Spicing up Gromacs

A collection of recipes to get started

Tools:

1 Check out Gromacs from Git

2 Set up an IDE project

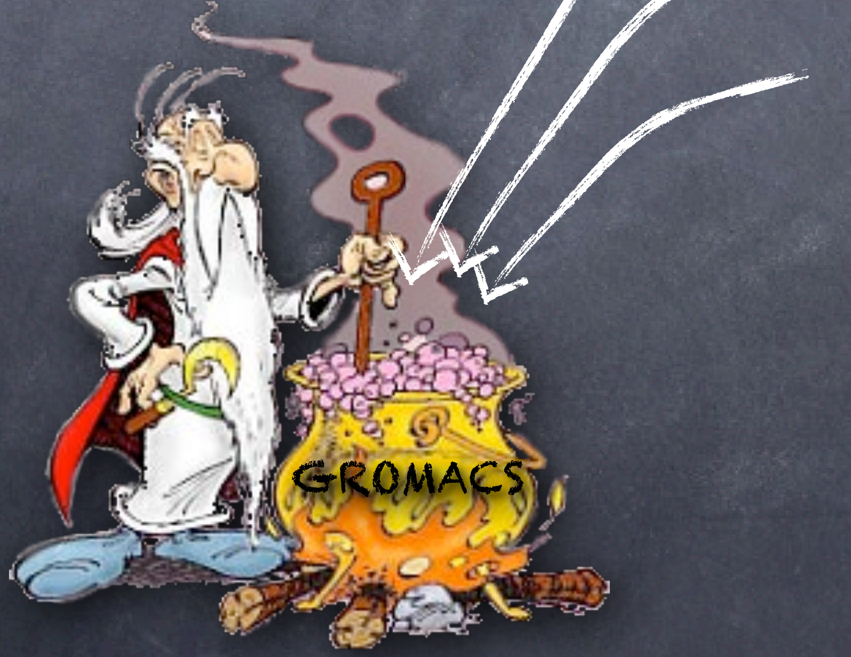
3 Configure with CMake/Autotools

4 Compile from Eclipse

5 Create a branch

6 Git how-to

7 Use an IDE



Recipes & how-tos:

8 MD time step

9 Gromacs source organization

10 Putting in extras:

- 11 Add a file
- 12 Add input parameters ...
- 13 ... and write them to TPR
- 14 gmxdump
- 15 Getting your file compiled
- 16 Interfacing mdrun
- 17 Read your TPR data
- 18 The MD loop
- 19 Output

Part 1: Prerequisites

Tools that make coo~~k~~ding easier

#1 Check out Gromacs from Git

- get a copy of the repository from the git server:

  ```
  git clone git://git.gromacs.org/gromacs.git

  cd gromacs
  git branch
  *master
  ```

- check out the latest stable branch:

  ```
  git checkout --track -b release-4-5-patches origin/release-4-5-patches

  git branch
   master
  *release-4-5-patches
  ```

- don't use `gromacs-4.5.x.tar.gz` for modifications!
  do create your own branch!

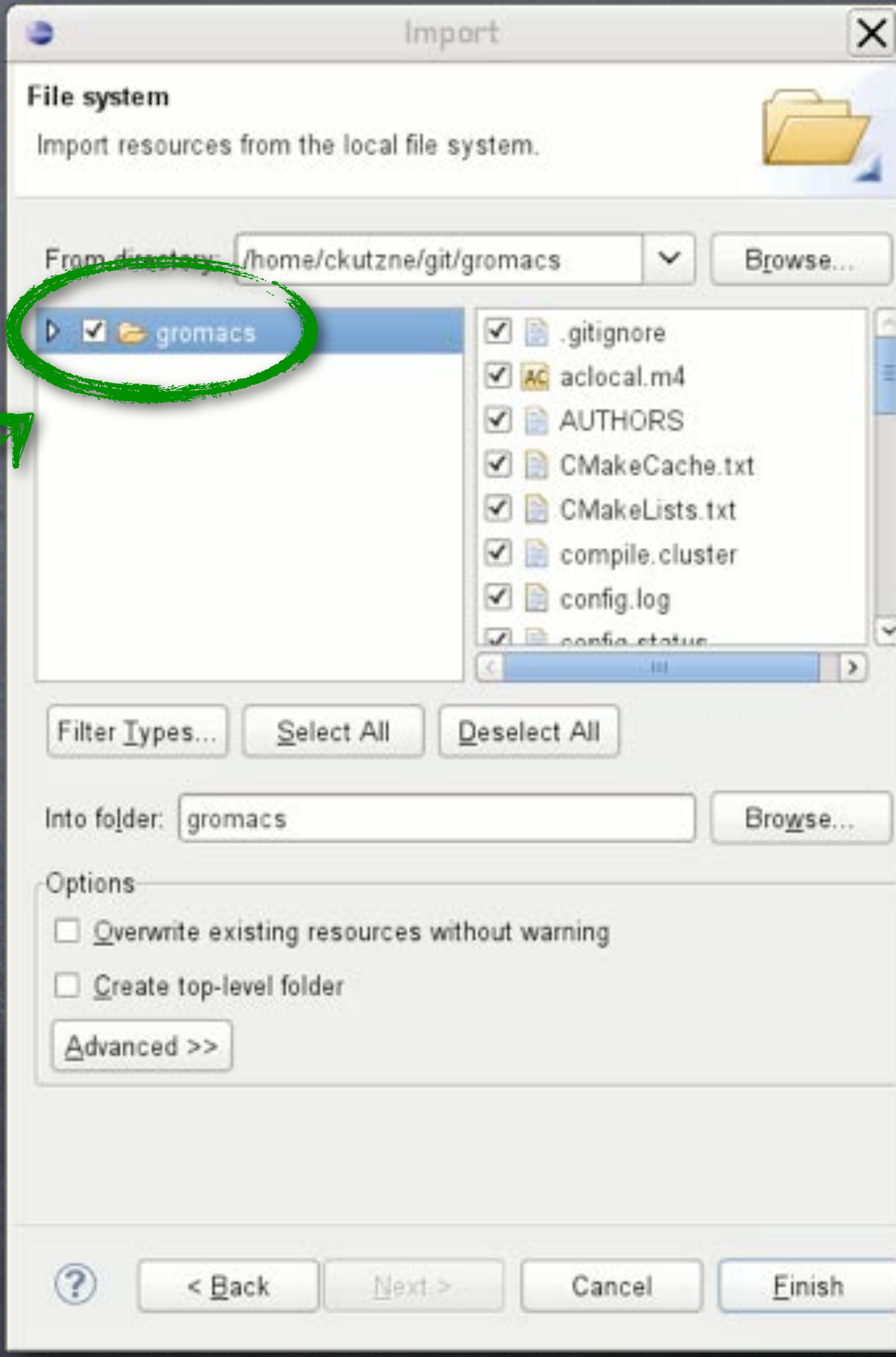
#2 Set up an IDE project

- /usr/local/bin/eclipse Ganymede (2008)
  or download Indigo/2011 at www.eclipse.org
  "Eclipse IDE for C/C++ Developers"

