Hacking Gromacs: Getting Your Feet Wet With CVS Code

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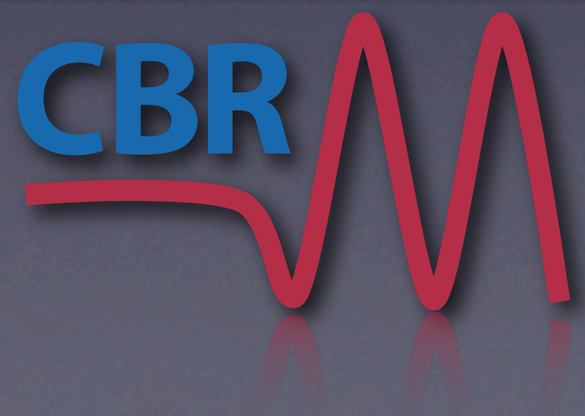
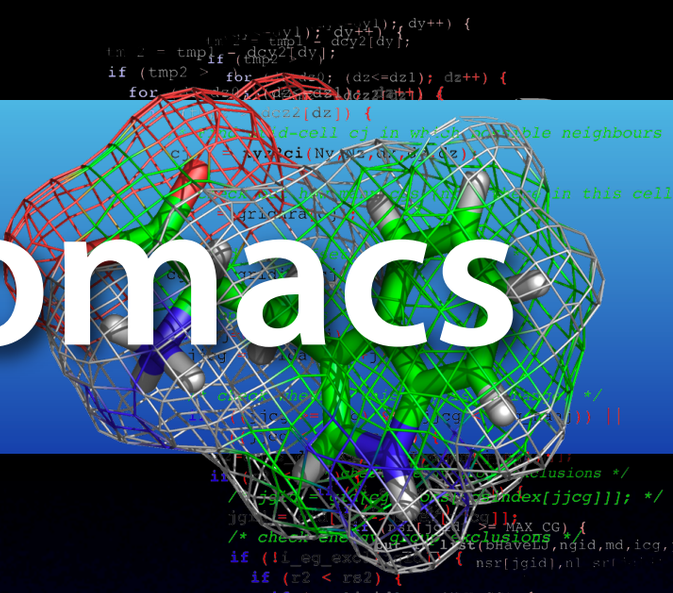
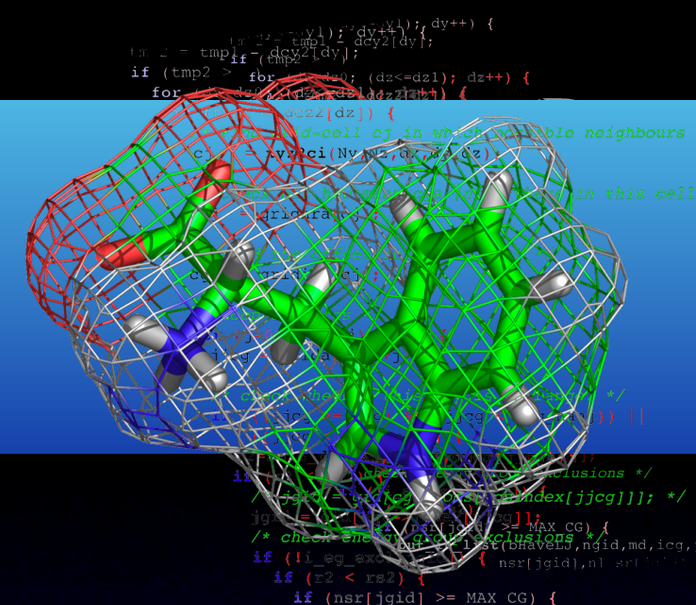


Outline: Hacking Gromacs



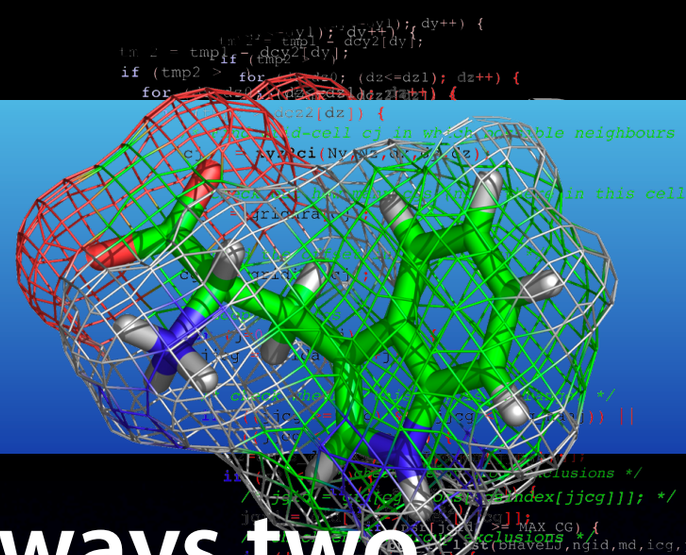
- Release vs. development codebase
- Building the CVS version(s) of Gromacs
- Configuration with automake & autoconf
- Architecture
- Organization of the source code
- Examples of modifications
- Good bug reports & patches
- Creating “distribution tarballs”

