Job Scheduling

A CPU can only do one thing at a time. When you run two programs at a time on your single-CPU workstation, the operating system uses "timeslicing" to give the illusion of running both at once: it runs one of the programs for a moment, then pauses that program to run the other one for a moment, and so on. If you are reading and editing documents, as most workstations are used for, this works fine - most of the time the computer is waiting for you to hit the next key anyway.

Running a simulation, however, uses the CPU heavily. When timeslicing between two simulations on a single-CPU workstation, you can expect each simulation to take roughly twice as long as if it had dedicated use of the CPU. This is obviously counter to the goals of high performance computing, so HPC clusters use batch job scheduling to ensure that each job has dedicated access to the resources it needs.

The principle behind batch job scheduling is:

- Each simulation is prepared (by the user) as a job, (batch job) which is a script that sets up and runs the simulation without interactive input from the user.
- Each job needs a certain set of resources for a certain amount of time. The user knows these needs in advance and can specify them in the job script.
  - "Resources" includes a number of CPUs and an amount of memory. Some jobs might also need a specific type of CPU or a specific software license.
  - The scheduler plans when and on which compute nodes to run each job.

The diagram below illustrates how jobs can be allocated to certain parts of the cluster at certain times. When a new job is submitted, the scheduler looks for a place and time to run the job, always aiming to start the job as soon as possible and to make the most efficient use of the full resources of the cluster:
On the NYU clusters, Torque and Moab manage the running and scheduling of jobs. As a user you will interact mostly with Torque, which accepts and runs job scripts and manages and monitors the cluster's compute resources. Moab does the heavy thinking: the planning of which job should be run where and when.

Avoid requesting vastly more CPUs, memory or walltime than you actually need. Jobs needing fewer resources are easier to schedule - in our scheduling diagram, a job requiring just 1 CPU for 1 hour could be inserted into the gap on Node 1 CPU 4. Smaller jobs are also more likely to receive priority when being scheduled.

Note that a small overestimate, such as 10%-20%, is wise, lest your job run out of time and be killed before it finishes, but requesting several times what you need will result in longer queueing time for your job and less efficient system utilization for everybody.