- File > New > C Project "my45proj"
  Project type: Makefile project > Empty > Linux GCC > Finish

- File > Import > General > File system
  select your gromacs git dir, check the checkbox with the gromacs source
  > Finish

- Right-Click on the newly created project > Team > Share project > Git



File system

Import resources from the local file system.

From directory: /home/ckutzne/git/gromacs

☑ gromacs

☑ .gitignore
☑ aclocal.m4
☑ AUTHORS
☑ CMakeCache.txt
☑ CMakeLists.txt
☑ compile.cluster
☑ config.log
☑ config.status

Into folder: gromacs

Options
□ Overwrite existing resources without warning
□ Create top-level folder

#3 Configure with CMake/Autotools

```
cd ~/workspace/my45proj
export LDFLAGS=-L/usr/local/fftw/312-gcc412/lib
export CPPFLAGS=-I/usr/local/fftw/312-gcc412/include
export CFLAGS="-g -O0 -Wall -Wno-unused"
```

A. Makefile generation

from Makefile.am
AutoTools
the GNU build system
(up to 4.5.x)

```
./bootstrap

./configure \
  --disable-shared \
  --prefix=/home/me/gmx
  (--enable-double)
```

from CMakeLists.txt
Cmake, cross-platform make
(4.5+)

```
mkdir build
cd build

cmake ..
 -DBUILD_SHARED_LIBS=off \
 -DCMAKE_INSTALL_PREFIX=/home/me/gmx \
 (-DGMX_DOUBLE=on)
```

src dir

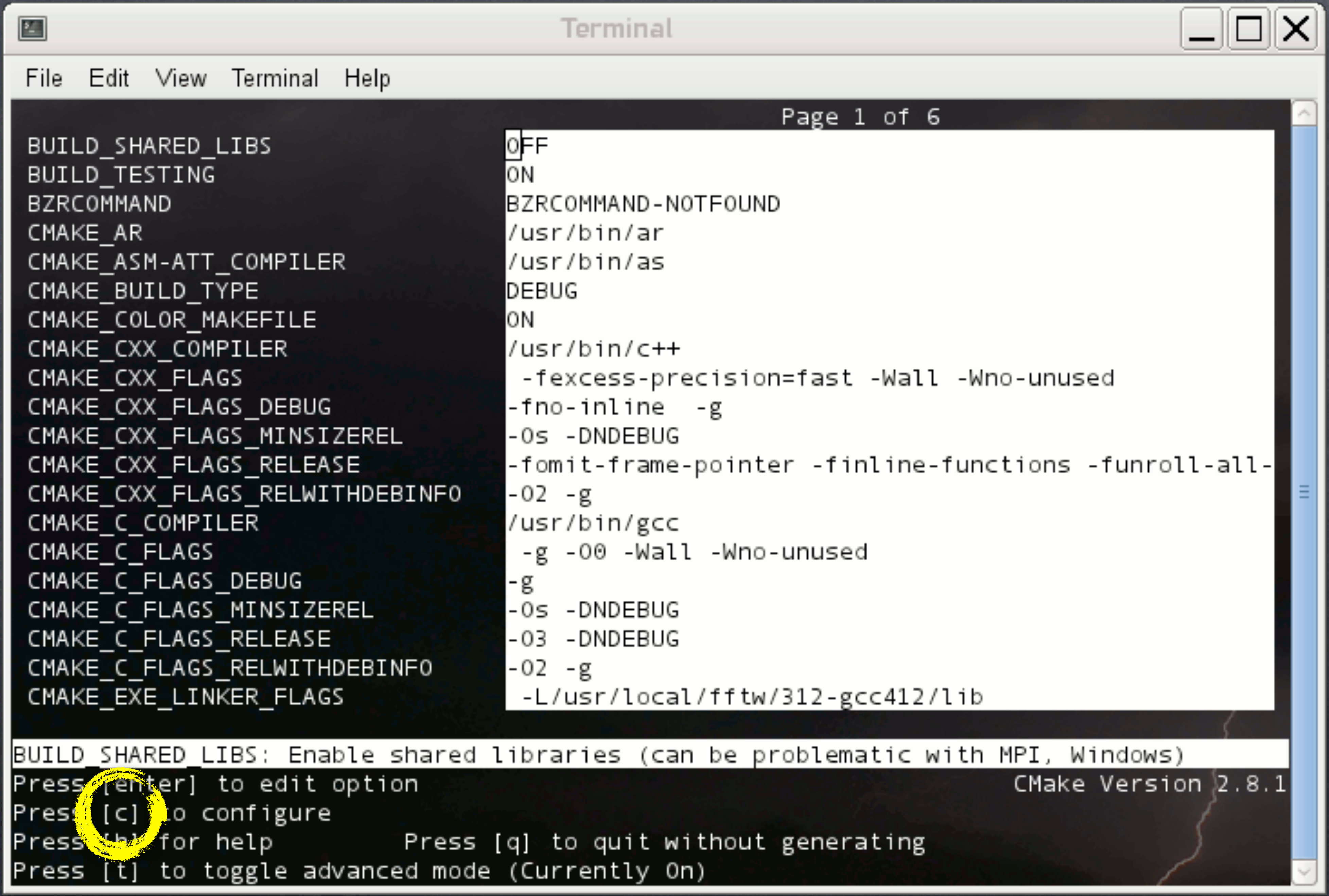
B. Compile & install

```
make -j 4
make install
```