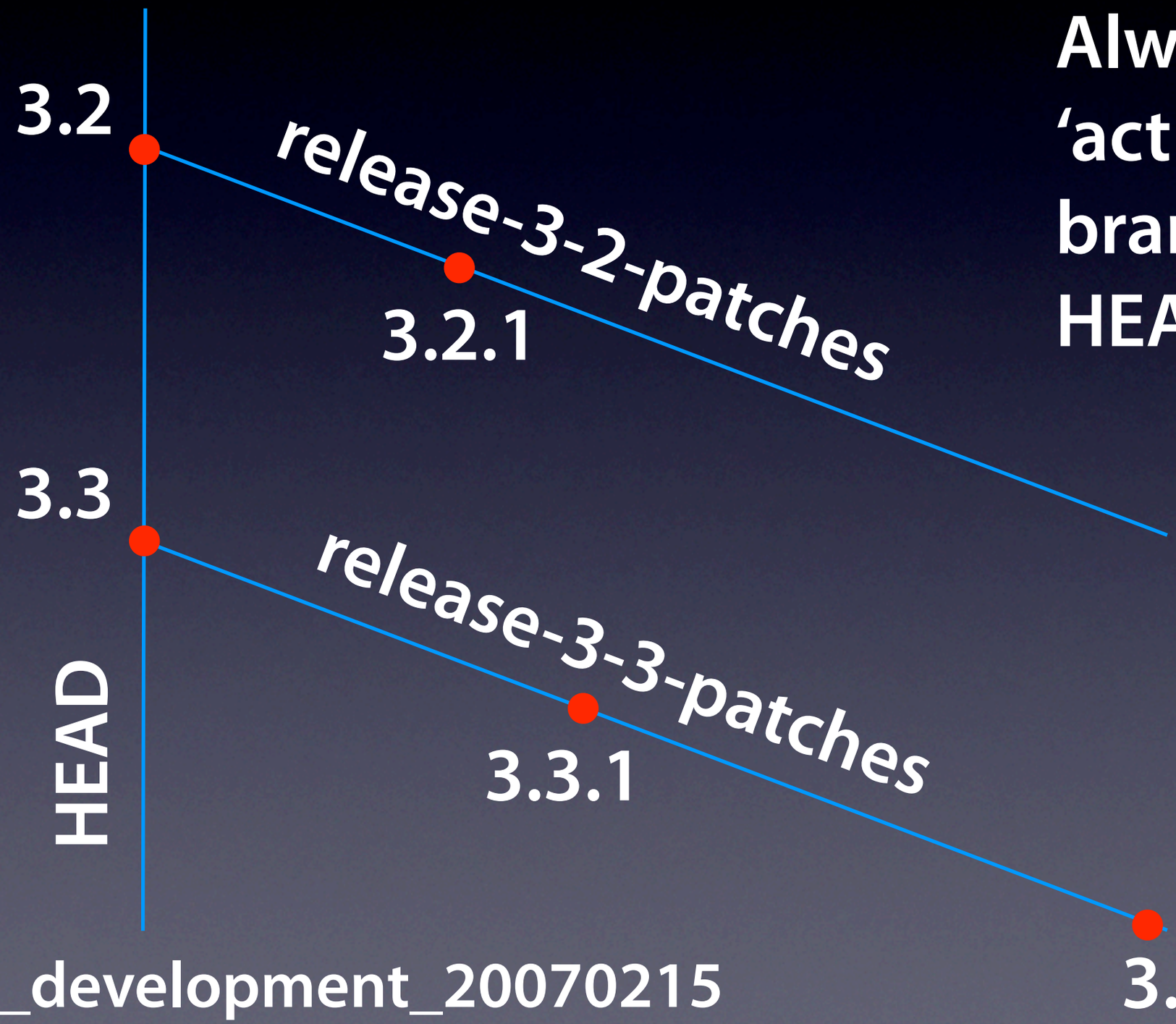
CVS repository



- Tracks all changes in Gromacs files
- Real-time update (whenever we check in)
- “How did stat.c change from 3.1.3 to 3.1.4?”
- Comments to all changes
- Immediate access to bug fixes
- Access to latest development version
- Test sets, manual source, etc.
- Completely public read-only access!

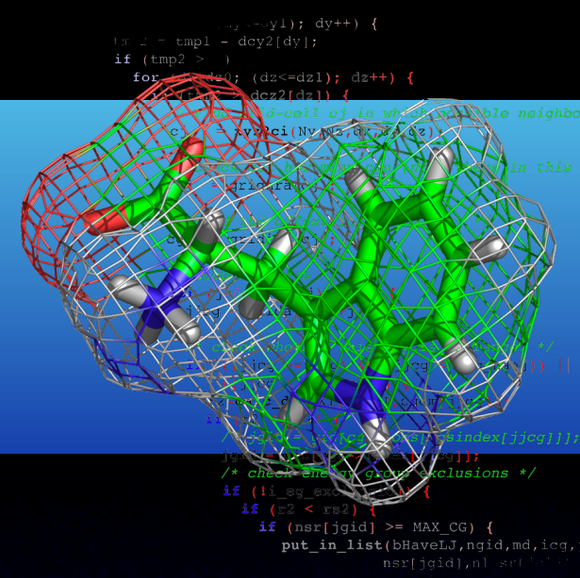
CVS branches





Always two ‘active’ branches: HEAD & patches

Using CVS



- You probably have it installed (‘which cvs’)
- Instructions available on Gromacs site
- First log in (anonymously)

```
$>cvs -z3 -d :pserver:anoncvs@cvs.gromacs.org:/home/gmx/cvs login
Password: [leave blank, hit return]
```

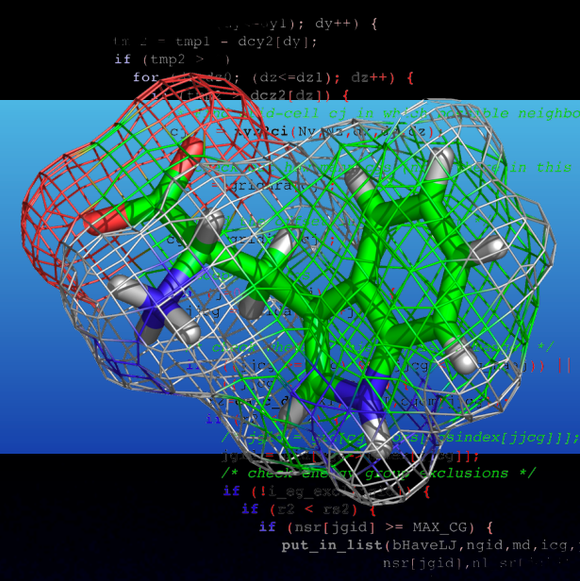
- “Check out” latest HEAD version:

```
$>cvs -z3 -d :pserver:anoncvs@cvs.gromacs.org:/home/gmx/cvs co gmx
```

