ARPACK - Arnoldi Package for sparse Eigenvalue Problems

Introductory Remarks

ARPACK is a collection of Fortran77 subroutines designed to solve large scale eigenvalue problems.

The package is designed to compute a few eigenvalues and corresponding eigenvectors of a general n by n matrix A. It is most appropriate for large sparse or structured matrices A where structured means that a matrix-vector product w Av requires order n rather than the usual order n² floating point operations. This software is based upon an algorithmic variant of the Arnoldi process called the Implicitly Restarted Arnoldi Method (IRAM). When the matrix A is symmetric it reduces to a variant of the Lanczos process called the Implicitly Restarted Lanczos Method (IRLM). These variants may be viewed as a synthesis of the Arnoldi/Lanczos process with the Implicitly Shifted QR technique that is suitable for large scale problems. For many standard problems, a matrix factorization is not required. Only the action of the matrix on a vector is needed.

ARPACK software is capable of solving large scale symmetric, nonsymmetric, and generalized eigenproblems from significant application areas. The software is designed to compute a few (k) eigenvalues with user specified features such as those of largest real part or largest magnitude. Storage requirements are on the order of n*k locations. No auxiliary storage is required. A set of Schur basis vectors for the desired k-dimensional eigen-space is computed which is numerically orthogonal to working precision. Numerically accurate eigenvectors are available on request.

Installations and Usage of ARPACK

On both Itanium and x86_64 based systems, sequential as well as parallel versions of ARPACK (the latter called PARPACK) are available. Parallel functionality is based on MPI. The following module stack is supported:

- **MPI-based version on all HPC systems**

| module load mkl  
module load arpack |

after which you link your application with

```
mpif90 -o myprog.exe <objects> $ARPACK_MPI_LIB $MKL_LIB
```

Notes:

1. The environment variable $ARPACK_LIB is also provided for linking purely serial (i.e., non-MPI) applications. In this case, the mpif90 wrapper can be replaced by a call to ifort.
2. All module stacks require the fortran module and an MPI environment to be loaded (one of these is usually contained in the default list of modules, depending on which system you logged in to). The MKL module is for the most part only required if your matrix-vector multiplication implementation (or another part of your program) contains BLAS/LAPACK calls.
3. By default, MKL may also run multi-threaded. You can set MKL_SERIAL=yes or load a sequential mkl module to enforce single-threaded operation.

Documentation

- Home page for the original ARPACK (version 96) on the Web. This version is not supported any more.
- Development of ARPACK is continued through the ARPACK-NG project.
- User's Guide to ARPACK

The ARPACK and PARPACK source packages, downloadable from the locations given above, also contains some example programs (for both the serial and parallel cases).