} use Eclipse

#3b Use Ccmake for special needs

ccmake .. will give you an interactive settings window,
          type (c)onfigure, (g)enerate



```
                                                 Page 1 of 6
 BUILD_SHARED_LIBS                OFF
 BUILD_TESTING                    ON
 BZRCOMMAND                       BZRCOMMAND-NOTFOUND
 CMAKE_AR                         /usr/bin/ar
 CMAKE_ASM-ATT_COMPILER           /usr/bin/as
 CMAKE_BUILD_TYPE                 DEBUG
 CMAKE_COLOR_MAKEFILE             ON
 CMAKE_CXX_COMPILER               /usr/bin/c++
 CMAKE_CXX_FLAGS                   -fexcess-precision=fast -Wall -Wno-unused
 CMAKE_CXX_FLAGS_DEBUG            -fno-inline  -g
 CMAKE_CXX_FLAGS_MINSIZEREL       -Os -DNDEBUG
 CMAKE_CXX_FLAGS_RELEASE          -fomit-frame-pointer -finline-functions -funroll-all-
 CMAKE_CXX_FLAGS_RELWITHDEBINFO   -O2 -g
 CMAKE_C_COMPILER                 /usr/bin/gcc
 CMAKE_C_FLAGS                     -g -O0 -Wall -Wno-unused
 CMAKE_C_FLAGS_DEBUG              -g
 CMAKE_C_FLAGS_MINSIZEREL         -Os -DNDEBUG
 CMAKE_C_FLAGS_RELEASE            -O3 -DNDEBUG
 CMAKE_C_FLAGS_RELWITHDEBINFO     -O2 -g
 CMAKE_EXE_LINKER_FLAGS            -L/usr/local/fftw/312-gcc412/lib

BUILD_SHARED_LIBS: Enable shared libraries (can be problematic with MPI, Windows)
Press [enter] to edit option                                 CMake Version 2.8.1
Press [c] to configure
Press [h] for help          Press [q] to quit without generating
Press [t] to toggle advanced mode (Currently On)
```

#4 Compile from Eclipse

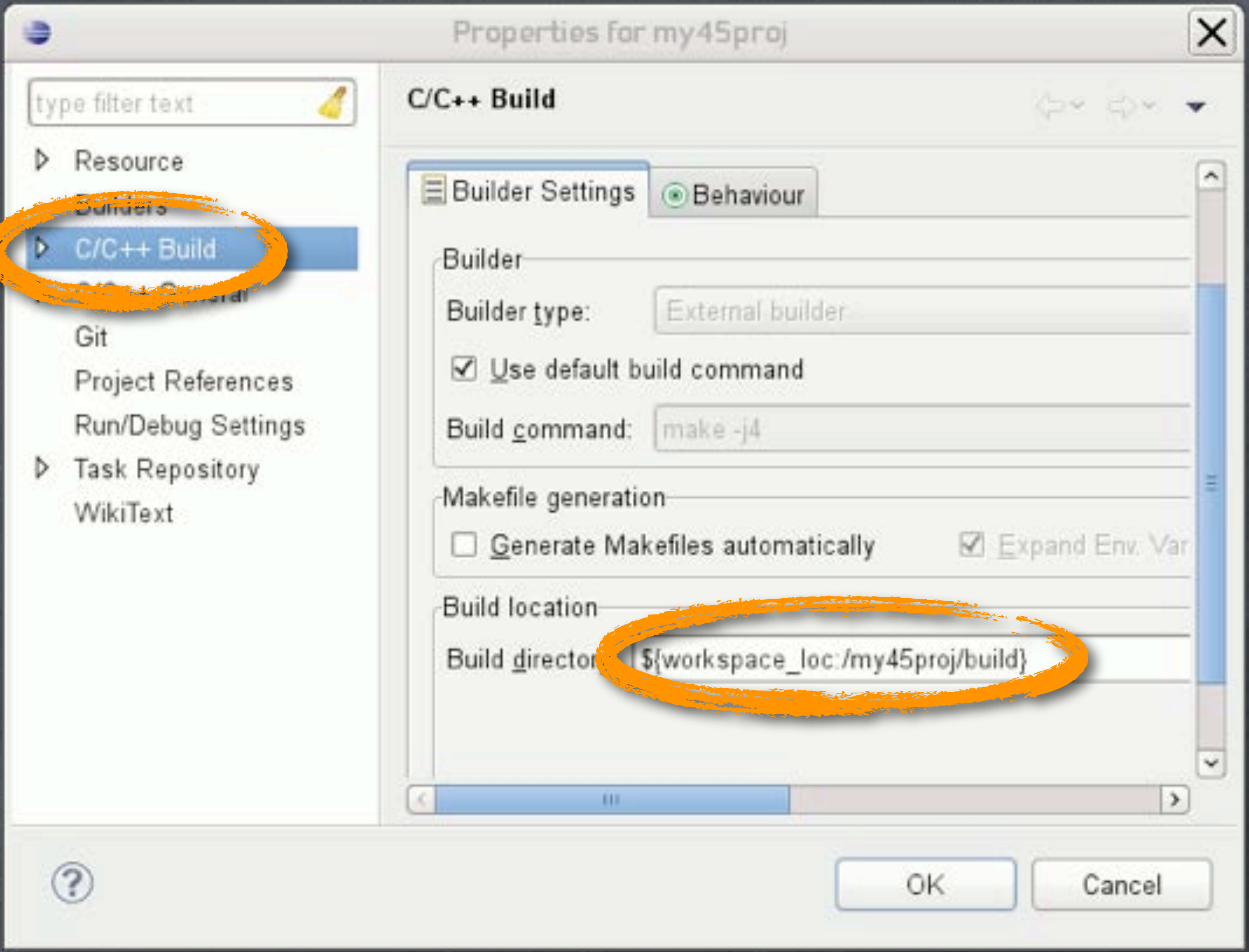
- Project > Properties > C/C++ Build

  set dir of Makefile

- Eclipse simply executes

  “make -j4”