- Check out the release branch instead: (1 line)

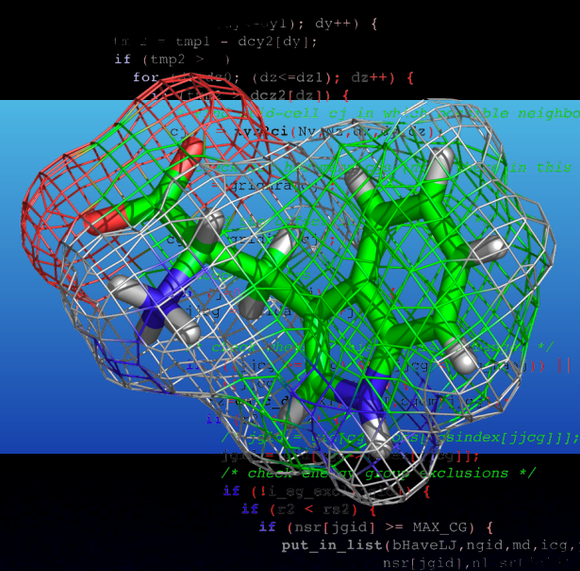
```
$>cvs -z3 -d :pserver:anoncvs@cvs.gromacs.org:/home/gmx/cvs \
      co -r release-3-3-patches gmx
```

Working with CVS



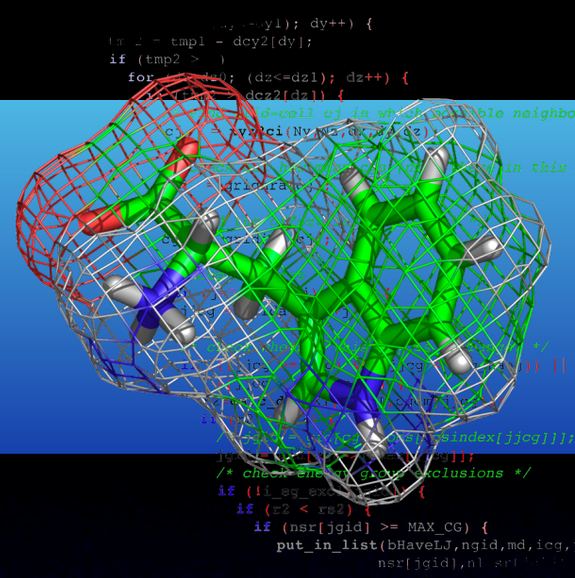
- The CVS ‘co’ command checks out a Gromacs version in a gmx subdirectory
- You cannot built yet - no configure script!
- Create it with command “./bootstrap”
- What is the configure script, really?

Configuration

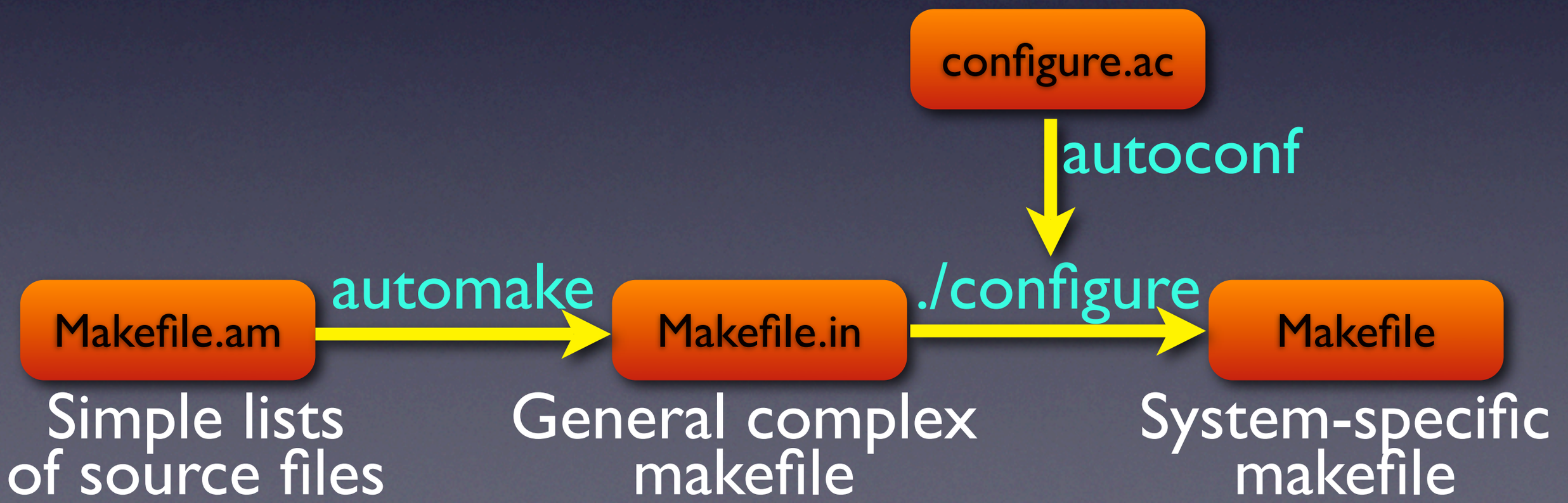


- “Where is the X11 library?”
- “What version is the FFTW library?”
- “Is the Intel Math Kernel Library installed?”
- “Do we have that buggy gcc version?”
- “Does the compiler understand assembly?”
- “Which flags should be used for this compiler?”
- “Is this a big or small endian system?”
- “Is a long integer 4 or 8 bytes?”
- “How do we build a shared library here?”

