From: Mark Jack <mark.a.jack@gmail.com>
Subject: **latest c++ code for armchair rings**
Date: August 7, 2011 12:33:31 AM EDT
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2 Attachments, 6.8 MB

Just as a review for Leon, Boyan or ME who might want to run the new code themselves:

C++:
This is the C++ code with a folder of different coordinate files for different size (m,m) armchair nanorings with N (=imax=rows=columns) atoms. The file names should be self-explanatory. The code now reads in the data file 'ARRAY_posr.dat' in subroutine 'general.h'.

Steps:
- Simply copy the data file you want to choose to 'ARRAY_posr.dat'.

- Make the necessary adjustments in the main 'cntor.cpp' for variables rows (=imax), columns (=imax) and idim (=4*m) and in 'classes'h' for variable blockDimension (= idim = 4*m).

- Compile with 'make cntor' and run sequentially on a single processor with './cntor'.

- Compile and immediately run in parallel with 2 processors on a MAC with 'make runcntor'

- Compile on a cluster with './cntor' and submit as a parallel MPI job with their job submission tool and a job submission script. See attached shell scripts (*.sh) as examples for FSU HPC and 'Pegasus' at U Miami HPC.

FORTRAN:
Generate your own coordinates by compiling and running the Fortran code just briefly for a second to create a file called 'ARRAY_posr.dat'.
E.g. on a MAC: gfortran contor... .f -o cntor.out -framework vecLib. Execute with './cntor'. You don't have to wait for the code to calculate its first DoS / T value, just stop it and use the generated file.

Don't forget to adjust 'imax', 'idim' everywhere with a general 'find/replace' and adjust the torus size to physical dimensions. Scroll down in the code to find the definitions for 'bigr' and 'smallr'. 1.42 Angstrom constant C-C bond lengths assumed everywhere. See Fortran code attached as well.

PETSC:
You will have to have PETSc installed for the C++. A step-by-step guide was created by Adam at:
https://docs.google.com/document/d/1MpUYaHmLKutfAkmTkmtWM7nAZgVtNDdawtdimpWkmfM/edit?authkey=CNPqxO8K&pli=1
(or search for 'Nanotorus Simulation' with Google).
A slight modification of the PETSc installation for the C++ code is necessary for 'Pegasus' / U Miami HPC compared to FSU HPC to get it to work. See google docs description.

You will need working C/C++ and Fortran compilers. You need MAC OSX Leopard v. 10.6 or later versions on a MAC for the right GNU gcc compiler [5 bucks or ask me for a copy] and download the proper GNU gfortran compiler gfortran-snwleo-intel-bin.tar.gz from http://hpc.sourceforge.net. The Fortran compiler is not provided with the Xcode development tools on the Apple installation CD. So you will have to download it and replace any older Fortran compiler on your MAC with it.

And modules have to be loaded on Pegasus (not at FSU) so compilers and MPICH are available. After logging in, type on the command line following sequence: module load lsf, module load intel, module load mpich2/intel. Don't forget to set your

ennvironment variables for PETSC_DIR and PETSC_ARCH. See docu above.

SUMMARY:

Both codes are now prepared for the electron-phonon calculation which we are planning with Mike Leamy's input files from GeorgiaTech (simply replace second file read-in 'ARRAY_posr.dat' by a new file name that will contain the displaced atomic coordinates at a specific phonon mode; reserved for later).

The zigzag torus code will be provided soon (already exists for Fortran).

MJ

PETScCntorEP.zip (6.8 MB)

cntor-curren...s.f (41.9 KB)