University of Science and Technology of China

Invoking REANN model in a Fortran program

- How to invoke a C/C++ function in a Fortran program

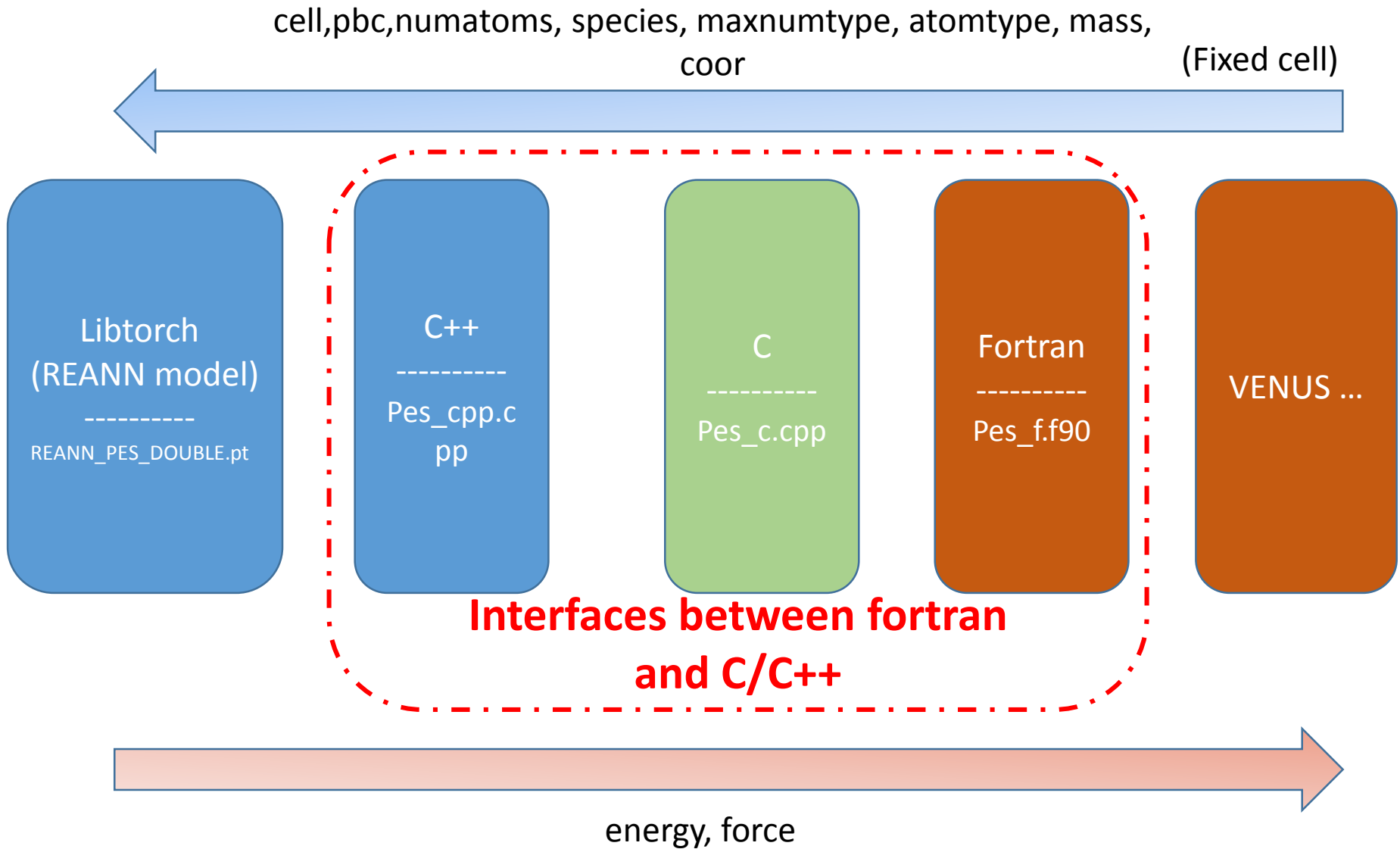Junfan Xia
2023.10.8

Outline

➢ **Code Architecture**

➢ **Code Compilation**

➢ **Example: VENUS**

Code architecture

Format to invoke REANN

```
!part-1 reann model initialization
call init_reann()
```

input_reann :

```
#cell    #DONNOT DELETE THE ANNOTATED LINES IN THIS INPUT FILE
 13.36712741   0.00000000   0.00000000
 -0.00000053  13.36712741   0.00000000
 -0.00000053  -0.00000053  13.36712741
#pbc
 1       1       1
#numatoms
192
#species masses
O  16.0
H  1.0
H  1.0
#maxnumtype
2
#atomtype
O
H
```

Order of species and atomtype should be as the same as that in the training process.

```
!part-2 reann model inference
call pes_ptr%reann_out(coor, energy_cal, force_cal)
```

```
!part-3 deallocate all variables realeated to reann
call delete_reann()
```