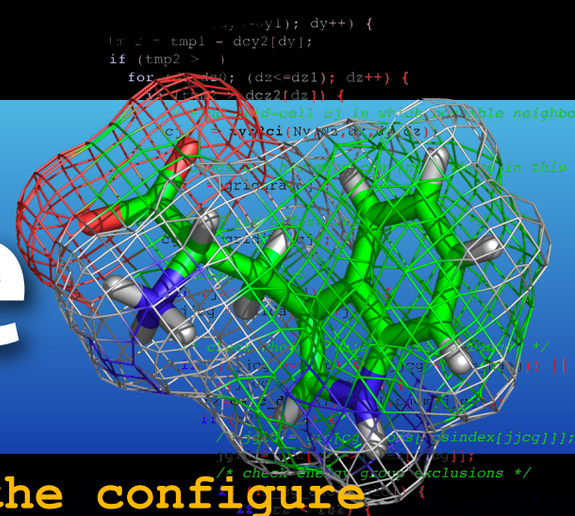
GNU autotools



- Automatic system configuration
- “Ugly tools for an ugly world”
- Avoid editing complicated makefiles



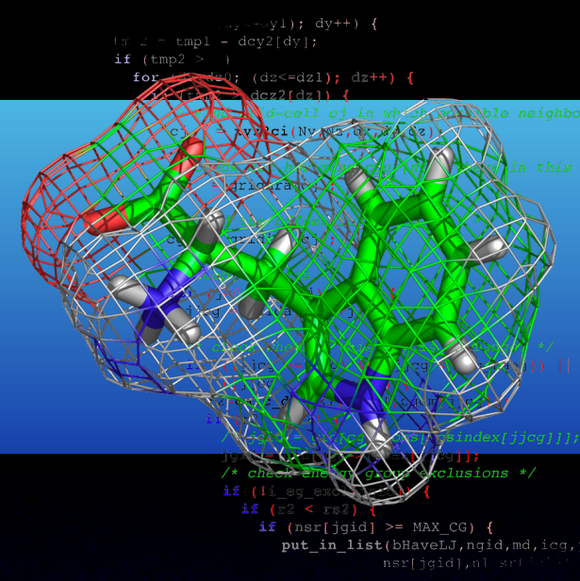
Makefile.am example



```
# Note: Makefile is automatically generated from Makefile.in by the configure
# script, and Makefile.in is generated from Makefile.am by automake.

AM_CPPFLAGS = -I$(top_srcdir)/include -DGMXLIBDIR=\"$(datadir)/top\"

LDADD = ../mdlib/libmd@LIBSUFFIX@.la ../gmxlib/libgmx@LIBSUFFIX@.la

bin_PROGRAMS = \
        grompp          mdrun           tpbconv         pdb2gmx         \
        protonate       luck            gmxdump                         \
        gmxcheck        x2top           ffscan
...
mdrun_SOURCES = \
        glaasje.c       glaasje.h       gctio.c         init_sh.c       \
        ionize.c        ionize.h        xmdrun.h        \
        do_gct.c        relax_sh.c      repl_ex.c       repl_ex.h       \
        xutils.c        compute_io.h    compute_io.c \
        md.c            mdrun.c         genalg.c        genalg.h
```

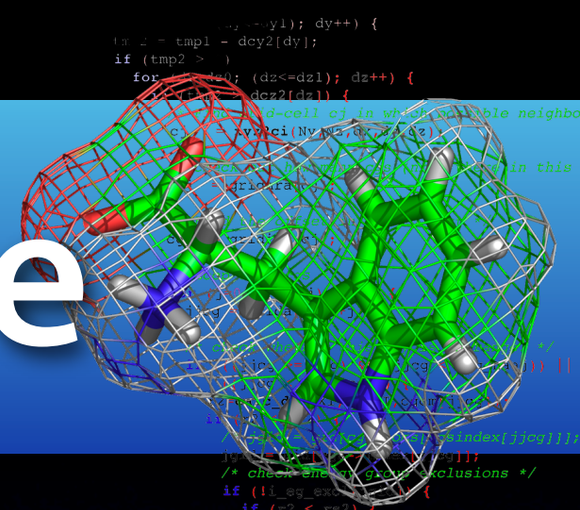
Note: No system-specific stuff or conditional libraries!
(We *never* look in the autogenerated complex Makefile.in)

Autoconf



- How do we do the system configuration?
  - Cannot count on anything being present
    - Use an extremely generic shell script!
- This script (configure) is generated automatically for us by autoconf, from an input specification in the file configure.ac (written in the M4 macrolanguage)

configure.ac example

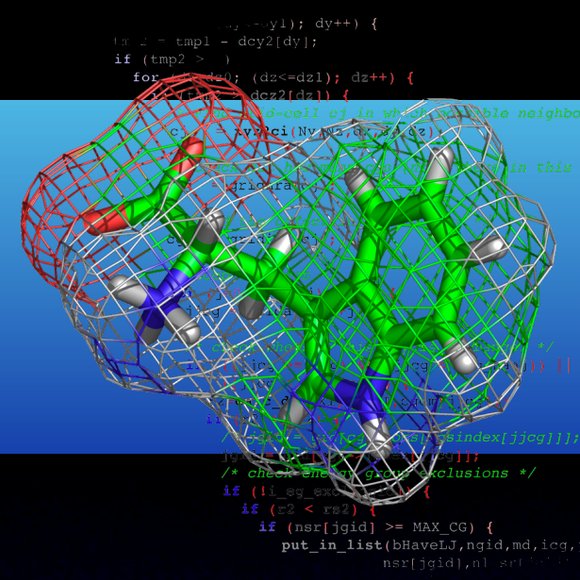


```
##############################################################
# Process this file wth autoconf to produce a configure script.
##############################################################

AC_PREREQ(2.50)
AC_INIT(GROMACS, 3.3.1, gmx-users@gromacs.org)
AC_CONFIG_SRCDIR(src/gmxlib/3dview.c)
AC_CONFIG_AUX_DIR(config)
AC_CANONICAL_HOST
```

```
...
### Single/Double
AC_ARG_ENABLE(float,
  [  --disable-float              use double instead of single precision],, enable_float=yes)
...
AC_CHECK_SIZEOF(int)
AC_CHECK_SIZEOF(long int)
...
#####
# Checks for additional and/or optional functions or libraries.
#AC_FUNC_MALLOC
AC_FUNC_MEMCMP
AC_TYPE_SIGNAL
```

