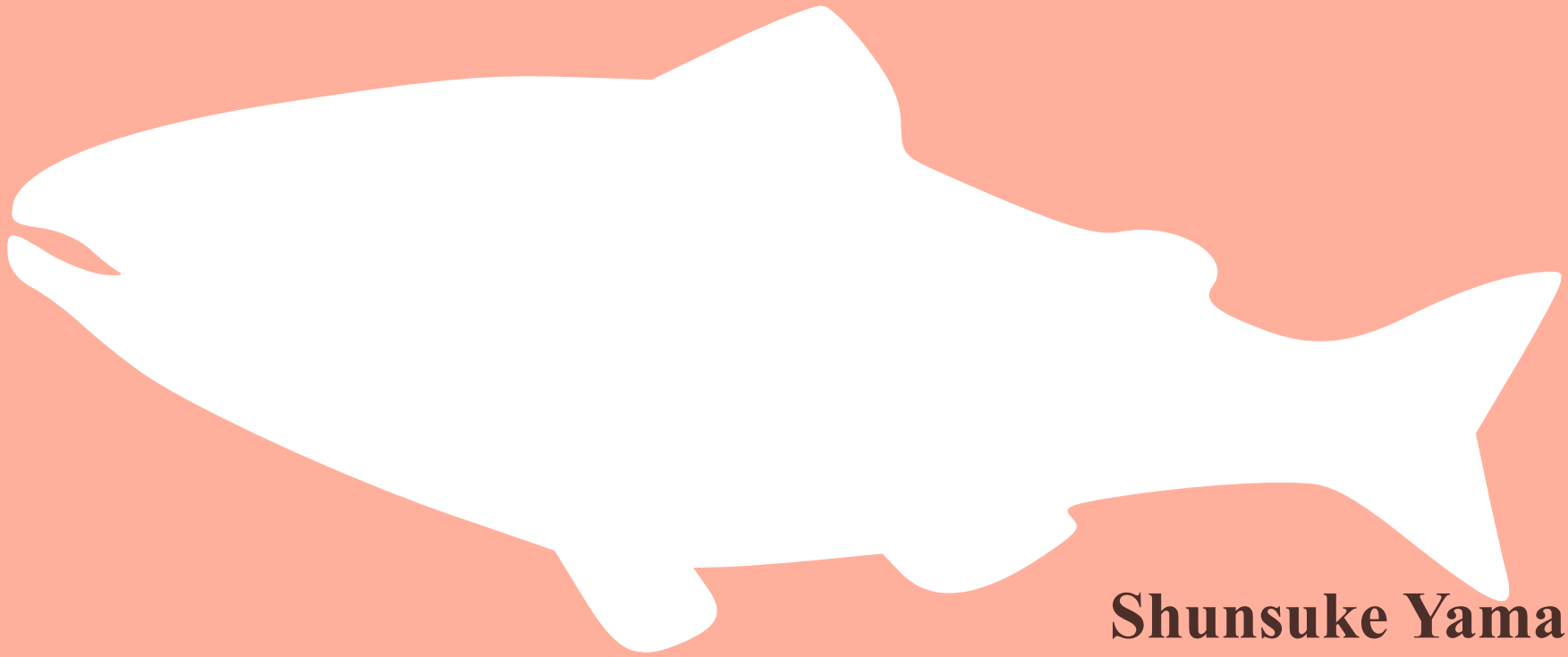
Installation

Quick start of SALMON



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Prerequisites

- Fortran90/C compiler with MPI
  - GCC (Gnu Compiler Collection)
  - Intel Fortran/C Compiler
  - Fujitsu Compiler (at FX100 / K-Computer)
- Library packages for linear algebra
  - BLAS/LAPACK
  - Intel Math Kernel Library (MKL)
  - Fujitsu Scientific Subroutine Library 2 (SSL-II)
- Build tool
  - CMake
  - Gnu Make

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Path setting

Modify ~/.bash_profile

* In this example, all programs will be installed in ~/work directory

Add $PATH settings as follows

```
# User specific environment and startup programs

PATH=$HOME/work/cmake/bin:$PATH
PATH=$HOME/work/SALMON/bin:$PATH

export PATH

module load intel intelmpi mkl
```

Location of executable files

Setting of compiler (if needed)

CMake: version check & install

Version check

```
$ cmake --version
```

CMake of version 3.0.2 or later is required.

Installation example of CMake version 3.9.6

```
$ cd ~/work
$ wget https://cmake.org/files/v3.9/cmake-3.9.6-Linux-x86_64.tar.gz
$ tar xvzf cmake-3.9.6-Linux-x86_64.tar.gz
$ mv cmake-3.9.6-Linux-x86_64 cmake
$ cmake --version

> cmake version 3.9.6
```

→ success!

Build of SALMON

Installation example for “intel-avx” architecture

```
$ cd ~/work/
$ wget http://salmon-tddft.jp/download/SALMON-v.1.2.0.tar.gz
$ tar xvfz SALMON-v.1.2.0.tar.gz
$ cd SALMON-v.1.2.0
$ mkdir build
$ cd build
$ ../configure.py --arch=intel-avx --prefix=~/work/SALMON
$ make && make install
$ which salmon.cpu

> ~/work/SALMON/bin/salmon.cpu
```

→ success!

* Specify an appropriate --arch (architecture of the CPU in your computer)

Build of SALMON: Compile options

View help

```
$ ../configure.py --help
```

For more information → Install and Run (SALMON web page)

Explicit specification of compile options (example: gnu compilers)

```
$ ../configure.py FC=gfortran CC=gcc FFLAGS=-O3 …
```

Optional: Gnu Make

```
$ cd ~/work/SALMON-v.1.2.0/makefiles
$ make -f Makefile.<PLATFORM>
```

Run SALMON

Copy example input files & job.sh

```
$ cd ~/work
$ mkdir tmp
$ cd tmp
$ cp ~/work/SALMON-v.1.2.0/examples/C2H2/* .
```

Run

```
$ salmon.cpu < C2H2_gs.inp > out.log
```

* Ground state calculation of acetylene

Quick check of output

1. Standard output (out.log)

   Syntax error → “error(s) in input”

2. variables.log

   For check of input variables (including default)

   #namelist: <Namelist>, status= 0 or -1 → OK

   otherwise → error