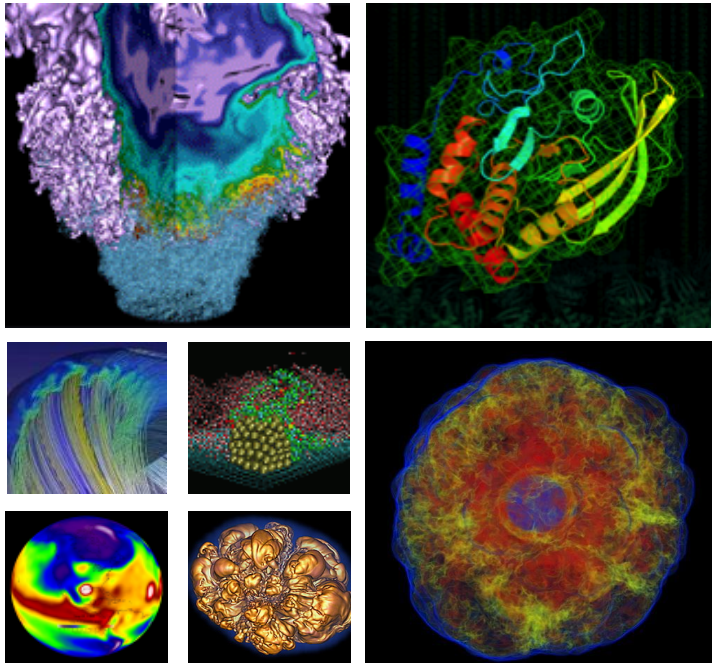
Brief Intro. to Quantum ESPRESSO at NERSC



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U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB

Quantum ESPRESSO

Open-source feature-full DFT application.

MPI + OpenMP!

Sub-Codes:

PW	Plane Wave DFT
CP	Car-Parrinello MD
PH	Phonons
XSPECTRA	X-Ray Absorption
NEB	Reaction Pathways Nudged Elastic Band
TDDFT	
PP	Post Processing

Quantum ESPRESSO

- Γ–point and k-point calculations, any crystal structure or supercell
- insulators and metals, with various flavors of broadening, or tetrahedra
- norm-conserving PPs in separable form, ultrasoft PPs, PAW • almost all flavours of LDA and of gradient-corrected exchangecorrelation functionals (PW91, PBE, B88-P86, BLYP,...), DFT+U, nonlocal (vdW-DF), hybrid functionals (PBE0, B3LYP), meta-GGA
- spin-polarized, magnetic systems (including noncolinear magnetism and spin-orbit interactions)