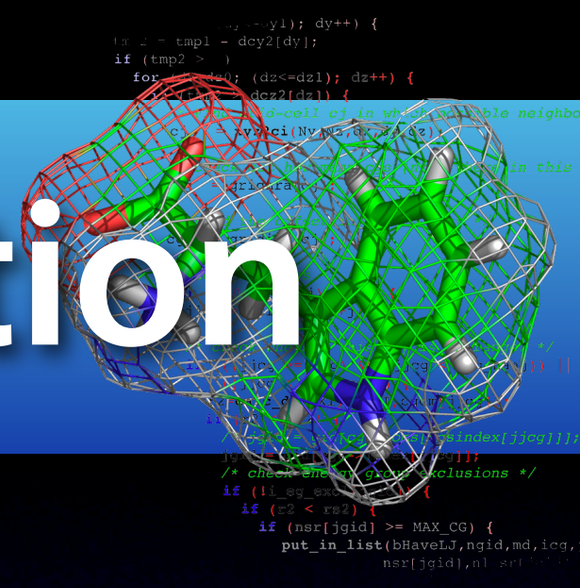
Many pre-existing macros (our own are in acinclude.m4)
autoconf uses libtool to create shared libraries portably

Building Gromacs



- After running ./bootstrap, you have the same setup as a Gromacs distribution
- Building Gromacs:
  - ./configure --prefix=/some/install/path (errors? read the end of config.log)
  - make -j # (#=number of CPUs you have)
  - make install

Source tree organization



- gmx
  - admin
  - config
  - scripts
  - man
  - share
    - html
    - tutor
    - template
    - top
  - include
    - types
  - src
    - gmxlib
      - nonbonded
    - mdlib
    - kernel
    - tools
    - ngmx
    - contrib

low-level routines

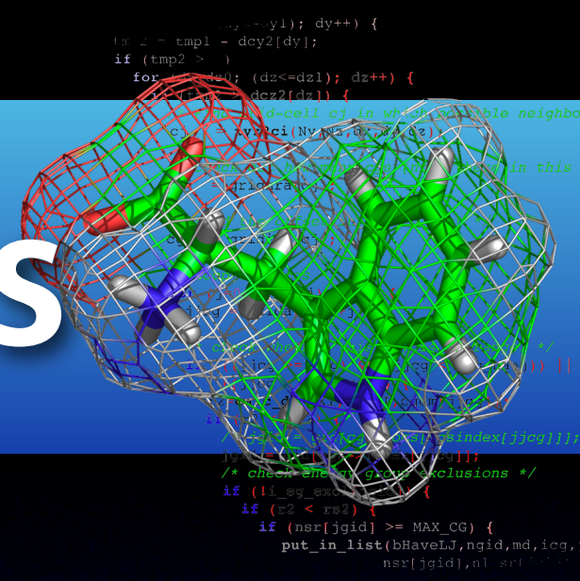
data structure definitions

assembly kernels

high-level routines

core programs

Gromacs flowcharts



- High level path through the source code during a simulation
- Calculating forces
- Data structures, neighbor lists
- Original charts by Gerrit Groenhof

mdrun -v -s topol.tpr

main()
kernel/mdrun.c

mdrunner()
kernel/md.c

do_md()
kernel/md.c

do_nm()
mdlib/minimize.c

do_lbfgs()
mdlib/minimize.c

do_cg()
mdlib/minimize.c

do_steep()
mdlib/minimize.c

Normal modes

Minimization

main loop over MD steps

do_force()
mdlib/sim_util.c

Details on next slide

write_traj()
mdlib/stat.c

update()
mdlib/update.c

do_update_md()
mdlib/update.c

constrain()
mdlib/constr.c

print statistics and quit
kernel/md.c

do_force()
mdlib/sim_util.c

ns()
mdlib/force.c

force()
mdlib/force.c

do_nonbonded()
gmxlib/nonbonded/nonbonded.c

gmx_pme_do()
mdlib/pme.c

calc_bonds()
gmxlib/bondfree.c

setup_kernels() called on first execution of do_nonbonded()

search_neighbors()
mdlib/ns.c

nb_kernel312()
../nonbonded/nb_kernel/nb_kernel312.c

nb_kernel312_x86_64_sse()
../nb_kernel312_x86_64_sse.s

Function pointers!

gmx_nb_free_energy_kernel()
gmxlib/nonbonded/nb_free_energy.c

spread_q_bsplines()
mdlib/pme.c

+3D FFT

solve_pme()
mdlib/pme.c

+3D iFFT

gather_f_bsplines()
mdlib/pme.c

bonds(), angles(), pdihs(), etc
gmxlib/bondfree.c

do_nonbonded14()
gmxlib/nonbonded/nonbonded.c

nb_kernel100_c.c:

