# Report: Comparison of Performance of Quantum Espresso Simulations for NFS and Scratch Space

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## Motivation

Performance of Quantum Espresso simulations depends on what file system is used for storing temporary files. The purpose of this report is to give some estimates of how NFS file system and scratch space affect the performance.

## Description

In this report I did some preliminary measurements of simulation performance of two systems metallic (Al) and isolator (MgB2) running on several number of cores (2 and 16) by varying single simulation parameter (K_POINTS).

## Experiment

PW

Results:

Case A: Running simulation on NFS

**[Al]**

| K points | FS | # cores | Time | Output Size, Mb |
|---|---|---|---|---|
| 60x60x60 | NFS | 2x12 | 01:31 | |
| 60x60x60 | NFS | 16x12 | 02:34 | |
| 100x100x100 | NFS | 2x12 | 10:48 | |
| 100x100x100 | NFS | 16x12 | 07:07 | 2.76 |

**[MgB2]**

| K points | FS | # cores | Time | Output Size, Mb |
|---|---|---|---|---|

| | | | | |
|---|---|---|---|---|
| 32x32x32 | NFS | 2x12 | 02:48 | 0.45 |
| 32x32x32 | NFS | 16x12 | 01:21 | 0.45 |
| 60x60x60 | NFS | 2x12 | 25:33 | 1.84 |
| 60x60x60 | NFS | 16x12 | 16:15 | 1.84 |

Case B: Running simulation on scratch space

**[Al]**

| **K points** | **FS** | **# cores** | **Time** | **Output Size, Mb** |
|---|---|---|---|---|
| 60x60x60 | Scratch | 2x12 | 00:40 | |
| 60x60x60 | Scratch | 16x12 | 00:54 | 1.04 |
| 100x100x100 | Scratch | 2x12 | 02:46 | |
| 100x100x100 | Scratch | 16x12 | 3:13, 3:19, 3:13 | 2.76 |

**[MgB2]**

| **K points** | **FS** | **# cores** | **Time** | **Output Size, Mb** |
|---|---|---|---|---|
| 32x32x32 | Scratch | 2x12 | 1:42 | 0.45 |
| 32x32x32 | Scratch | 16x12 | 0:46 | 0.45 |
| 60x60x60 | Scratch | 2x12 | 09:27 | 1.84 |
| 60x60x60 | Scratch | 16x12 | 02:45 | 1.84 |

Cluster: foxtrot.danse.us 34x12
The cluster was not used during these measurements.

Conclusions:
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Appendix A: Example of PW files for Al and MgB2 for scratch space

# Al

```
&CONTROL
    calculation = 'scf',
    restart_mode = 'from_scratch',
    tprnfor = .true.,
    outdir = '/scratch/dexity/test',
    pseudo_dir = '../pseudo/',
/

&SYSTEM
    ibrav = 2,
    degauss = 0.02,
    smearing = 'gauss',
    occupations = 'smearing',
    ecutwfc = 27.0,
    ecutrho = 300.0,
    celldm(1) = 7.63449299556,
    celldm(2) = 1.0,
    celldm(3) = 1.0,
    celldm(4) = 0.0,
    ntyp = 1,
    nat = 1,
/

&ELECTRONS
    conv_thr = 1.0d-8,
    mixing_beta = 0.7,
/

ATOMIC_SPECIES
 Al  26.9815 Al.bp-n-van_ak.UPF

ATOMIC_POSITIONS (crystal)
 Al      0.00000000  0.00000000  0.00000000

K_POINTS (automatic)
 100 100 100 0 0 0
```

# MgB2

```
&CONTROL
    calculation = 'scf',
    pseudo_dir = '../pseudo/',
    tprnfor = .true.,
    prefix = 'mgb2',
    outdir = '/scratch/dexity/test',
    tstress = .true.,
/

&SYSTEM
    nbnd = 12,
```

```
    nspin = 1,
    ecutwfc = 64,
    celldm(4) = -0.5,
    occupations = 'smearing',
    celldm(1) = 5.81347171,
    ibrav = 4,
    celldm(3) = 1.141104624,
    degauss = 0.025,
    smearing = 'methfessel-paxton',
    celldm(2) = 1.0,
    nat = 3,
    ecutrho = 256,
    ntyp = 2,
    la2f = .false.,
/

&ELECTRONS
    conv_thr = 1.0d-12,
/

ATOMIC_SPECIES
 Mg 24.305 mg.ncpp
 B 11.0 B.pbe-n-van_ak.UPF

ATOMIC_POSITIONS (alat)
 Mg    0.0  0.0         0.0
 B     0.5  0.28867513  0.570552312
 B     0.0  0.57735027  0.570552312

K_POINTS (automatic)
 60 60 60 0 0 0
```