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HOW TO INSTALL AND IMPLEMENT THE MD-R– MOLECULAR DYNAMICS LIBRARY TO REPAST

The MD-R toolkit utilizes the developed 3D space projection to run short-range molecular dynamics simulations. The user is re required to install Repast HPC and all its components. The tutorial and details on Repast HPC can be found on its main website at:

http://repast.sourceforge.net/hpc_tutorial/TOC.html.

How to Install the MD-R Toolkit with Repast HPC

1. Go to http://engr.uconn.edu/~gelyko/md-repast-3d.html and download the MD-R toolkit library.

2. Add the header files, and the source files or the library files accordingly to the path in your makefile for compilation and linking.

3. Include in your code the appropriate header files from the MD-R library.

How to Run the Provided MD-R Demo

A demo of the MD-R toolkit is provided at http://engr.uconn.edu/~gelyko/md-repast-lib.html. It shows 3D simulations of (i) a Lennard-Jones liquid, (ii) a lipid bilayer model and (iii) a 2D network of particles moving in a 3D space and interacting via a worm-like chain potential.

Instructions for the demo:

1. Download and extract the demo file from the site above.

2. Modify the paths in the Makefile to specify the location of Repast HPC, the 3D projection, and MD-R. For example:

```
# Specify path for Repast HPC

BASE_DIR=[name of repast HPC folder]/RHPC_2.0

# Specify path for the 3D projection

MDR_3D_DIR=mdr-3d-projection/

# Specify path for MDR

MDR_DIR=mdr-lib/
```

3. Use the provided command "make clean" to clear all the object files and the executable file, if necessary, before recompilations.

4. Recompile the files by typing "make" to generate the executable file.

5. Confirm that boost mpi has been added to the path and then run the program by typing "mpirun -n 8 ./bin/mdr.exe props/config.props props/model.props".

Users can visualize the result of the program using the configuration viewer AtomEye, which can be downloaded at http://li.mit.edu/Archive/Graphics/A/