version	Description
build01	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.

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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
- Hybrid functionals: ACE is now the default
- Hybrid functionals with PAW now work
- Optimized tetrahedron method, contributed by Mitsuaki Kawamura, U. Tokyo

For fixes and incompatible changes in 6.1 version see the full release notes.

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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:

```
module load buildenv-intel/2017
```

Configure line:

Caveats

- Common issue:

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

crash?!

instead use

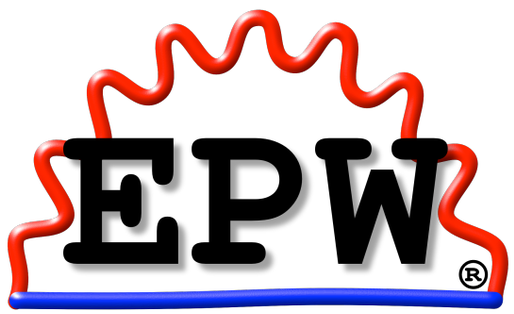
```
mpprun pw.x –inp job.in > job.out
```

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

see NSC web site for setting up!

Beskow: no local disks!

Together with QE installation



http://epw.org.uk

electron-phonon interaction using Wannier functions

http://west-code.org

large scale GW calcs.

http://www.yambo-code.org

optics from BSE

Outlook

- Increasing user interest in Quantum Espresso?
- Benchmarks
- Best practices
- Advanced user help

Virtual NanoLab (VNL)

Quantum Wise

Virtual NanoLab

NSC

National Supercomputer Centre in Linköping Sweden

Information

http://quantumwise.com **examples, tutorials**

- Building supercells, surfaces, interfaces etc.
- 2 concurrent licenses at NSC
  - VASP functionality with paid license
  - Academic license (win/linux/mac)
- Easier to use via remote desktop, ThinLinc

```
$ module add vnl/2016.4
$ vnl &
```