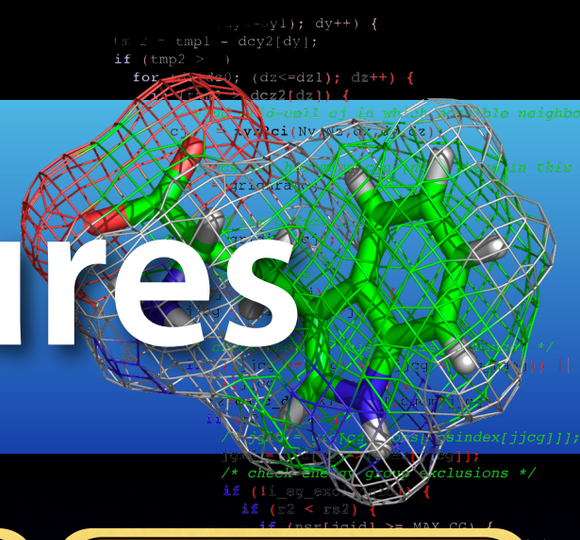
```
...
        for(k=nj0; (k<nj1); k++)
        {
          jnr             = jjnr[k];
          j3              = 3*jnr;
          jx1             = pos[j3+0];
          jy1             = pos[j3+1];
          jz1             = pos[j3+2];
          dx11            = ix1 - jx1;
          dy11            = iy1 - jy1;
          dz11            = iz1 - jz1;
          rsq11           = dx11*dx11+dy11*dy11+dz11*dz11;
          rinv11          = 1.0/sqrt(rsq11);
          qq              = iq*charge[jnr];
          rinvsq          = rinv11*rinv11;
          vcoul           = qq*rinv11;
          vctot           = vctot+vcoul;
          fscal           = (vcoul)*rinvsq;
          tx              = fscal*dx11;
          ty              = fscal*dy11;
          tz              = fscal*dz11;
          fix1            = fix1 + tx;
          fiy1            = fiy1 + ty;
          fiz1            = fiz1 + tz;
          faction[j3+0] = faction[j3+0] - tx;
          faction[j3+1] = faction[j3+1] - ty;
          faction[j3+2] = faction[j3+2] - tz;
        }
...
```

x4

nb_kernel100_x86_64_sse.s

```
;# calculate rinv=1/sqrt(rsq)
rsqrtps xmm5, xmm1
movaps xmm2, xmm5
mulps xmm5, xmm5
unpcklps xmm0, xmm7  ;# jqa jqb jqc jqd
movaps xmm4, [rsp + nb100_three]
mulps xmm5, xmm1 ;# rsq*lu*lu
subps xmm4, xmm5 ;# 30-rsq*lu*lu
mulps xmm4, xmm2
mulps xmm0, [rsp + nb100_iq]
mulps xmm4, [rsp + nb100_half]
movaps xmm1, xmm4
mulps  xmm4, xmm4
;# xmm1=rinv
;# xmm4=rinvsq

;# calculate coulomb interaction, xmm0=qq
mulps  xmm0, xmm1   ;# xmm0=vcoul
mulps  xmm4, xmm0   ;# xmm4=fscal

;# add potential to vctot (sum in xmm12)
addps  xmm12, xmm0

mov rsi, [rbp + nb100_faction]
;# the fj's - accumulate x & y forces from memory
movlps xmm0, [rsi + r8*4] ;# x1 y1 - -
movlps xmm1, [rsi + r10*4] ;# x3 y3 - -
movhps xmm0, [rsi + r9*4] ;# x1 y1 x2 y2
movhps xmm1, [rsi + r11*4] ;# x3 y3 x4 y4

;# calculate scalar force by multiplying dx with fscal
mulps  xmm9, xmm4
mulps  xmm10, xmm4
mulps  xmm11, xmm4

;# xmm0-xmm2 contains tx-tz (partial force)
;# accumulate i forces
addps xmm13, xmm9
addps xmm14, xmm10
addps xmm15, xmm11
```

Common data structures



topology

name
guess!
idef
bonded interactions
atoms
mass, charge, etc.
block[]
block definitions
symtab
name references

inputrec

all the mdp options
nsteps
ns_type
nstlist
nstxout
pme_order
...
userint1-4
userreal1-4

forcerec

derived options
rlist
neighborlist cutoff
epsilon_r
eeltype
cutoff/RF/PME
vdwtype
cutoff/bham/tables
nnblists
nblists[]
neighborlists
nbfp
nonbonded params

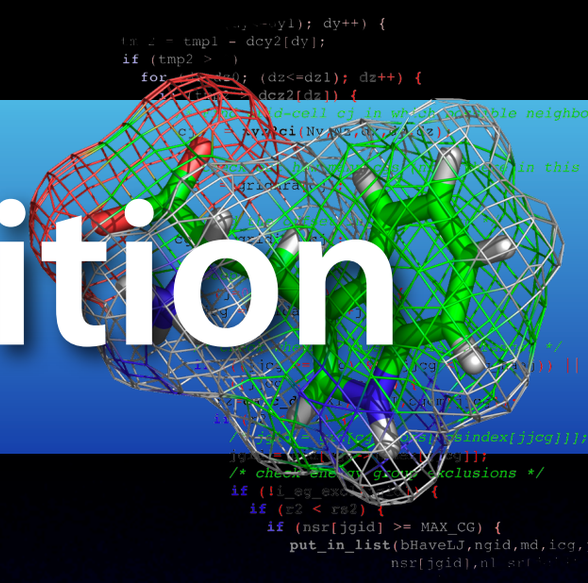
mdatoms

massA/B
particle mass
chargeA/B
particle charge
typeA/B
particle LJ type
cTC[]
T-coupling groups
cENER[]
Energy groups
cFREEZE[]
Freeze groups