on many different hardware and software configurations

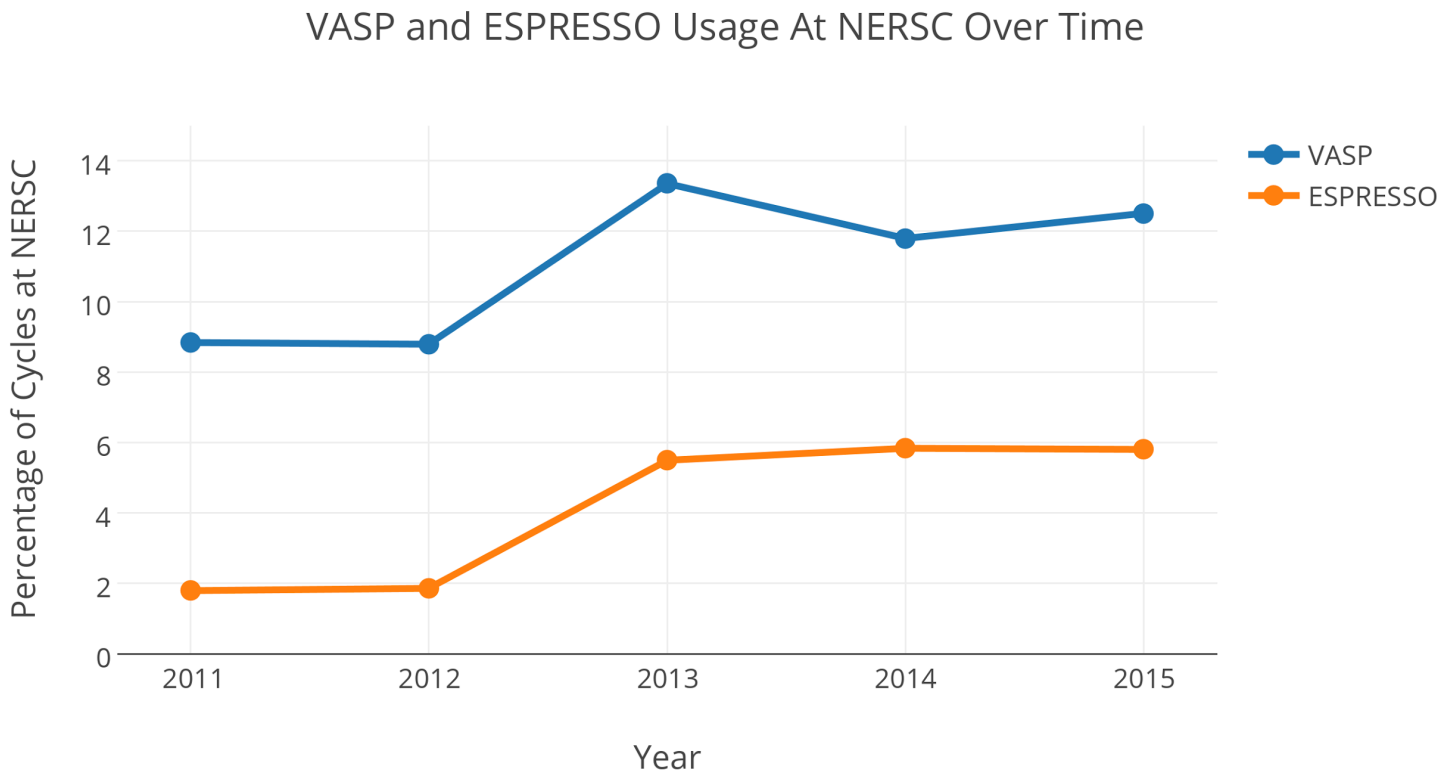
From: http://www.fisica.uniud.it/~giannozz/QE-Tutorial/tutorial_overview.pdf

Other Reasons to Use QE

- Quantum ESPRESSO is a Tier 1 NESAP code. Actively being ported to Xeon-Phi.
  - Fabio Affinito (CINECA)
  - Paul Kent (ORNL)
  - Intel IPCC

- It is an open-source application with a lot of community involvement
  - Integration with advanced MBPT codes like Yambo, BerkeleyGW (and newer methods from Umari et al.), EPW, ShirleyXAS etc.
  - Advances in Hybrid and MD from Distasio et al. (USA)

QE Usage at NERSC



QE Usage at NERSC

How to use QE at NERSC:

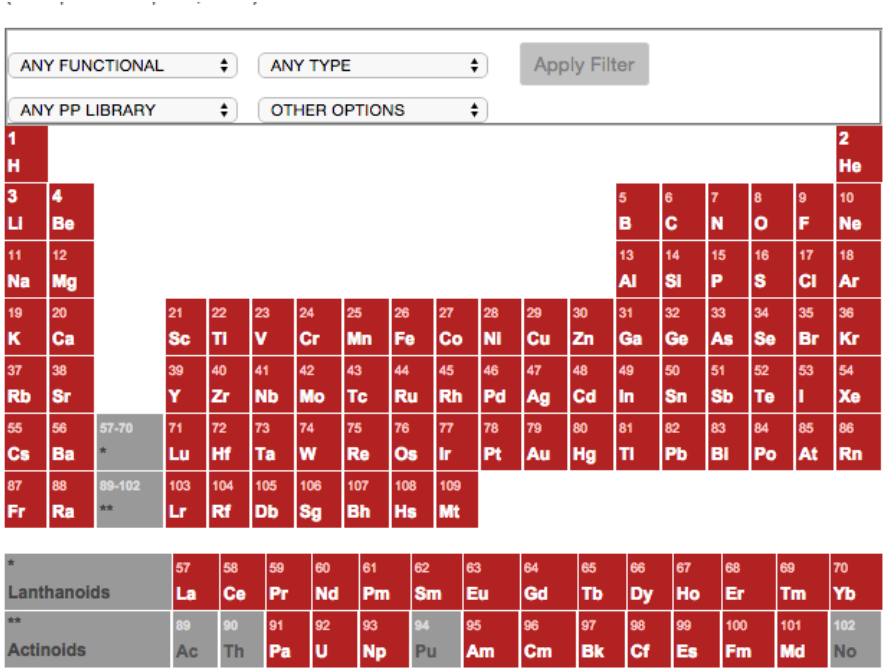
```
% module avail espresso

----------------------------/usr/common/usg/Modules/modulefiles ---------------------------------
espresso/5.0.0          espresso/5.0.2-2        espresso/5.0.3-2(default) espresso/5.1.1
espresso/5.0.2          espresso/5.0.3          espresso/5.1              espresso/5.1.2

% module load espresso

#in batch script

aprun -n 48 pw.x -ntg 5 -in infile.in > outfile.out
```