  in the chosen directory when we hit Ctrl-B



Properties for my45proj

C/C++ Build

Builder Settings | Behaviour

Builder

Builder type: External builder

☑ Use default build command

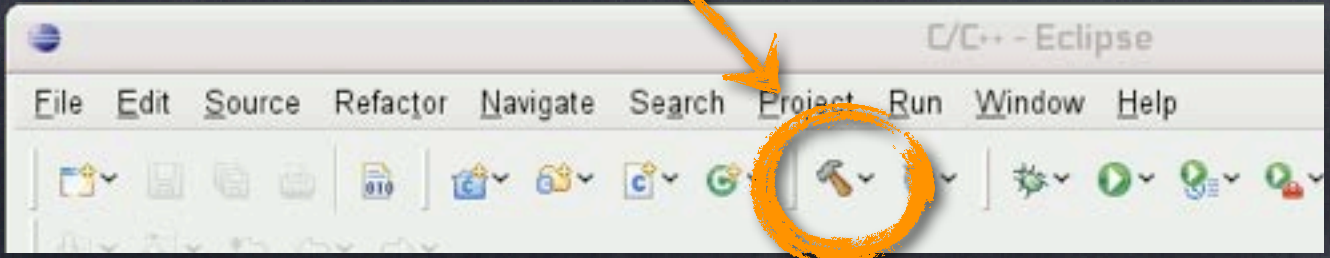
Build command: make -j4

Makefile generation

□ Generate Makefiles automatically ☑ Expand Env. Var

Build location

Build director ${workspace_loc:/my45proj/build}



#5 Create a branch

- create a branch, start from current:

```
git branch   - shows current branch
 master
*release-4-5-patches
```

-
```
git branch my45feature   - create branch
git branch
 master
 my45feature
*release-4-5-patches
```

-
```
git checkout my45feature - check out branch
git branch
 master
*my45feature
 release-4-5-patches
```

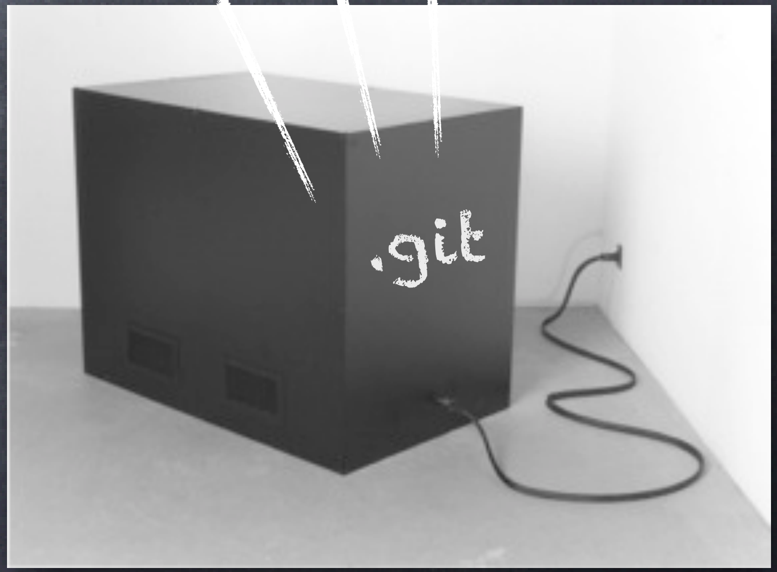
- At any time merge newest bugfixes into my45feature

```
git pull
git merge release-4-5-patches
```

- .git contains all history about every file/version ever checked in

- git checkout <branch> puts the latest state of files of <branch> into your working tree:

```
./gromacs/src/kernel/mdrun.c
./gromacs/src/kernel/grompp.c
./gromacs/src/kernel/*.c
./gromacs/src/tools/*.c
./gromacs/include/*.h
./gromacs/share/*
./gromacs/.git/
```



#6 Git how-to

- after some programming, you have a first version working.

```
git status
# On branch my45feature
# Changed but not updated:
#  modified:   src/mdlib/pull.c
#  modified:   src/kernel/md.c
#
# Untracked files:
#   src/mdlib/anewfile.c
```

- !@XX!! Did I change md.c?

```
git checkout -- src/kernel/md.c
```

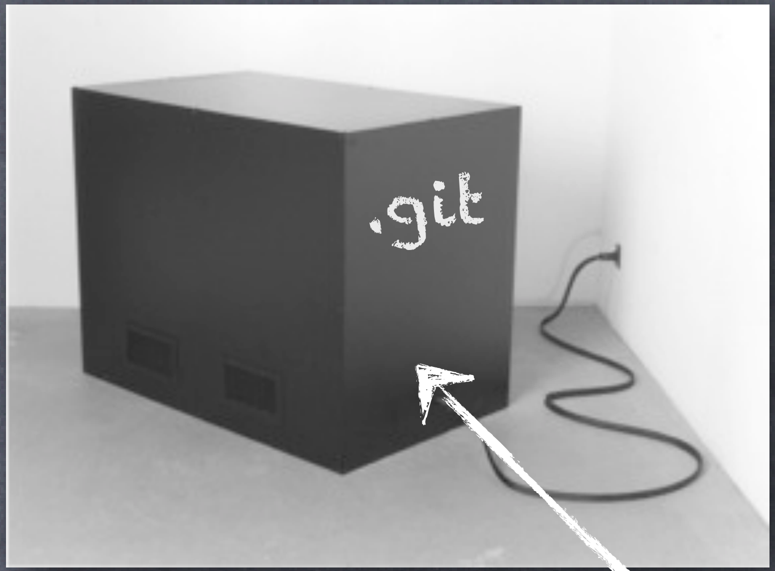
- undoes changes

- What was it I changed in pull.c?:

```
git diff ./src/mdlib/pull.c
```

- Not OK, this is a pile of !@XX. Let's start over again!

