

Resources

As part of the Molecular Foundry's Theory Facility we use a number of local compute clusters as well as [The National Energy Research Scientific Computing Center \(NERSC\)](#). Cluster resources are managed by the High Performance Computing Services (HPCS) group at LBNL. The Foundry annual allocations of computer time at NERSC are obtained through a yearly competitive proposal process; NERSC computer time is well-suited to and extensively used by Foundry Scientists and Users for long-term projects and "production" runs that require large-scale computation.

Vulcan

Purchased with ARRA Stimulus Funds, Vulcan is a 242-node cluster with Infiniband interconnect connected to a 41.7TB LUSTRE parallel file system. Each node has two 2.4GHz Intel Xeon E5530 Quad-core Nehalem processors with 3GB RAM per core. Vulcan is also connected to an additional 57.0TB BlueArc NFS file system. Theoretical performance is 18.1TFLOPS with 5.7TB of total memory.

Vulcan is used exclusively by Theory Facility Staff and Users. Ideal for exploratory research, Vulcan provides the Theory Facility with the flexibility to address exciting new problems as they arise, allows fast turnaround for development projects, and is highly scalable for future expansion.

Nano

The Theory Facility's first in-house parallel Linux cluster, Nano is a 624 core Intel Xeon processor machine (consisting of a mix of 2-, 4-, and 8-core nodes) networked with high-speed, low-latency Infiniband interconnects; it has 824 GB of total memory, uses a 10.1TB Panasas parallel file system, and has a theoretical peak performance of 3.1 Teraflops.

Lawrencium

The Theory Facility supplements its cluster computing resources with access to [Lawrencium](#), an LBNL-wide computing resource.

Mako

The University of California Office of the President (UCOP) sponsors the [Shared Research Computing Services Pilot Project](#) in collaboration with the ten UC Universities and LBNL. The Theory Facility has access to its North Cluster, known as [Mako](#). This cluster comprises 272 dual quad-core (Nehalem) nodes and is quite similar in architecture to Vulcan.