Materials Studio on Aang

Add Gateway:

1. Go to Tools -> Server Console. Click “yes” at the prompt.
2. Right click Server Gateways -> New -> Server Gateway
3. Fill out window as follows, and click “Run Diagnostics”:
Running a calculation:

1. Select the Job Control tab - > Gateway location -> Select “Aang”. If you do not see the Aang gateway, you might have to restart materials studio or your computer.
2. Max number of cores is 32 but ONLY use up to 30. Also if applicable select “Optimize number of cores on the fly”. Click “Run”
3. Job status can be found in the “Jobs” window. It should show “Gateway” as aang.engr.arizona.edu:18888.
4. Files will be automatically downloaded once calculation has finished.
5. NOTE: If you close Materials Studio while a job is running, it will still run on Aang. When you re-launch Materials Studio and open that project it will ask if you want to reconnect to job. Click “yes”

6. You can submit multiple jobs in the same project or another and materials studio will handle the queue, however this might reduce performance.
7. To kill a job right click it and select actions->stop.