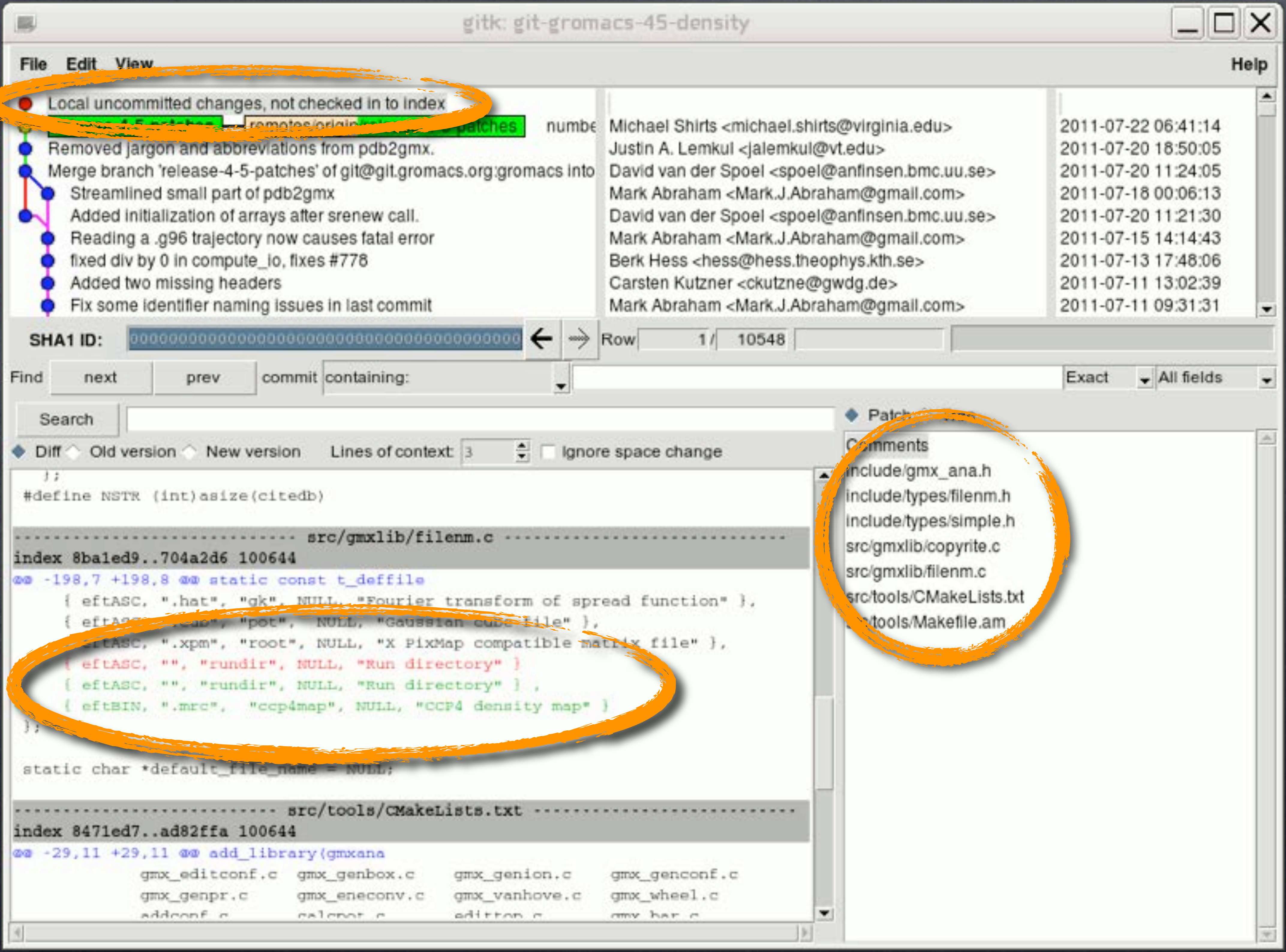
```
git reset --hard
```



- OK, now it looks good.

```
git add src/mdlib/pull.c
git add src/kernel/md.c
git add src/mdlib/anewfile.c
git commit -m "Added feature XY"
```

#6b Use gitk before you commit



```
● Local uncommitted changes, not checked in to index
  release-4-5-patches  remotes/origin/release-4-5-patches   numbe   Michael Shirts <michael.shirts@virginia.edu>      2011-07-22 06:41:14
  Removed jargon and abbreviations from pdb2gmx.                   Justin A. Lemkul <jalemkul@vt.edu>                 2011-07-20 18:50:05
  Merge branch 'release-4-5-patches' of git@git.gromacs.org:gromacs into   David van der Spoel <spoel@anfinsen.bmc.uu.se>   2011-07-20 11:24:05
    Streamlined small part of pdb2gmx                              Mark Abraham <Mark.J.Abraham@gmail.com>           2011-07-18 00:06:13
    Added initialization of arrays after srenew call.             David van der Spoel <spoel@anfinsen.bmc.uu.se>    2011-07-20 11:21:30
    Reading a .g96 trajectory now causes fatal error               Mark Abraham <Mark.J.Abraham@gmail.com>           2011-07-15 14:14:43
    fixed div by 0 in compute_io, fixes #778                       Berk Hess <hess@hess.theophys.kth.se>             2011-07-13 17:48:06
    Added two missing headers                                      Carsten Kutzner <ckutzne@gwdg.de>                 2011-07-11 13:02:39
    Fix some identifier naming issues in last commit               Mark Abraham <Mark.J.Abraham@gmail.com>           2011-07-11 09:31:31
```

