Brief user guide / essentials for

QSpace / MPS Pack © A. Weichselbaum

Public / Open directory
`WBX=/home/a/Andreas.Weichselbaum/Matlab/X/`

most recent version: `MPSPACK_v3.0`

Brief comments on essential subdirectories

- `lib/` - bunch of frequently matlab routines
- `bin/` - QSpace mex routines (C++ QSpace library already compiled into matlab routines)
- `util/` - bunch of frequently used mex routines that are independent of QSpace
- `Source/` - C++ source files (just to give an idea; not necessarily up to date)
- `Class/@QSpace/` - (mostly) Matlab wrapper routines to C++ QSpace library
- `NRG/` - elementary (fdm)NRG routines
- `setup/` - exemplary NRG setup scripts
- `MCC/` - when you run jobs on the cluster, you will need to mcc-compile your Matlab program (this way, the cluster job won't need a Matlab license for every job that is submitted; there is no advantage in speed, otherwise; talk to one of the students using QSpace the first time you submit jobs to the cluster)

On the departments workstations as well as the ASC cluster, there is no need to recompile the mex files, since all systems work identical. I keep the binaries up to date. For help on the individual mex-routines, type on the matlab prompt `<name-of-mex-routine> -?`

Copy entire package to your home directory, e.g.
`rsync -rptv $WBX/MPSPACK_v3.0 <your-home-directory>/Matlab/`

General strategy

- use C++ routines (mex-routines) for actual calculations; input / output is either from / to the Matlab command line, or storage to files in matlab binary format
- do model setup and (graphical) analysis entirely within matlab

When starting matlab

- I usually use command-line mode only, therefore the logging of the routines is optimized for this type of usage (e.g. in terms of overwriting lines during calculations, etc.); feel free to use the matlab desktop, though, if you prefer.
- I myself stick to fixed matlab version (since matlab has a tendency to change things not always to the better); currently used version: `R2016a` (since Aug 2016)
- Matlab sources the `startup.m` file in the current directory if it finds one
- therefore to streamline the matlab startup, I put a shell script `ml` into `$WBX/bin/`; this sets environmental variables (such as matlab version to be used), as well as environmental variables used in `MPSPACK_v3.0/startup.m`
- see also `MPSPACK_v3.0/.*` files:
  `.bashrc, .functions, .matlab_setup.pl`

Default script to run NRG: `rnrg[.m]`

(in MPSPACK_v3.0/NRG; this call `NRGWilsonQS[.mexa64]`)

(Subsequent) default script to calculate correlation functions: `rdma[.m]`
(in MPSPACK_v3.0/NRG; this call `fdmNRG_QS[.mexa64]`)

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