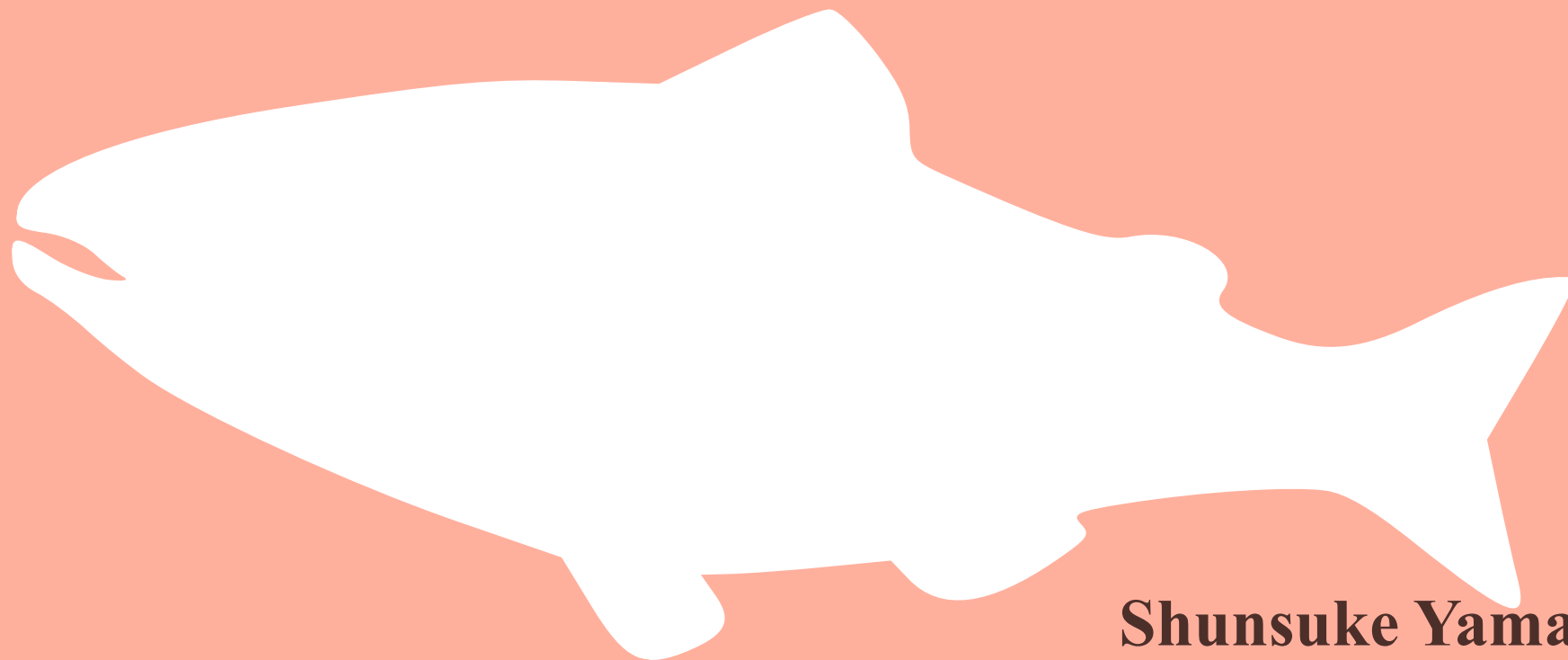


# Installation of SALMON



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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
```

Set compiling environment (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  
  -<PLATFORM>.tar.gz  
$ tar xvzf cmake-3.9.6-<PLATFORM>.tar.gz  
$ mv cmake-3.9.6-<PLATFORM> cmake  
$ cmake --version  
> cmake version 3.9.6
```

# Building of SALMON

## Installation example for “intel-avx” architecture

```
$ cd ~/work/  
$ wget http://salmon-tddft.jp/download/SALMON-v.1.0.0.tar.gz  
$ tar xvfz SALMON-v.1.0.0.tar.gz  
$ cd SALMON-v.1.0.0  
$ mkdir build  
$ cd build  
$ ../configure.py --arch=intel-avx --prefix=~/work/SALMON  
$ make && make install  
$ which salmon.cpu
```

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

# Building of SALMON: Compiler options

For more information

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

Manual specification of compiler options (example: gnu compilers)

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

Optional: Gnu Make

```
$ cd ~/work/SALMON-v.1.0.0/makefiles  
$ make -f Makefile.<PLATFORM>
```

# Run SALMON

## Copy example input files

```
$ cd ~/work  
$ mkdir tmp  
$ cd tmp  
$ cp ~/work/SALMON-v.1.0.0/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