NOVA
NERSC’s Online VASP Application

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Why VASP?

Codes Used by the Most Projects at NERSC

- CPMD
- WRF
- NIMROD
- NAMD
- LAMMPS
- NWChem
- Quantum Espresso
- Gaussian
- VASP

Number of Projects as of Sep 2010
Why run VASP in a browser?

Making interacting with HPC more efficient

- Error checking
- Organizing and retrieving jobs
- Real-time job monitoring
- Integrated analysis tools
- Integration with other online tools
- Meaningful UI controls
SYSTEM = Hg

NWRITE = 2
IALGO = 48 ! uncomment this line to get timings
NELM = 13
ENMAX = 140 eV ; IALGO = -1 ; NELMIN = 3 ; NELMDL = 7
NGX=31 ; NGY=31 ; NGZ=31 ; NGXF=48 ; NGYF=48 ; NGZF=48
NBANDS=316
NSIM =4
LREAL = .TRUE.   real space projections
BMIX = 2.5      mixing parameter
ISYM = 0        switch of symmetry
EDIFF = 1E-4
LWAVE=.FALSE.
LCHARG=.FALSE.

Ionic Relaxation
NSW =      0    number of steps for IOM
NBLOCK = 1 ; KBLOCK =  5
SMASS = 0.5 Nose mass-parameter (am)
POTIM = 5.00 time-step for ion-motion
TEBEG = 423 temperature

PC-function
APACO = 10.0 distance for P.C.

Mass of Ions in am
POMASS = 200.59000
ZVAL = 12.00
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Files
- POSCAR
- POTCAR
- KPOINTS
- INCAR

Computational Settings
- Run this job

Recommended Minimal Settings

- Precision:
- Cutoff energy for plane wave basis set:
- Projection done in:
- Method to determine partial occupancies:
- Order:

Optional Settings
- Optional Initialization Settings
- Optional Iteration Settings
- Optional Quality Settings
- Optional Algorithm Settings
### VASP with a modern interface

+ **Optional Initialization Settings**

- **Optional Iteration Settings**

<table>
<thead>
<tr>
<th>Setting</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max number of electronic steps:</td>
<td>61</td>
</tr>
<tr>
<td>Min number of electronic steps:</td>
<td>6</td>
</tr>
<tr>
<td>Max number of ionic steps:</td>
<td>51</td>
</tr>
<tr>
<td>Calculate pair correlation function and DOS each ionic steps</td>
<td>NBMCC</td>
</tr>
<tr>
<td>Max number of steps in Broyden mixer:</td>
<td></td>
</tr>
<tr>
<td>□ Only reset if storage exceeded</td>
<td></td>
</tr>
<tr>
<td>Begin updating charge density</td>
<td></td>
</tr>
<tr>
<td>□ according to default</td>
<td></td>
</tr>
<tr>
<td>□ immediately</td>
<td></td>
</tr>
<tr>
<td>□ after [ ] steps, □ with delay after each ionic step</td>
<td>NELMDL</td>
</tr>
</tbody>
</table>
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Inside NERSC, NOVA

Files

POSCAR
POTCAR
KPOINTS
INCAR

Computational Settings

VASP version

4.6.35 = default

VASP executable

collinear (vasp) = default

Queue

regular

Run On

1 nodes x 8 procs per node = 8 cores

Maximum Walltime

2 Hours 3 Minutes

Node Memory

First Available

Process Memory Limit

GB

Email Notifications

On begin

On end

On abort

Repository

Default

Save  Cancel
VASP with a modern interface

Job Control

Jobs to Be Run

Oxygen in a box [View All Files] [Copy Job]

Jobs Running

LiOAI [View All Files] [Copy Job] [Stop Job]
Queued April 3, 2011, 8:12 p.m.
Not yet started.

Jobs Recently Completed

Oxygen Atom in a Box [View Convergence] [View All Files] [Copy Job]
Started April 3, 2011, 2:58 p.m.
Completed April 3, 2011, 2:58 p.m.
Real-Time Monitoring

**Oxygen in a box** [View All Files] [Copy Job]

Stop this job at the next opportunity? This will write a STOPCAR file to the directory.

- Stop at next ionic step (recommended)
- Stop at next electronic step

[Cancel]
Real-Time Monitoring

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Convergence

Free Energy

Ionic Step

Job Information

System: carver

PBS Job ID: 606410.cvrsvc09-ib
Current State of NOVA

• Django application using the NEWT API
• Early version implements some graphical features
• Checks INCAR keywords and values
• Can set up jobs, copy, submit, monitor, stop, import files from outside NOVA
Future Features

• Real-time convergence monitoring
• POSCAR file generation
• Ensured coherency across input files
• Visualization tools
• Advanced error detection
• File sharing
• Connection to Materials Genome Project
Test version of NOVA

https://portal-auth.nersc.gov/nova

Comments and suggestions to
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