Pseudopotentials

UPF Format

http://www.quantum-espresso.org/pseudopotentials/

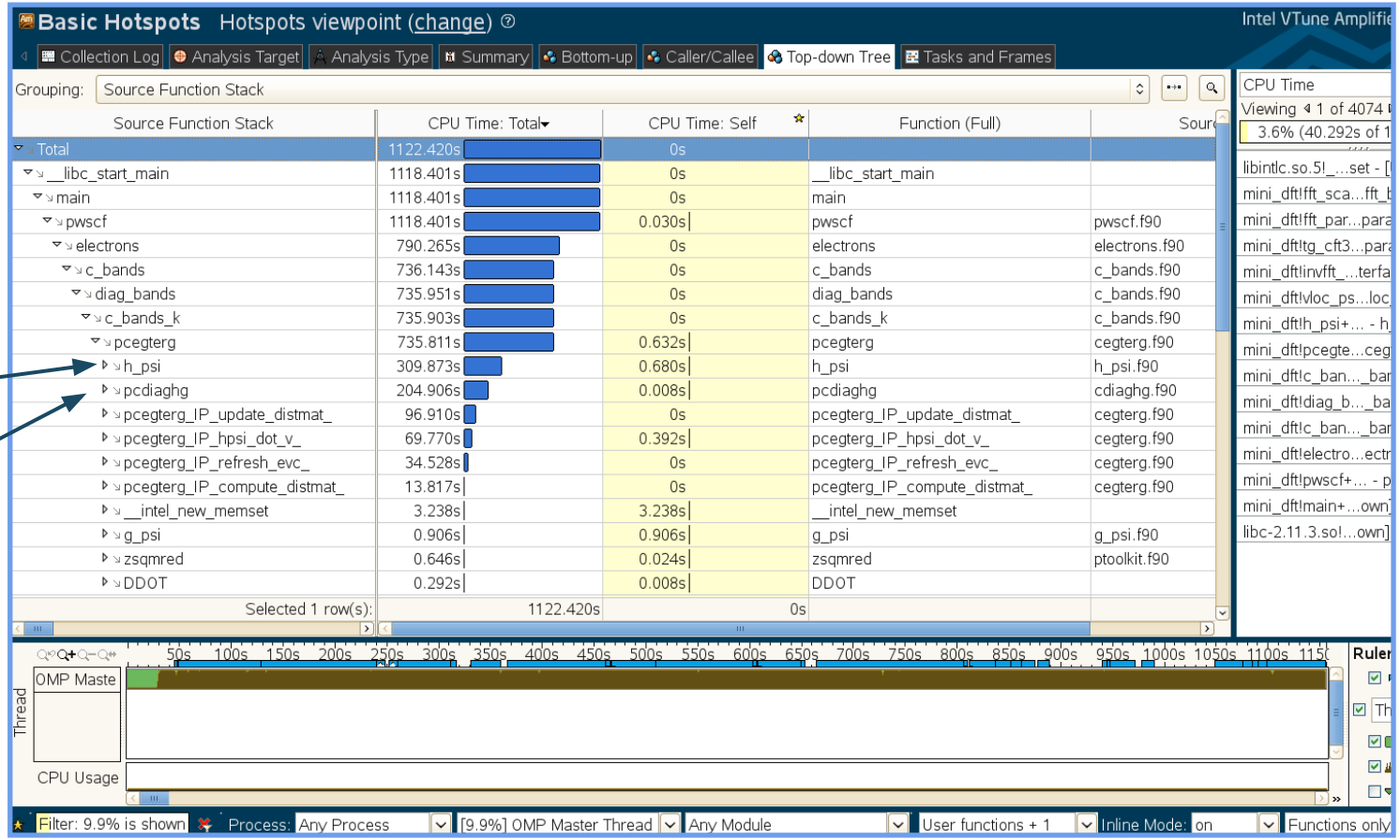
Supports many types and functionals



Profile (2000 atom MgO)