SHA1 ID: 0000000000000000000000000000000000000000   Row 1 / 10548

Find next prev commit containing: Exact All fields

Search

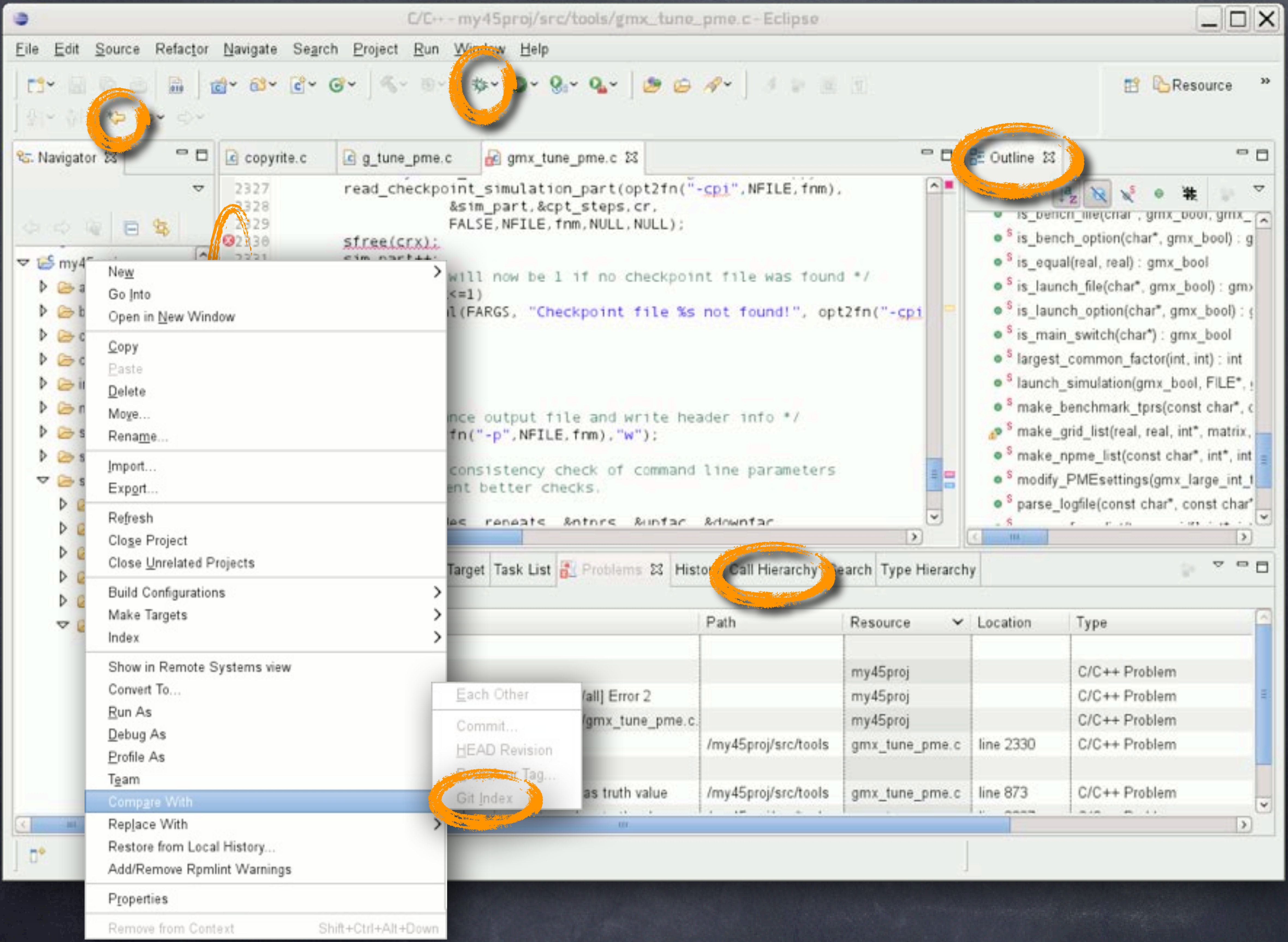
◆ Diff ◇ Old version ◇ New version   Lines of context: 3   □ Ignore space change

```
  };
#define NSTR (int)asize(citedb)

---------------------------- src/gmxlib/filenm.c ----------------------------
index 8ba1ed9..704a2d6 100644
@@ -198,7 +198,8 @@ static const t_deffile
    { eftASC, ".hat", "gk", NULL, "Fourier transform of spread function" },
    { eftASC, ".cub", "pot", NULL, "Gaussian cube file" },
    { eftASC, ".xpm", "root", NULL, "X PixMap compatible matrix file" },
-   { eftASC, "", "rundir", NULL, "Run directory" }
+   { eftASC, "", "rundir", NULL, "Run directory" } ,
+   { eftBIN, ".mrc",  "ccp4map", NULL, "CCP4 density map" }
 };

 static char *default_file_name = NULL;

-------------------------- src/tools/CMakeLists.txt --------------------------
index 8471ed7..ad82ffa 100644
@@ -29,11 +29,11 @@ add_library(gmxana
            gmx_editconf.c  gmx_genbox.c    gmx_genion.c    gmx_genconf.c
            gmx_genpr.c     gmx_eneconv.c   gmx_vanhove.c   gmx_wheel.c
            addconf.c       calcpot.c       edittop.c       gmx_bar.c
```

◆ Patch ◇ Tree

Comments
include/gmx_ana.h
include/types/filenm.h
include/types/simple.h
src/gmxlib/copyrite.c
src/gmxlib/filenm.c
src/tools/CMakeLists.txt
src/tools/Makefile.am

#7 Use an IDE (Eclipse, KDevelop, SourceNav)

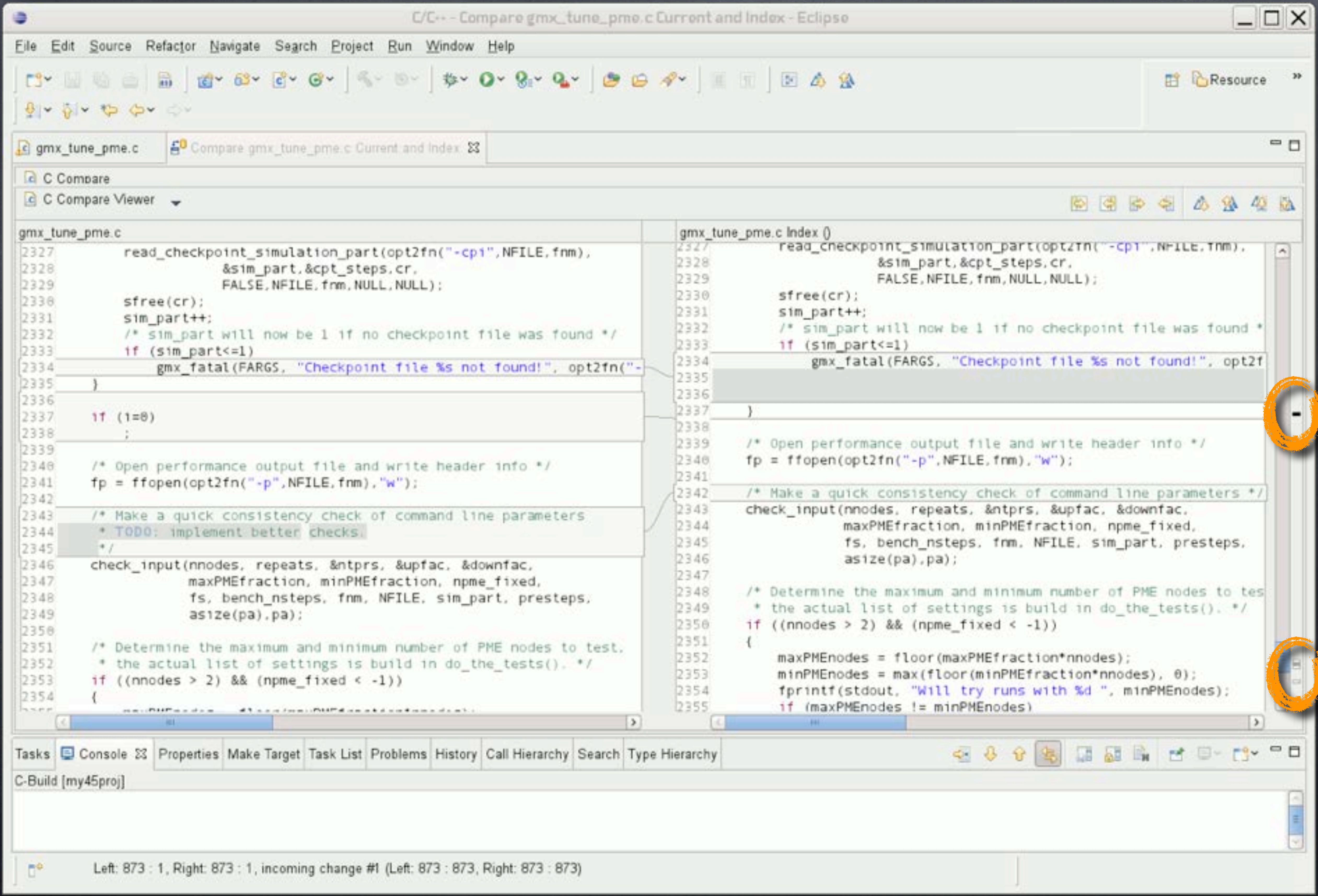


```
        read_checkpoint_simulation_part(opt2fn("-cpi",NFILE,fnm),
                                        &sim_part,&cpt_steps,cr,
                                        FALSE,NFILE,fnm,NULL,NULL);
        sfree(crx);
        sim_part++;
will now be 1 if no checkpoint file was found */
<=1)
l(FARGS, "Checkpoint file %s not found!", opt2fn("-cpi

nce output file and write header info */
fn("-p",NFILE,fnm),"w");

consistency check of command line parameters
ent better checks.

es, repeats, &ntprs, &upfac, &downfac
```

