We have two different computing environments for fitting demanding models to large space and/or time data sets.

1. A distributed system consists of multiple autonomous computers (nodes) that communicate through a computer network. A computer program that runs in a distributed system is called a distributed program. Message Passing Interface (MPI) is a specification for an Application Programming Interface (API) that allows many computers to communicate with one another (implementations in C, C++, and Fortran.)

2. A shared memory multiprocessing system consists of a single computer with memory that may be simultaneously accessed by one or more programs running on multiple central processing units (CPUs). The OpenMP (Open Multi-Processing) is an API that supports shared memory multiprocessing programming (implementations in C, C++, and Fortran).

My lab currently favors shared memory multiprocessing system.

We buy rack mounted units (e.g., Sun Fire X4170 Server with 2 quad-core Intel Xeon Processor 5500 Series and 48 GB of RAM ∼10-15k) running the Linux operating systems. Software includes OpenMP coupled with Intel Math Kernel Library (MKL) http://software.intel.com/en-us/non-commercial-software-development. MKL is a library of highly optimized, extensively threaded math routines (e.g., BLAS, LAPACK, ScalAPACK, Sparse Solvers, Fast Fourier Transforms, and vector RNGs).

See http://blue.for.msu.edu/comp-notes for some simple examples of C++ with MKL and Rmath libraries along with associated Makefile files (I’ll add more examples shortly and upon request).
Computing environments

Many core and contributed packages (including spBayes) call Basic Linear Algebra Subprograms (BLAS) and LAPACK (Linear Algebra PACKage) Fortran libraries.

Substantial computing gains:
- Processor specific threaded BLAS/LAPACK implementation (e.g., MKL or AMD’s Core Math Library (ACML))
- Processor specific compilers (e.g., Intel’s icc/ifort)

Compiling R to call MKL’s BLAS and LAPACK libraries (rather than stock serial versions).

```
MKL_LIB_PATH="/opt/intel/composer_xe_2011_sp1.10.319/mkl/lib/intel64"
export LD_LIBRARY_PATH=$MKL_LIB_PATH
MKL="-L$MKL_LIB_PATH -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -liomp5 -lpthread -lm"
./configure --with-blas="$MKL" --with-lapack
```

Time needed to collect 100 MCMC samples using `spLM` and threaded vs. non-threaded BLAS/LAPACK on an Intel Core 2 Quad processor and Ubuntu 8.10 Linux OS. R compiled with GNU gcc and gfortran.

![Graph showing time needed to collect 100 MCMC samples using threaded vs. non-threaded BLAS/LAPACK](image.png)