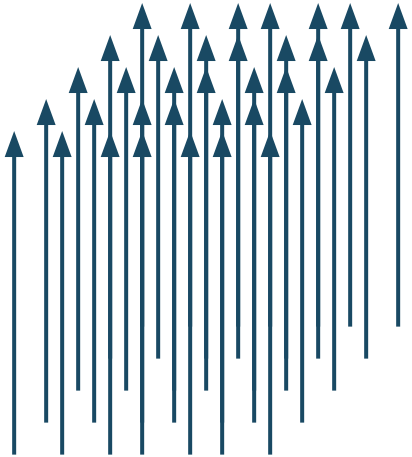
H * Psi

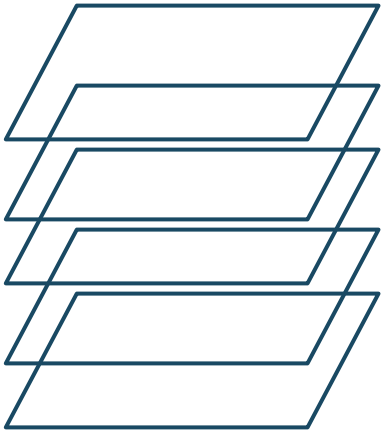
Subspace Diagonalization



Parallelization levels

By Default QE parallelizes over plane-waves (G Vectors). By default, FFTs are parallelized via rods in z direction and planes perpendicular to z direction.





By default, can't scale number of processors beyond number of planes (G Vectors in z direction)

Parallelization levels

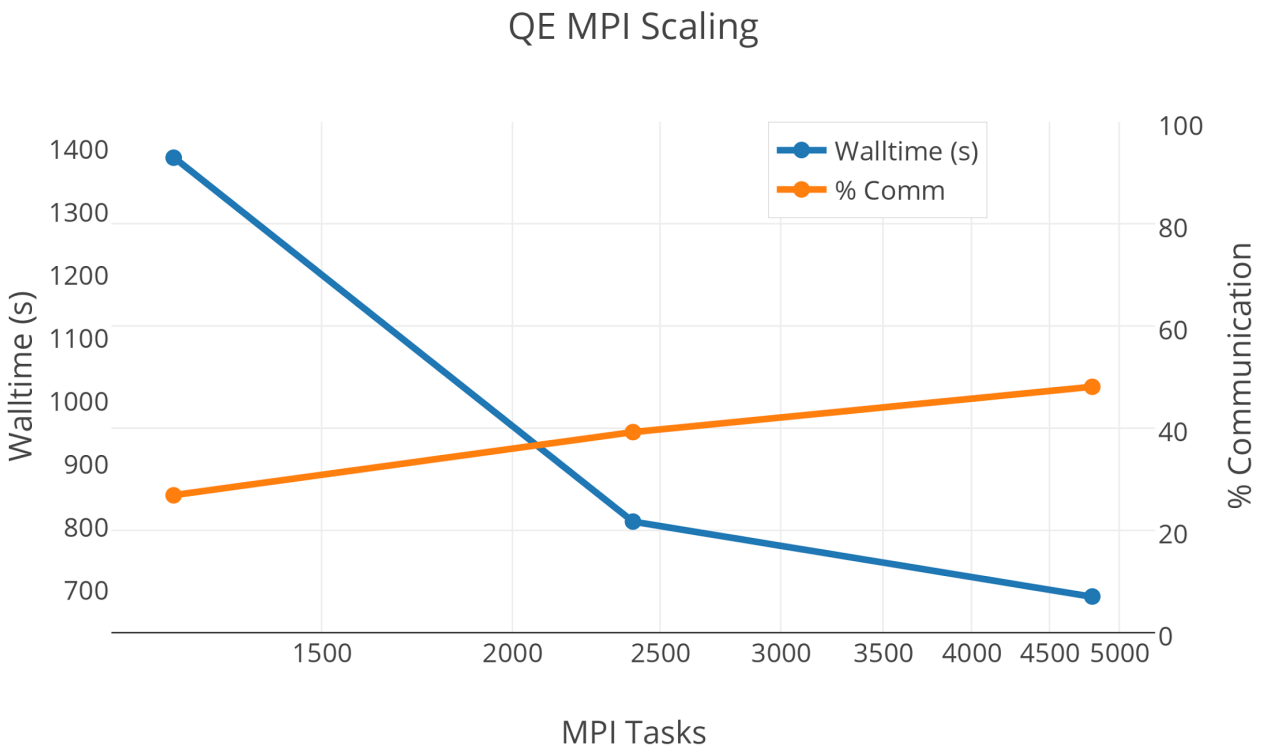
Going beyond the default. You can give pw.x several command line arguments to improve parallelism.