	Path	Resource	Location	Type
		my45proj		C/C++ Problem
all] Error 2		my45proj		C/C++ Problem
/gmx_tune_pme.c		my45proj		C/C++ Problem
	/my45proj/src/tools	gmx_tune_pme.c	line 2330	C/C++ Problem
as truth value	/my45proj/src/tools	gmx_tune_pme.c	line 873	C/C++ Problem

C/C++ - my45proj/src/tools/gmx_tune_pme.c - Eclipse
File Edit Source Refactor Navigate Search Project Run Window Help
Resource
Navigator
copyrite.c
g_tune_pme.c
gmx_tune_pme.c
Outline
is_bench_option(char*, gmx_bool) : g
is_equal(real, real) : gmx_bool
is_launch_file(char*, gmx_bool) : gmx
is_launch_option(char*, gmx_bool) :
is_main_switch(char*) : gmx_bool
largest_common_factor(int, int) : int
launch_simulation(gmx_bool, FILE*,
make_benchmark_tprs(const char*,
make_grid_list(real, real, int*, matrix,
make_npme_list(const char*, int*, int
modify_PMEsettings(gmx_large_int_t
parse_logfile(const char*, const char*
New
Go Into
Open in New Window
Copy
Paste
Delete
Move...
Rename...
Import...
Export...
Refresh
Close Project
Close Unrelated Projects
Build Configurations
Make Targets
Index
Show in Remote Systems view
Convert To...
Run As
Debug As
Profile As
Team
Compare With
Replace With
Restore from Local History...
Add/Remove Rpmlint Warnings
Properties
Remove from Context Shift+Ctrl+Alt+Down
Each Other
Commit...
HEAD Revision
Branch or Tag...
Git Index
Target
Task List
Problems
History
Call Hierarchy
Search
Type Hierarchy

#7b IDE benefits


C/C++ - Compare gmx_tune_pme.c Current and Index - Eclipse
File Edit Source Refactor Navigate Search Project Run Window Help
Resource
gmx_tune_pme.c
Compare gmx_tune_pme.c Current and Index
C Compare
C Compare Viewer
Tasks
Console
Properties
Make Target
Task List
Problems
History
Call Hierarchy
Search
Type Hierarchy
C-Build [my45proj]

gmx_tune_pme.c

```
        read_checkpoint_simulation_part(opt2fn("-cpi",NFILE,fnm),
                    &sim_part,&cpt_steps,cr,
                    FALSE,NFILE,fnm,NULL,NULL);
        sfree(cr);
        sim_part++;
        /* sim_part will now be 1 if no checkpoint file was found */
        if (sim_part<=1)
            gmx_fatal(FARGS, "Checkpoint file %s not found!", opt2fn("-
    }

    if (1=0)
        ;

    /* Open performance output file and write header info */
    fp = ffopen(opt2fn("-p",NFILE,fnm),"w");

    /* Make a quick consistency check of command line parameters
     * TODO: implement better checks.
     */
    check_input(nnodes, repeats, &ntprs, &upfac, &downfac,
                maxPMEfraction, minPMEfraction, npme_fixed,
                fs, bench_nsteps, fnm, NFILE, sim_part, presteps,
                asize(pa),pa);

    /* Determine the maximum and minimum number of PME nodes to test.
     * the actual list of settings is build in do_the_tests(). */
    if ((nnodes > 2) && (npme_fixed < -1))
    {
```

gmx_tune_pme.c Index ()

```
        read_checkpoint_simulation_part(opt2fn("-cpi",NFILE,fnm),
                    &sim_part,&cpt_steps,cr,
                    FALSE,NFILE,fnm,NULL,NULL);
        sfree(cr);
        sim_part++;
        /* sim_part will now be 1 if no checkpoint file was found *
        if (sim_part<=1)
            gmx_fatal(FARGS, "Checkpoint file %s not found!", opt2f


    }

    /* Open performance output file and write header info */
    fp = ffopen(opt2fn("-p",NFILE,fnm),"w");

    /* Make a quick consistency check of command line parameters */
    check_input(nnodes, repeats, &ntprs, &upfac, &downfac,
                maxPMEfraction, minPMEfraction, npme_fixed,
                fs, bench_nsteps, fnm, NFILE, sim_part, presteps,
                asize(pa),pa);

    /* Determine the maximum and minimum number of PME nodes to tes
     * the actual list of settings is build in do_the_tests(). */
    if ((nnodes > 2) && (npme_fixed < -1))
    {
        maxPMEnodes = floor(maxPMEfraction*nnodes);
        minPMEnodes = max(floor(minPMEfraction*nnodes), 0);
        fprintf(stdout, "Will try runs with %d ", minPMEnodes);
        if (maxPMEnodes != minPMEnodes)
```