Preparation for Code Compilation

- ## Requirement

Software/Library	Version
CMake	3.19.3
GCC/Gfortran/G++	9.2.0
Pytorch	1.12.1
Libtorch-cpu/gpu	1.12.1
Cuda	11.3

- ## Environment variables

```
#gcc-9.2
source /public/software/gcc-9.2.0/gcc-9.2.sh
#cmake-3.19.3
export PATH=/public/software/cmake-3.19.3/bin:$PATH
#cuda
export CUDA_TOOLKIT_ROOT_DIR=/usr/local/cuda-11.3/
## setting for cuda CMAKE_CUDA_COMPILER
export PATH=/usr/local/cuda-11.3/bin/:$PATH
```

CMake

```
.
├── build                          Part III
│   ├── build.sh
│   └── clean-cmake.sh
├── cmake                          Part I
│   └── CMakeLists.txt
├── README
├── src                            Part II
│   ├── CMakeLists.txt
│   ├── interfaces
│   │   ├── CMakeLists.txt
│   │   ├── pes_c.cpp
│   │   ├── pes_c.h
│   │   ├── pes_cpp.cpp
│   │   ├── pes_cpp.hpp
│   │   └── pes_f.f90
│   └── test.f90
└── test
    ├── configuration
    ├── input_reann
    ├── REANN_PES_DOUBLE.pt
    ├── REANN_PES_FLOAT.pt
    └── test.sh
```

```
 1 cmake_minimum_required(VERSION 3.5 FATAL_ERROR)
 2
 3 project(recipe LANGUAGES Fortran CXX)
 4
 5 SET(CMAKE_CXX_RELEASE_FLAGS "$ENV{CXXFLAGS} -O3 -Wall -Wextra")
 6 SET(CMAKE_Fortran_FLAGS_RELEASE "-Wall -Wextra -lstdc++ -cpp -O3")
 7
 8 set(CMAKE_CXX_STANDARD 14)
 9 set(CMAKE_CXX_STANDARD_REQUIRED ON)
10 set(CMAKE_CXX_EXTENSIONS OFF CACHE BOOL "Use compiler extensions")
11
12 set(CMAKE_ARCHIVE_OUTPUT_DIRECTORY ${CMAKE_CURRENT_BINARY_DIR}/lib)
13 set(CMAKE_LIBRARY_OUTPUT_DIRECTORY ${CMAKE_CURRENT_BINARY_DIR}/lib)
14 set(CMAKE_RUNTIME_OUTPUT_DIRECTORY ${CMAKE_CURRENT_BINARY_DIR}/bin)
15 set(CMAKE_Fortran_MODULE_DIRECTORY ${CMAKE_CURRENT_BINARY_DIR}/modules)
16
17 message(STATUS "CMAKE_CURRENT_BINARY_DIR:  ${CMAKE_CURRENT_BINARY_DIR}")
18 message(STATUS "CMAKE_CURRENT_SOURCE_DIR:  ${CMAKE_CURRENT_SOURCE_DIR}")
19
20 get_filename_component(REANN_DIR ${CMAKE_CURRENT_SOURCE_DIR}/.. ABSOLUTE)
21
22 set(REANN_SOURCE_DIR ${REANN_DIR}/src)
23 add_subdirectory(${REANN_SOURCE_DIR} ./trash)
```

Compilation options

Path containing the final executable file

Path of the source code

```
 1  enable_language(C)
 2
 3  if(BUILD_CUDA)
 4      SET(CMAKE_PREFIX_PATH       /public/home/xjf/proj-22-0117/lammps/lammps-li
    btorch-1.10/pkg/libtorch-1.12.1-gpu)    # add to link the libtorch
 5      set(CUDA_TOOLKIT_ROOT_DIR "/usr/local/cuda-11.3/")
 6      set(CUDNN_LIBRARY "/usr/local/cuda-11.3/lib64/")
 7      set(CUDNN_INCLUDE_DIR "/usr/local/cuda-11.3/include/")
 8      message(STATUS "Building with libtorch ON GPU
 9         -- libtorch        :     ${CMAKE_PREFIX_PATH}
10         -- CUDA  ROOT      :     ${CUDA_TOOLKIT_ROOT_DIR}
11         -- CUDNN libraries :     ${CUDNN_LIBRARY}
12         -- CUDNN includes  :     ${CUDNN_INCLUDE_DIR};
13      ")
14  else()
15      SET(CMAKE_PREFIX_PATH       /public/home/xjf/proj-22-0117/lammps/lammps-li
    btorch-1.10/pkg/libtorch-1.12.1-cpu)    # add to link the libtorch
16      message(STATUS "Building with libtorch ON CPU
17         -- Libtorch        :     ${CMAKE_PREFIX_PATH}
18      ")
19  endif()
20
21  find_package(Torch REQUIRED)    #to find the torch in the path
```
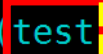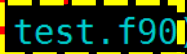
Path of Libtorch