1. **-npools** k-point parallelism. Near perfect level of parallelism. Downside is big systems don't use many k-points
2. **-ntg** instructs QE to do multiple FFTs concurrently in different "task groups". Allows you to scale to processor counts beyond the number of planes. Downside is not for hybrids.
3. -**nbgrp** band parallelism. For hybrid functionals only.
4. -**ndiag** Number of processors with which to call scalapack

MPI Scalability (-ntg 5)

MgO

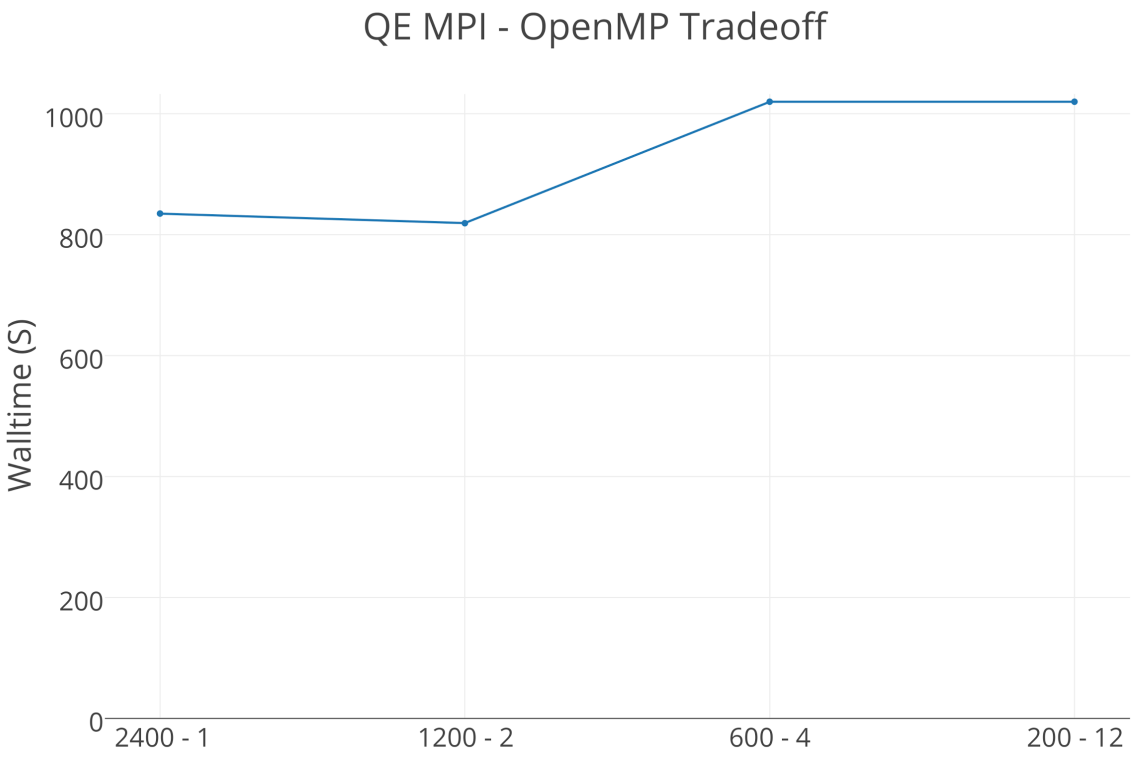
2000 atoms



OpenMP

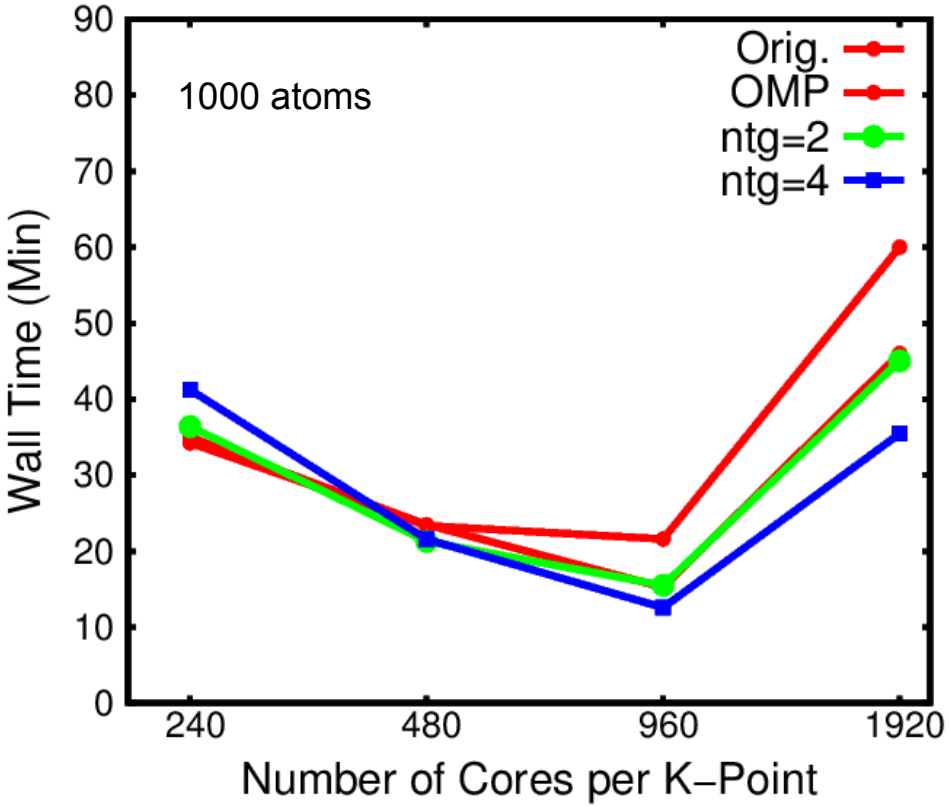
OpenMP

MgO
2000 atoms



