Embedded Parameters computations

Makefile\_embd\_mpi --- make file for compiling and creating the executable embdrun.exe (MPI version); To be used as: make -f Makefile\_embd\_mpi

Makefile\_embd\_ser --- make file for compiling and creating the executable embdrun\_ser.exe (serial version); To be used as: make -f Makefile\_embd\_ser

# This MODULE contains the following files:

# demo\_embd.f90:

This file is initializing the EMBD\_CLASS, which is the module used for calculations of the embedded # parameters. It contains the subroutines/functions

It is used to read the input parameters for the computations of the embedded parameters.

This subroutine calls the function 'EMBD\_DRIVER', which is part of the module EMBD\_CLASS found in these fortran files:

# embdmodule.f90 -- Parallel (using MPI protocols) of the EMBD\_CLASS

# embdmodule\_ser.f90 -- Serial version of the EMBD\_CLASS

# EMBD\_CLASS contains the following functions:

# subroutine EMBD\_DRIVER(Nf, Nd, Na, M1, M2, Tau1, tau2, db, frmt) -- it is the driver subroutine of the EMBD\_CLASS

# subroutine MPI\_Broadcast() -- it used to broad coast to all processors all attributes of the class EMBD\_CLASS

# subroutine read\_xyz() -- it is used to read the input time series representing the dynamical variables

# subroutine print\_embdparam() -- It prints out the embedded dimension parameters

# subroutine Allocate\_embeddedDim() -- It is used to allocate memory for the global dynamical variables of the EMBD\_CLASS

# subroutine deAllocate\_EmbeddedDim() -- It is used to free the memory allocated for the global dynamical variables of the EMBD\_CLASS

# subroutine CompEmbeddedDimensions\_fast() -- Computes the time shift and state vector dimension of time series - fast routine of MPI

# subroutine getTimeLag\_fast(Idof, tau\_arg) -- Calculates the time Lag using the fast routine - MPI version

# subroutine getOptEmbDim\_fast(idof, Mopt\_arg) -- Calculates the embedded dimension using the fast routine - MPI version

# subroutine CompEmbeddedDimensions\_slow() -- Computes the time shift and state vector dimension of time series - slow routine of MPI

# subroutine getTimeLag\_slow(N, x, tau\_min, tau\_max, tau\_arg, MI) -- Calculates the time Lag using the slow routine - MPI version

# subroutine getOptEmbDim\_slow(n, X, m1, m2, tau, Mopt, count\_fnn) -- Calculates the embedded dimension using the slow routine - MPI version

# subroutine CompEmbeddedDimensions(gtau, gmopt) -- Computes the time shift and state vector dimension of time series - serial routine

# subroutine getTimeLag(N, x, tau\_min, tau\_max, tau\_arg, MI) -- Calculates the time Lag using the serial routine

# subroutine getOptEmbDim(n, X, m1, m2, tau, Mopt, count\_fnn) -- Calculates the embedded dimension using the serial routine

# The input parameters of the module are:

Number of Time Frames - **Nframes**

Number of time series - **Natoms**

Dimensionality of the problem - **Ndim**

Time lag minimum value - **T1**

Time lag maximum value - **T2**

Embedded dimension minimum value - **M1**

Embedded dimension maximum value - **M2**

Set debugging flag value - **Debug**

Chose the format of Input/Output data **– frmt**

A bash shell script is given below:

*!#/bin/bash*

*root=../fortran*

*nframes=10000*

*natoms=2*

*ndim=1*

*T1=1*

*T2=100*

*M1=2*

*M2=20*

*Debug=1*

*parallel=0*

*NP=2*

*frmt=’csv’*

*if [ parallel == 1 ]; then*

*mpirun -np $NP ${root}/embdrun.exe ${nframes} ${natoms} ${ndim} ${T1} ${T2} ${M1} ${M2} ${Debug} ${frmt}*

*else*

*${root}/embdrun.exe ${nframes} ${natoms} ${ndim} ${T1} ${T2} ${M1} ${M2} ${Debug} ${frmt}*

*fi*