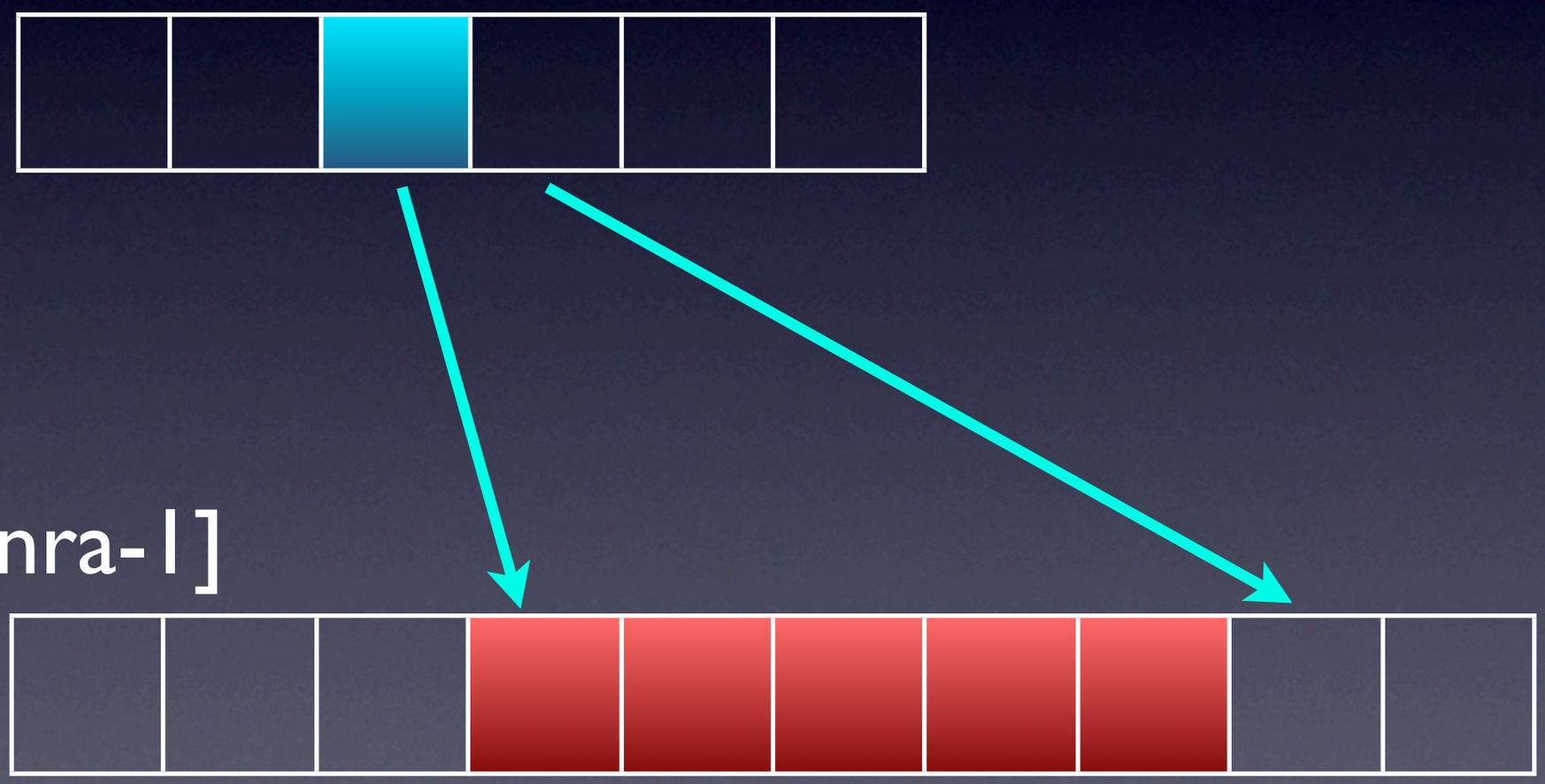
block

nr
#blocks
index[]
array with indices in a[]
nra
number of atoms
a[]
array with atom numbers in each group

Gromacs block definition

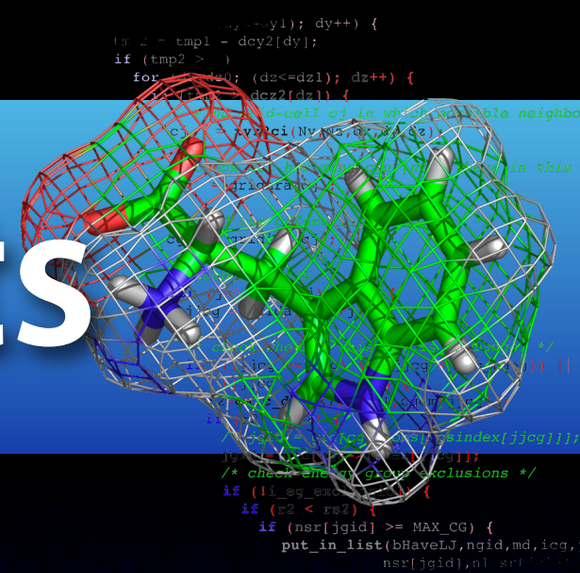


index[0,..,nr-1]



index[0,..,nra-1]

