The Atomic Energy Network (ænet) Package

Nongnuch Artrith

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1 What is ænet?

The Atomic Energy NETwork (**ænet**) package is a collection of tools for the construction and application of atomic interaction potentials based on artificial neural networks (ANN). The **ænet** code allows the accurate interpolation of structural energies, e.g., from electronic structure calculations, using ANNs. ANN potentials generated with **ænet** can then be used in larger scale atomistic simulations and in situations where extensive sampling is required, e.g., in molecular dynamics or Monte-Carlo simulations.

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3 Installation

3.1 Short installation summary

1. Compile the L-BFGS-B library

   - Enter the directory "./lib"
     `$ cd ./lib`
   - Adjust the compiler settings in the "Makefile"
   - Compile the library with
     `$ make`

   The library file `liblbfgsb.a`, required for compiling **ænet**, will be created.

2. Compile the **ænet** package

   - Enter the directory "./src"
     `$ cd ./src`
   - Compile the ænet source code with
     `$ make -f makefiles/Makefile.XXX`
     where `Makefile.XXX` is an approproiate Makefile.
     To see a list of available Makefiles just type:
     `$ make`

   The following executables will be generated in "./bin":

   - `generate.x`: generate training sets from atomic structure files
   - `train.x`: train new neural network potentials
   - `predict.x`: use existing ANN potentials for energy/force prediction

3.2 Detailed installation instructions

Except for a number of Python scripts, **ænet** is developed in Fortran 95/2003. Generally, the source code is tested with the free GNU Fortran compiler and the commercial Intel Fortran compiler, and the Makefile settings for these two compilers are provided. While the **ænet** source code should be platform independent, we mainly target Linux and Unix clusters and **ænet** has not been tested on other operating systems.

ænet requires three external libraries:

1. BLAS (Basic Linear Algebra Subprograms),
2. LAPACK (Linear Algebra PACKage),
3. And the L-BFGS-B optimization routines by Nocedal et al.

Usually, some implementation of BLAS and LAPACK comes with the operating system or the compiler. If that is not the case, the libraries can be obtained from Netlib.org. `libblas.a` and `liblapack.a` have to be in the system library path in order to compile **ænet**.

The L-BFGS-B routines, an implementation of the bounded limited-memory Broyden-Fletcher-Goldfarb-Shanno algorithm, is distributed on the homepage of the authors (Nocedal et al.). For the user's convenience we have decided to distribute the original L-BFGS-B files along with **ænet** package, so you do not have to actually download the library yourself. However, each application of **ænet** should also acknowledge the use of the L-BFGS-B library by citing:

R. H. Byrd, P. Lu and J. Nocedal, *SIAM J. Sci. Stat. Comp.* **16** (1995) 1190-1208.

3.2.1 Compilation of external libraries that are distributed with ænet

All external libraries needed by the ænet code are in the directory "./lib". Currently, only one external library is distributed with **ænet**, the L-BFGS-B library (see above).

To compile the external libraries

1. Enter the directory "./lib"

   ```
   $ cd ./lib
   ```

2. Adjust the compiler settings in the "Makefile"

   The Makefile contains settings for the GNU Fortran compiler (`gfortran`) and the Intel Fortran compiler (`ifort`). Uncomment the section that is appropriate for your system.

3. Compile the library with

   ```
   $ make
   ```

The static library "liblbfgsb.a", required to build **ænet**, will be created.

3.2.2 Build ænet

The **ænet** source code is located in "./src".

1. Enter "./src"

   ```
   $ cd ./src
   ```

2. To see a short explanation of the Makefiles that come with **ænet**, just run `make` without any options.

   ```
   $ make
   ```

   Select the Makefile that is appropriate for your computer.

3. Compile with

   ```
   $ make -f makefiles/Makefile.XXX
   ```

   where `Makefile.XXX` is the selected Makefile.

Three executables will be generated and stored in "./bin":

- `generate.x`: generate training sets from atomic structure files
- `train.x`: train new neural network potentials
- `predict.x`: use existing ANN potentials for energy/force prediction