

Case Studies of Existing Rolls

Building MGL roll

Rocks-A-Palooza I

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Prepare for the build

Check out CVS Rocks distribution

- cvs d:pserver:anonymous@cvs.rocksclusters.org:/home/cvs/CVSROOT login
- cvs d:pserver:anonymous@cvs.rocksclusters.org:/home/cvs/CVSROOT checkout -r ROCKS_3_3_0 rocks

Go to the roll's directory

- # cd rocks/src/roll/mgl
- > # Is

CVS/ graphs/ Makefile nodes/ src/ version.mk



File graphs/default/mgl.xml

```
<?xml version="1.0" standalone="no"?>
<!DOCTYPE kickstart SYSTEM "@GRAPH_DTD@">
<graph>
                                         color specified
    <description>
                                         in version.mk
    MGL Roll
    </description>
                                                              mgl
    <changelog>
    $Log: mgl.xml,v $
                                    root
                                                 server
    </changelog>
    <edge from="server" to="mgl"/>
</graph>
```

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File nodes/mgl.xml

```
<?xml version="1.0" standalone="no"?>
<!DOCTYPE kickstart SYSTEM "@KICKSTART_DTD@">
<kickstart>
   <description>
   Python based software developed at the Molecular Graphics Lab (MGL)
   </description>
   <copyright></copyright>
   <changelog>$Log: mgl.xml,v $<changelog>
   <package>mgl-tools</package>
   <package>mgl-swig</package>
   <package>rocks-mgl</package>
   <package>roll-mgl-usersguide</package>
   <post></post>
</kickstart>
```



Contents of src/

- # mkdir rocks
 - user profile files
- # mkdir tools
 - ⇒ mgl tarball
- # mkdir swig
 - prerequisite software for mgl tools
- # mkdir usersguide
 - users guide placeholder, used for real guide development



src/rocks/

create mgl.sh (and mgl.csh)

```
export MGL_ROOT="/opt/mgl"
export PATH="$MGL_ROOT/bin:$PATH"
if [-z "$LD_LIBRARY_PATH"]; then
export LD_LIBRARY_PATH="$shlibdirs"
else
export LD_LIBRARY_PATH="$shlibdirs:$LD_LIBRARY_PATH"
fi
```

Makefile

```
install::
```

mkdir -p \$(ROOT)/etc/profile.d install -m755 mgl.* \$(ROOT)/etc/profile.d

version.mk

```
NAME = rocks-mgl
RELEASE = 0
VERSION = 3.3.0
5/20/05
```



src/swig/

Is src/swig

CVS/ Makefile SWIG-1.3.22.tar.gz mgl-swig.spec.in version.mk

version.mk

```
NAME = mgl-swig
RELEASE = 0
VERSION = 1.3.22
SWIG = SWIG
```

◆ Makefile

```
PKGROOT=/opt/mgl
install::
    mkdir -p $(ROOT)/$(PKGROOT)
    (cd $($WIG)-$(VERSION); make prefix=$(ROOT)/$(PKGROOT) install;)
build:
    gunzip -c $($WIG)-$(VERSION).tar.gz I tar -x
    (cd $($WIG)-$(VERSION); ./configure --prefix=$(PKGROOT); make)
```



src/tools/

Is src/tools

CVS/ Makefile.mgl.in mgl-tools.spec.in

Install.sh.in mgl-tools-1.3.alpha1.tar.gz patch-files/

Makefile mgl-tools-1.3.alpha2.tar.gz version.mk

patch-files/

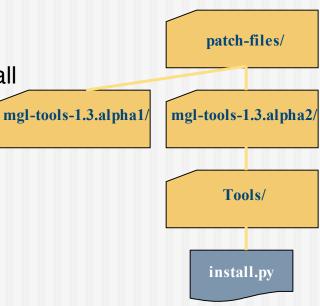
- drop-in files to substitute originals
- same directory structure as in the tarball

version.mk

NAME = mgl-tools

RELEASE = 0

VERSION = 1.3.alpha2





src/tools/Makefile

```
PKGROOT = /opt/mgl
MGL_ROOT = $(PKGROOT)
SEDSPEC += \
    -e 's%@MGL_ROOT@%$(MGL_ROOT)%g'
install::
    mkdir -p $(ROOT)/$(PKGROOT)
    (cd $(NAME)-$(VERSION); make prefix=$(ROOT)/$(PKGROOT) install;)
build:
    gunzip -c $(NAME)-$(VERSION).tar.gz I tar -x
    $(SED) $(SEDSPEC) Install.sh.in > $(NAME)-$(VERSION)/Install.sh
    $(SED) $(SEDSPEC) Makefile.mgl.in > $(NAME)-$(VERSION)/Makefile
    cd patch-files && find . -type f I grep -v CVS I cpio -pduv ../
```



Sedspec substitution

Install.sh.in

```
export MGL_ROOT="@ROOT@/@MGL_ROOT@"
export MGL_PURE_ROOT="@MGL_ROOT@"
....

Install.sh
```

export MGL_ROOT="<path-where-building>/opt/mgl" export MGL_PURE_ROOT="/opt/mgl"

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Building

- Build rpms
 - # cd mgl/src/rocks; make rpm
- Build roll
 - ⇒ # cd mgl; make roll
- Result

mgl/RPMS/i386:

- mgl-swig-1.3.22-0.i386.rpm
- mgl-tools-1.3.alpha2-0.i386.rpm

mgl/RPMS/noarch:

- rocks-mgl-3.2.0-0.noarch.rpm
- roll-mgl-usersguide-3.3.0-0.noarch.rpm
- roll-mgl-kickstart-3.3.0-0.noarch.rpm

mgl:

or roll-mgl-3.3.0-0.i386.iso