Gromacs neighborlists



topology

il_code
index to nb kernel

icoul / ivdw
Coul & vdw type

nri
number of lists

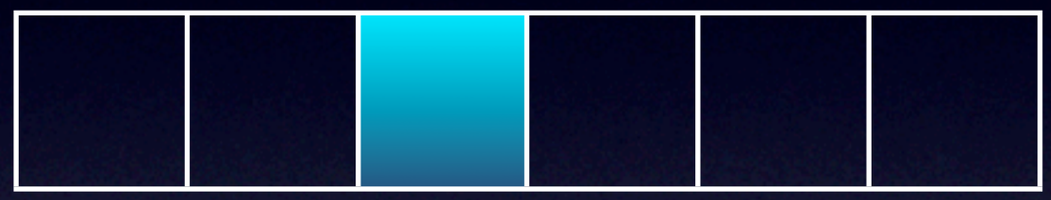
nrj
 # neighbors

iinr
index of list owners

jindex
list limits

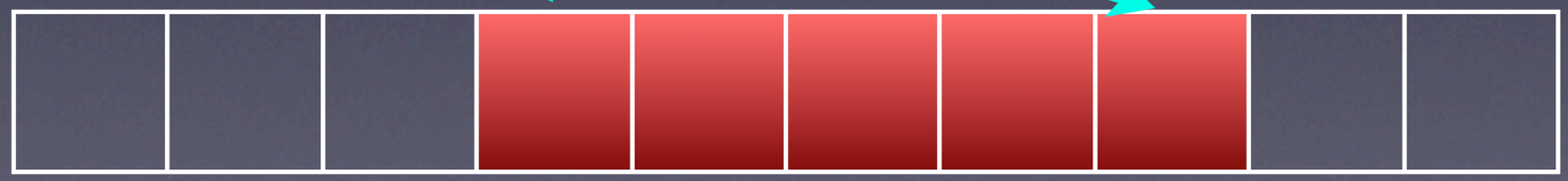
jjnr
neighbor indices

iinr[0,..,nri-1]

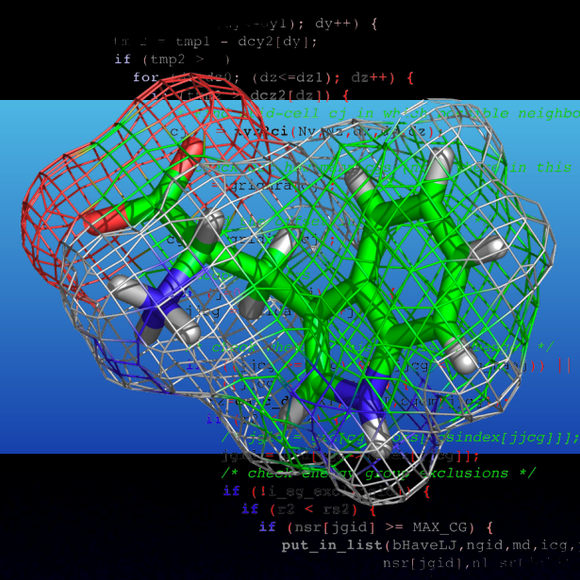


jindex[0,..,nri]

jjnnr[0,..,nri-1]

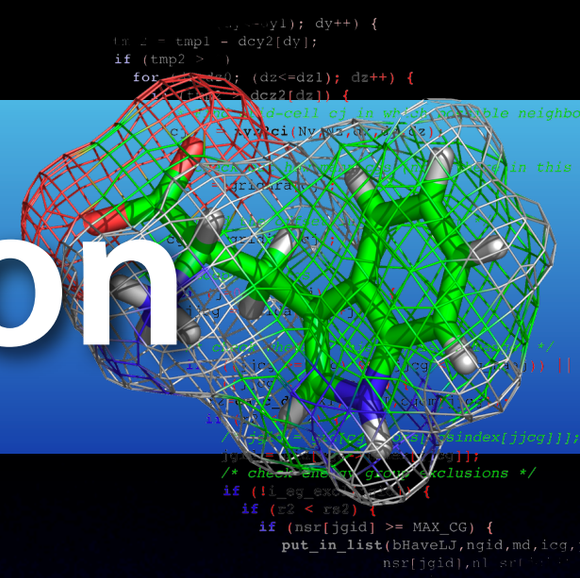


Bugzilla



- http://bugzilla.gromacs.org
- Report, track, and find patches for bugs
- NOT for support, though - we often don't comment at all on a bugzilla entry until we have had time to test/confirm it
- Mailing list is better if you are not sure
- Good bug reports have lots of information
- Always try to provide a (small) test case

Creating a distribution



- **Autoconf comes with built-in capabilities to create source 'tarballs' (like ours) that include your modifications:**

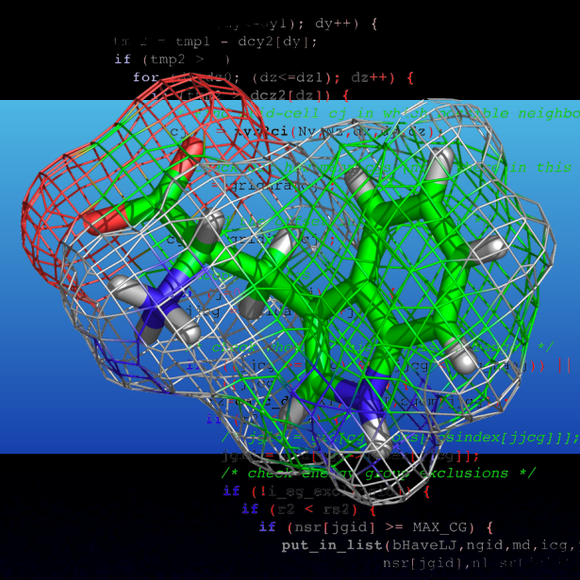
```
$> make dist
```

Just creates gromacs-<RELEASE>.tar.gz

```
$> make distcheck
```

1. Create gromacs-<RELEASE>.tar.gz
2. Check that all files are there
3. Try to build it in a temporary directory
4. Make sure that it cleans up fine

Creating a patch



- Once you have created a new feature or fixed a bug, how do you contribute it back?
- In the top (gmx) directory, issue:
  `cvs diff > fix.patch` (better: `cvs diff -U 3`)
- Try to clean the resulting fix.patch so it only contains the important changes!
- To apply it to another source tree:
  `patch < fix.patch`