

rpmbuild protocol on centos nodes

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Easy version

- Build dir: /groups/rccg/rpmbuild
- download source file in SOURCES
- do a test build first: extract file, configure, make, make install

with: prefix=/opt/apps_test/xxx

- write down the best configure and make options, avoid a buggy and slow build
- prepare the SPECS/xxx.spec file, R-3.1.2 and gromacs is a good template
- rpmbuild using the spec file
- install the RPMS/x86_64/xxx.rpm binary
- Clean up SOURCES and /opt/apps_test/

Decide LMOD dependency tree

- Core, Compiler, MPI
- Core: doesn't depend on anything,
like: gcc, intel, atlas, python, java, Matlab
- Compiler: depend on compiler,
like: openmpi, R
- MPI: depend on MPI version,
like: gromacs, VinaLC, VASP, ...

The purpose

- When a program runs, the environment is in agreement with when it was build
--automatically set up by Lmod
- e.g. you build your Gromacs with openmpi-1.8 and run it with openmpi-1.3, it will error out
- e.g. you build your R with Intel and runs it with gcc, you error out

Start to use LMOD

- `ssh clarinet001-198`
- `source /opt/centos/use_lmod.sh`
- Or put these in your `.bashrc`

```
if [ -e /etc/centos-release ]
then
    export PATH=/opt/centos/sys/bin:$PATH

    if [ -d /opt/centos/sys/profile.d ]; then
        for i in /opt/centos/sys/profile.d/*.sh; do
            if [ -r $i ]; then
                . $i
            fi
        done
    fi
fi
```

SPEC file break down

(pink-do not edit, black-edit)

R spec file

Summary: R statistics package

Name: R

Version: 3.1.2

Release: gcc48 --the dependency and release number, like: gcc48-openmpi18-02

License: GNU General Public License

Vendor: <http://www.r-project.org/>

Group: statistics/graphics

Source: R-3.1.2.tar.gz

Packager: HMS- jimi_chu@hms.harvard.edu

AutoReqProv: no

%description

R is a free software environment for statistical computing and graphics.

```
%define debug_package %{nil}
```

```
%define comp_fam gcc
```

```
%define comp_ver 4.8.2
```

```
%define mpi_fam openmpi
```

```
%define mpi_ver 1.8.4
```

```
##do not modify these
```

```
%define APPS      /opt/centos/apps
```

```
%define MODULES  modulefiles
```

```
%define comp_fam_ver %{comp_fam}-${comp_ver}
```

```
%define mpi_fam_ver %{mpi_fam}-${mpi_ver}
```

```
%define set_tree error
```

```
##end do not
```

```
## MUST set ONLY one of the three to 1
```

```
%define dep_mpi 0
```

```
%define dep_comp 1
```

```
%define is_core 0
```

##do not change these

%if "%{is_core}" == "1"

%define PKG_BASE %{APPS}/%{name}

%define INSTALL_DIR %{PKG_BASE}/%{version}

%define MODULE_DIR %{APPS}/%{MODULES}/Core/%{name}

%define set_tree 1

%endif

%if "%{dep_comp}" == "1"

%define PKG_BASE %{APPS}/%{comp_fam_ver}/%{name}

%define INSTALL_DIR %{PKG_BASE}/%{version}

%define MODULE_DIR %{APPS}/%{MODULES}/Compiler/%{comp_fam}/%{comp_ver}/%{name}

%define set_tree 1

%endif

%if "%{dep_mpi}" == "1"

%define PKG_BASE %{APPS}/%{comp_fam_ver}/%{mpi_fam_ver}/%{name}

%define INSTALL_DIR %{PKG_BASE}/%{version}

%define MODULE_DIR %{APPS}/%{MODULES}/MPI/%{comp_fam}/%{comp_ver}/%{mpi_fam}/%{mpi_ver}/%{name}

%define set_tree 1

%endif

%if "%{set_tree}" == "error"

%{error: You must set the compiler/mpi/core tree !}

exit

%endif

##end do not

%prep

rm -rf \$RPM_BUILD_ROOT/%{INSTALL_DIR}

%setup -n R-%{version}

---R-%{version} is the actual extracted folder name,

---it may vary from tar file

%build

mkdir -p \$RPM_BUILD_ROOT/%{INSTALL_DIR}

mkdir -p %{INSTALL_DIR}

```
cat >> config.site << 'EOF'
```

```
CFLAGS='-g -O3'
```

```
FFLAGS='-g -O3'
```

```
CXXFLAGS='-g -O3'
```

```
FCFLAGS='-g -O3'
```

```
BLAS_LIBS="-L${HMS_OPENBLAS_LIB} -lopenblas"
```

```
EOF
```

```
##make sure the modules agree with the parameters
```

```
module purge
```

```
module load gcc/4.8.2
```

```
module load openblas/0.2.13
```

```
./configure --prefix=%{INSTALL_DIR} --with-blas --with-lapack --with-x=no
```

```
make
```

```
make install
```

```
##make the R_LIB built-in
```

```
sed -i.old '1s;^;rlibname <- paste0(Sys.getenv("HOME"),"/R/library/",getRversion(),"_", "%  
{comp_fam_ver}")\ninvisible(system(paste("mkdir","-p",rlibname), intern =  
TRUE))\nSys.setenv("R_LIBS" = rlibname)\nSys.setenv("R_LIBS_USER" = rlibname)\n;' %  
{INSTALL_DIR}/lib64/R/library/base/R/Rprofile
```

--content of this page are learned from test compile

--typically just: configure, make, make install

--addition contents are for optimization and automation

```
cp -rp %{INSTALL_DIR}/ $RPM_BUILD_ROOT/%{INSTALL_DIR}/..
```

```
##create modulefiles
```

```
rm -rf $RPM_BUILD_ROOT/%{MODULE_DIR}
```

```
mkdir -p $RPM_BUILD_ROOT/%{MODULE_DIR}
```

```
cat > $RPM_BUILD_ROOT/%{MODULE_DIR}/%{version}.lua << 'EOF'
```

```
load("openblas/0.2.13")
```

--additional dependencies load here

```
help([[
```

The R modulefile defines the following environment variables

HMS_R_DIR for the location of the R distribution.

--every env variable start with HMS_name_

```
Version %{version}
```

```
]])
```

```
whatis("Name: R")
```

```
whatis("Version: %{version}")
```

```
whatis("Category: statistics")
```

```
whatis("Keywords: statistics, graphics, ")
```

```
whatis("Description: R is a language and environment for statistical computing and graphics.")
```

```
whatis("URL: http://www.r-project.org/")
```

```
setenv( "HMS_R_DIR", "%{INSTALL_DIR}")
```

--depends, may also need _BIN, _INC, _LIB

```
-- Append/prepend path
```

```
prepend_path("PATH", "%{INSTALL_DIR}/bin")
```

--may also need LD_LIBRARY_PATH

```
EOF
```

finish

%files

%defattr(-,rc200,rccg,-) --set this to your userID

%{INSTALL_DIR}

%{MODULE_DIR}

%post

%postun

%clean

rm -rf \$RPM_BUILD_ROOT

Build and Install RPM

```
$ rpmbuild -ba SPECS/xxx.spec
```

```
$ sudo rpm -ivh RPMS/x86_64/xxx.rpm
```

- clean up SOURCES, keep only tar files and
- clean up /opt/apps_test/
- test the module you just put up