CUDA-related paths

Path of Libtorch

```
22
23 add_executable(test test.f90)
24 target_sources(test
25   PRIVATE
26     interfaces/pes_cpp.cpp
27     interfaces/pes_c.cpp
28     interfaces/pes_f.f90
29   )
30
31 target_link_libraries(test
32   PRIVATE
33     ${TORCH_LIBRARIES}
34   )
```

Name of project name and executable file

Name of the main file

Names of other files

Build the program – Part III

build.sh :

```
cmake -D BUILD_CUDA=OFF -D CMAKE_Fortran_COMPILER=$(which gfortran) -D CMA
KE_CXX_COMPILER=$(which g++) -D CMAKE_C_COMPILER=$(which gcc) ../cmake
```

Compiling GPU version code requires a machine with GPU (CUDA).

```
(base) [xjf@R740xdproj-reann_cpp2f-fixedcell]$ ls
build   cmake   README   src   test
(base) [xjf@R740xdproj-reann_cpp2f-fixedcell]$ cd build/
(base) [xjf@R740xdbuild]$ sh clean-cmake.sh
(base) [xjf@R740xdbuild]$ sh build.sh
-- The Fortran compiler identification is GNU 9.2.0
-- The CXX compiler identification is GNU 9.2.0
-- Detecting Fortran compiler ABI info
```

······

```
-- Configuring done
-- Generating done
-- Build files have been written to: /public/home/xjf/code_tmp/cpp/cpp2fortran
/reann2venus/proj-reann_cpp2f-fixedcell/build
(base) [xjf@R740xdbuild]$ make
Scanning dependencies of target test
[ 20%] Building Fortran object trash/CMakeFiles/test.dir/interfaces/pes_f.f90.
o
[ 40%] Building Fortran object trash/CMakeFiles/test.dir/test.f90.o
[ 60%] Building CXX object trash/CMakeFiles/test.dir/interfaces/pes_cpp.cpp.o
[ 80%] Building CXX object trash/CMakeFiles/test.dir/interfaces/pes_c.cpp.o
[100%] Linking CXX executable ../bin/test
[100%] Built target test
```

Example: VENUS

```
(base) [xjf@R740xdproj-venus]$ ls
build  cmake  trash  VENUS-20200403
(base) [xjf@R740xdproj-venus]$ cd VENUS-20200403/
(base) [xjf@R740xdVENUS-20200403]$ ls
ADAMSM.f                GLPAR.f            NMODE.f         SELECT.f
ANGVEL.f                GPATH.f            nnmod.mod       SIZES
ArbitraryAxisRotation.f GRCONV.f           ORTHAN.f        STATPT.f
BAREXC.f                HEIGHT.f           others          SURF.f
CENMAS.f                HOMOQP.f           PARTI.f         SYBMOL.f
CMakeLists.txt          INITEBK.f          POTEN.f         SYMPLE.f
constant.mod            INITQP.f           POTENZ.f        tags
CPUSEC.f                interfaces_reann   PRINFO.f        test_t.py
DENQ.f                  JMAXCALC.f         PROBJ.f         t.f
DVDQ.f                  LMEXCT.f           QMMICRO.f       THERMBATH.f
EBOND.f                 LMODE.f            RADAU.f         THERMO.f
EIGN.f                  log                RAND0.f         THRMAN.f
EIGOUT.f                log_t              RAND1.f         uesr-co2
ENERGY.f                ma                 RANDST.f        VENUS.f
ENMODE.f                MAINLZ.f           readme          VERLET.f
FGMTRX.f                Makefile           ROTATE.f        VFDATE.f
FINAL.f                 makefile_eann      ROTATEJKM.f     VOLPSCONE.f
FINLNJ.f                makefile_eann_g    ROTATEJM.f      WEBOND.f
FMTRX.f                 makefile_eann_goon ROTATEX.f       WENMOD.f
GAMA.f                  Makefile_ini       ROTATEY.f       WLBOND.f
GASDEV.f                MICROCI.f          ROTATEZ.f       xgasdev.f
GFINAL.f                MPATH.f            ROTEN.f
GINROT.f                MPATHO.f           ROTN.f
GLO.f                   NMA.f              RUNGEK.f
```

```
set(REANN_SOURCE_DIR ${REANN_DIR}/VENUS-20200403)

add_executable(venus VENUS.f)
target_sources(venus
  PRIVATE
    ADAMSM.f ANGVEL.f BAREXC.f CENMAS.f
    DVDQ.f EBOND.f EIGN.f
    EIGOUT.f ENERGY.f ENMODE.f VFDATE.f FGMTRX.f
    FINAL.f FINLNJ.f FMTRX.f GAMA.f GFINAL.f MPATHO.f
    GINROT.f GLPAR.f GPATH.f GRCONV.f
    HOMOQP.f INITEBK.f INITQP.f
    LMEXCT.f LMODE.f MPATH.f NMODE.f ORTHAN.f
    PARTI.f POTEN.f RAND0.f RAND1.f RANDST.f ROTATE.f
    ROTEN.f ROTN.f RUNGEK.f SELECT.f SURF.f SYBMOL.f
    THRMAN.f VENUS.f
    WEBOND.f WENMOD.f WLBOND.f STATPT.f
    HEIGHT.f CPUSEC.f RADAU.f SYMPLE.f
    THERMO.f THERMBATH.f GASDEV.f
    POTENZ.f VERLET.f PRINFO.f MAINLZ.f
    MICROCI.f QMMICRO.f VOLPSCONE.f DENQ.f
    JMAXCALC.f PROBJ.f
    ROTATEX.f ROTATEY.f ROTATEZ.f
    ArbitraryAxisRotation.f ROTATEJM.f ROTATEJKM.f
    GLO.f
    interfaces_reann/pes_cpp.cpp
    interfaces_reann/pes_c.cpp
    interfaces_reann/pes_f.f90
    interfaces_reann/interface.f
    interfaces_reann/friction.f
    interfaces_reann/GWRITE.f
    interfaces_reann/cart_to_frac.f90
    interfaces_reann/TEST.f
)
```

```
SET(CMAKE_Fortran_FLAGS "-lstdc++ -cpp -std=legacy -fno-automatic -ffast-m
ath -W -fno-second-underscore -L/public/software/compiler/intel/intel-comp
iler-2017.5.239/mkl/lib/intel64 -lmkl_rt")
```

