BLAS and LAPACK: Numerical Linear Algebra

BLAS

The Basic Linear Algebra Subroutines provide a standardized interface for baseline numeric vector and matrix operation that is often needed in scientific codes. The interface is documented as part of the BLAS project, and a reference implementation is also supplied. However, in practice one should always use a vendor optimized implementation (see below) of this library to achieve high usage efficiency.

LAPACK

The Linear Algebra Package supplies a standardized interface for solution of more advanced and complex problems (e.g. matrix decompositions or eigenvalue problems) from linear algebra. The interface is documented as part of the LAPACK project, and a reference implementation is also supplied. Again, a vendor optimized implementation should normally be used. Note that LAPACK builds upon BLAS for its implementation, so the two libraries usually come bundled.

Use of BLAS and/or LAPACK on LRZ HPC systems

Note that the libraries from the reference implementation usually are linked with a command like

```
f90 -o myprog.exe myprog.f90 -llapack -blas
```

(using the generic name "f90" for the Fortran compiler here), and therefore many build systems use this linkage. However this will usually not work on the LRZ HPC systems; you will need to replace the library specification by something like

```
f90 -o myprog.exe myprog.f90 $MKL_LIB
```

assuming that you are using Intel's Math Kernel Library (MKL) implementation of BLAS and LAPACK.

Available implementations

- Intel MKL
- NAG libraries
- GNU Scientific Library (unoptimize C interface to BLAS only)

Further implementations

The versions listed here are not currently supported by LRZ on its HPC systems; however you might want to try them out on your own:

- OpenBLAS
- ATLAS

Furthermore, implementations exist that are targeted at different architectures:

- ACML (targeted to AMD processors, but retired)
- ESSL (an IBM product built for use on POWER processors)
- cuBLAS / CULA (targeted for use on NVidia GPUs)

Further information

On the NAG web site, some examples for invocations of LAPACK routines are provided.