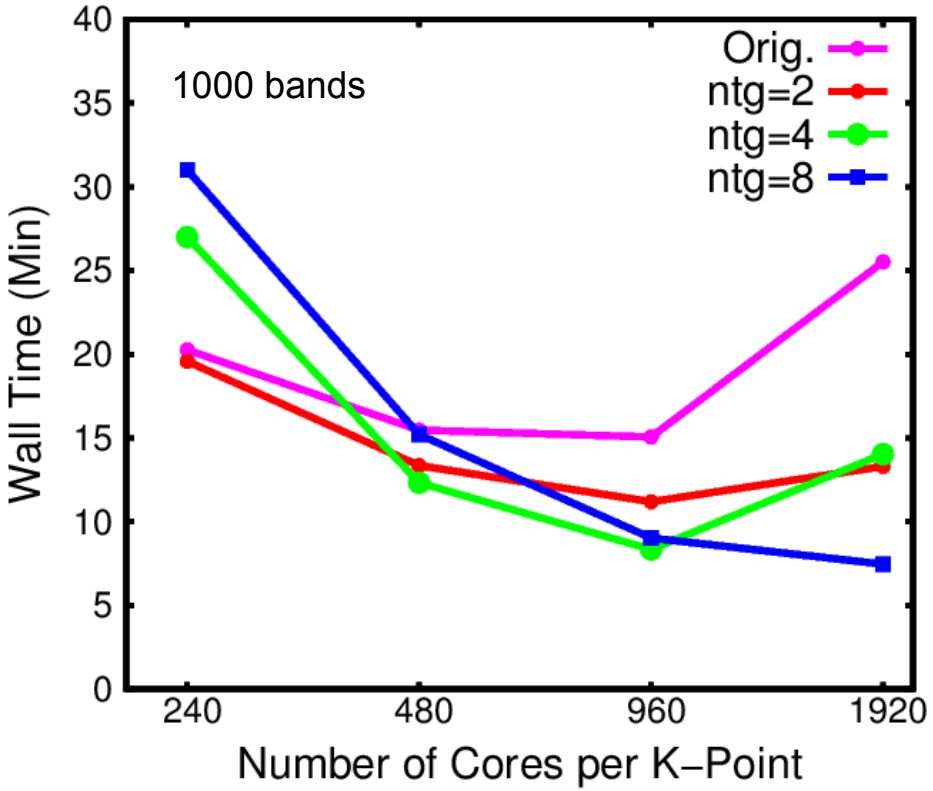
SCF Scaling

-ntg



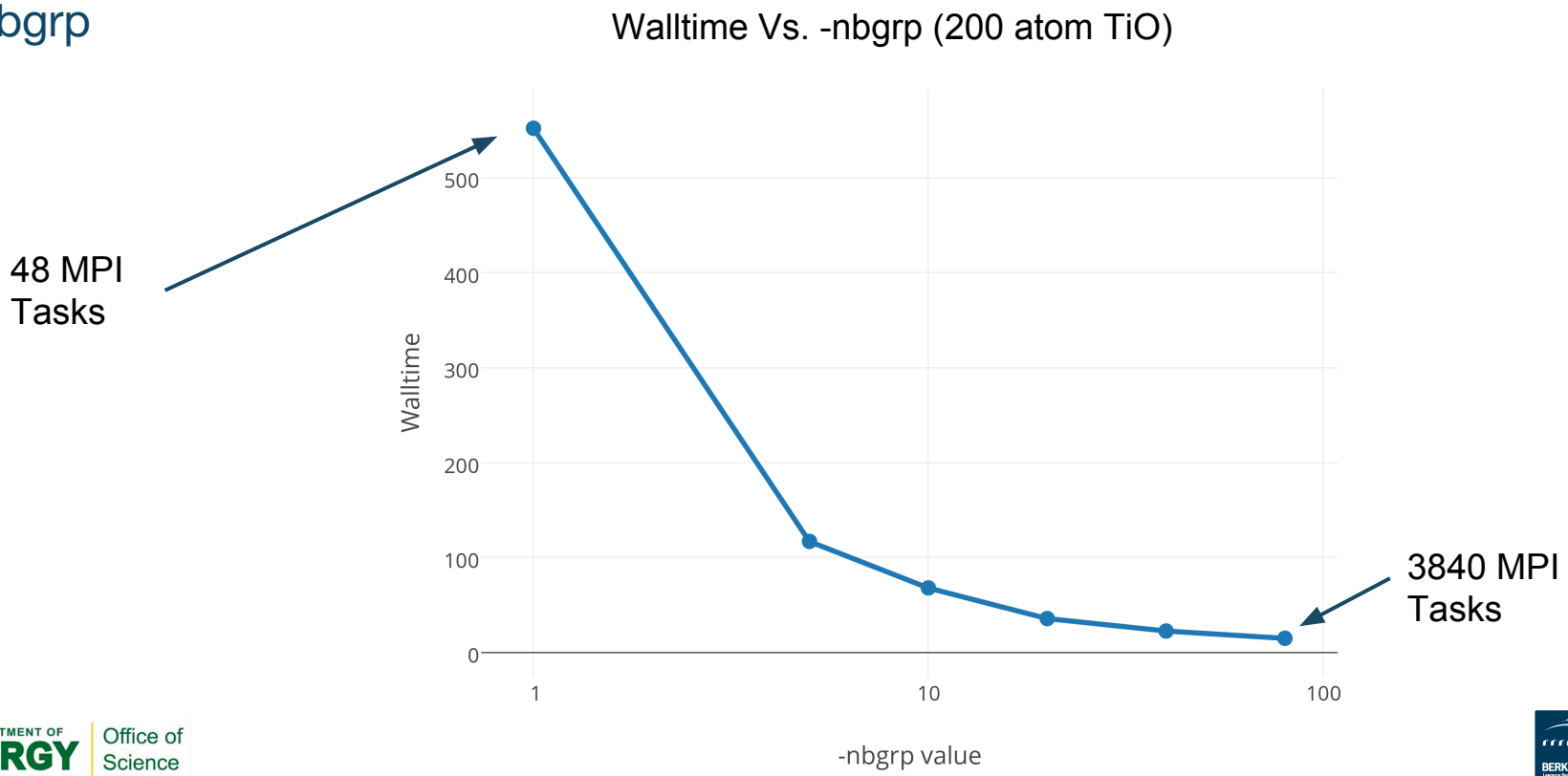
NSCF Scaling

-ntg



Hybrid Scaling

-nbgrp



Known Issues

Certain arrays are not distributed (e.g. becp)

Must use internal FFT library for Threaded FFTs

Band parallelization is still in progress