Example: VENUS


```fortran
!-->..ADDED BY BIN 12/29/2015
!-->..FOR GENERATING INITIAL RANDOM SEED
      SUBROUTINE INIT_RANDOM_SEED()
         IMPLICIT NONE
         INTEGER I,N,CLOCK
         INTEGER SEED(33) !(2) !
         CALL SYSTEM_CLOCK(COUNT=CLOCK)
         SEED=CLOCK+37*(/(I-1,I=1,33)/) !2
         CALL RANDOM_SEED(PUT=SEED)
      END SUBROUTINE
!-->..END
```

```
/public/home/xjf/code_tmp/cpp/cpp2fortran/reann2venus/proj-venus/VENUS-2020040
3/VENUS.f:2103:30:

 2103 |          CALL RANDOM_SEED(PUT=SEED)
      |                              1
Error: Size of 'put' argument of 'random_seed' intrinsic at (1) too small (2/3
3)
make[2]: *** [trash/CMakeFiles/venus.dir/VENUS.f.o] Error 1
```

Example: VENUS

```fortran
!-->Define your own potential for Venus below
!-->Initialize your potential parameters
      subroutine POTPRE()
      use pes_mod
      implicit real*8 (a-h,o-z)

      call init_reann()

      return
      end subroutine POTPRE
```

Example: VENUS

```fortran
!-->Link your own potenial here
       subroutine POT0(NATOMS,V)
       use pes_mod
       implicit real*8 (a-h,o-z)
       PARAMETER(NDA=160,NDA3=NDA*3,NDP=10,NDG=20)
       COMMON/QPDOT/Q(NDA3),PDOT(NDA3),FCOEF(NDA3,NDA3)
       COMMON/PQDOT/P(NDA3),QDOT(NDA3),W(NDA)
       COMMON/FRAGB/WTA(NDP),WTB(NDP),LA(NDP,NDA),LB(NDP,NDA),QZA(NDP,
     &NDA3),QZB(NDP,NDA3),NATOMA(NDP),NATOMB(NDP)
       COMMON/CONSTN/C1,C2,C3,C4,C5,C6,C7,PI,HALFPI,TWOPI
       common/surfpara/zbase
!forces shape should be (3, natoms-NRGD),which is general ,not (3,natoms-8)
       COMMON/VRSCAL/THERMOTEMP,NSEL,NSCALE,NEQUAL,NRGD
       dimension coor(3,natoms),forces(3,natoms-NRGD)
       do i=1,natoms
          coor(1,i)=Q((i-1)*3+1)
          coor(2,i)=Q((i-1)*3+2)
          coor(3,i)=Q(3*i)
       enddo

       call pes_ptr%reann_out(coor, vpot, forces)

       V=vpot*23.0605d0
       V=V*C1             ! to integration unit

       return
       end subroutine POT0
```

Example: VENUS

```fortran
!-----------------------------------------------------------
      subroutine deallocate_pes
      use pes_mod
      implicit none
      call delete_reann()
      return
      end subroutine
```