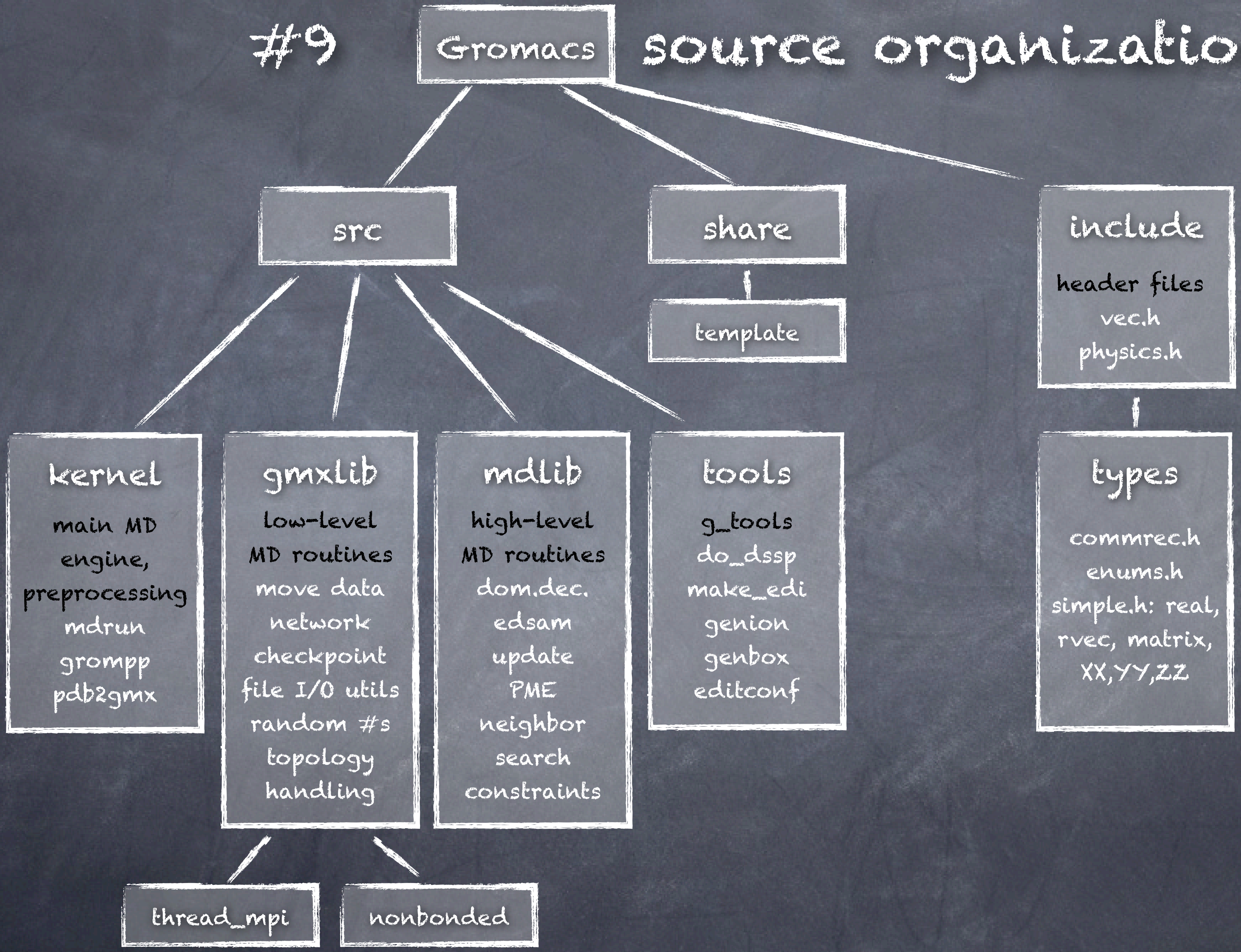
Left: 873 : 1, Right: 873 : 1, incoming change #1 (Left: 873 : 873, Right: 873 : 873)

Part 2: Spicing up Gromacs

#8 Molecular dynamics time step

What?	Where in Gromacs?	File name
— Read in r_i, v_i, m_i, q_i, potential U	— read from tpr & cpt	— tpxio.c, checkpoint.c
— Loop over MD steps	— do_md( )	— md.c
— Calculate forces f_i	— do_force( )	— sim_util.c
— make neighbor lists for f_{nb}	— ns( )	— ns.c
— evaluate f_{Coul} and f_{vdW} up to r_c	— do_nonbonded( )	— nonbonded.c
— evaluate long-range f_c (PME)	— gmx_pme_do( )	— pme.c
— evaluate bonded forces	— calc_bonds( )	— bondfree.c
— Update positions and velocities	— update_coords( )	— update.c
— (constrain positions)	— update_constraints( )	
$\mathbf{v}(t+\frac{\Delta t}{2}) = \mathbf{v}(t-\frac{\Delta t}{2}) + \frac{\mathbf{F}(t)}{m}\Delta t$	$\mathbf{r}(t+\Delta t) = \mathbf{r}(t) + \mathbf{v}(t+\frac{\Delta t}{2})\Delta t$	
— Output r_i, v_i, T, p, energies, ...	— write_traj -> xtc, cpt, trr	— stat.c

#9 Gromacs source organization



Gromacs

src

share

include

header files
vec.h
physics.h

template

kernel

main MD engine, preprocessing
mdrun
grompp
pdb2gmx

gmxlib

low-level MD routines
move data
network
checkpoint
file I/O utils
random #s
topology handling

mdlib

high-level MD routines
dom.dec.
edsam
update
PME
neighbor search
constraints

tools

g_tools
do_dssp
make_edi
genion
genbox
editconf

types

commrec.h
enums.h
simple.h: real, rvec, matrix, XX,YY,ZZ

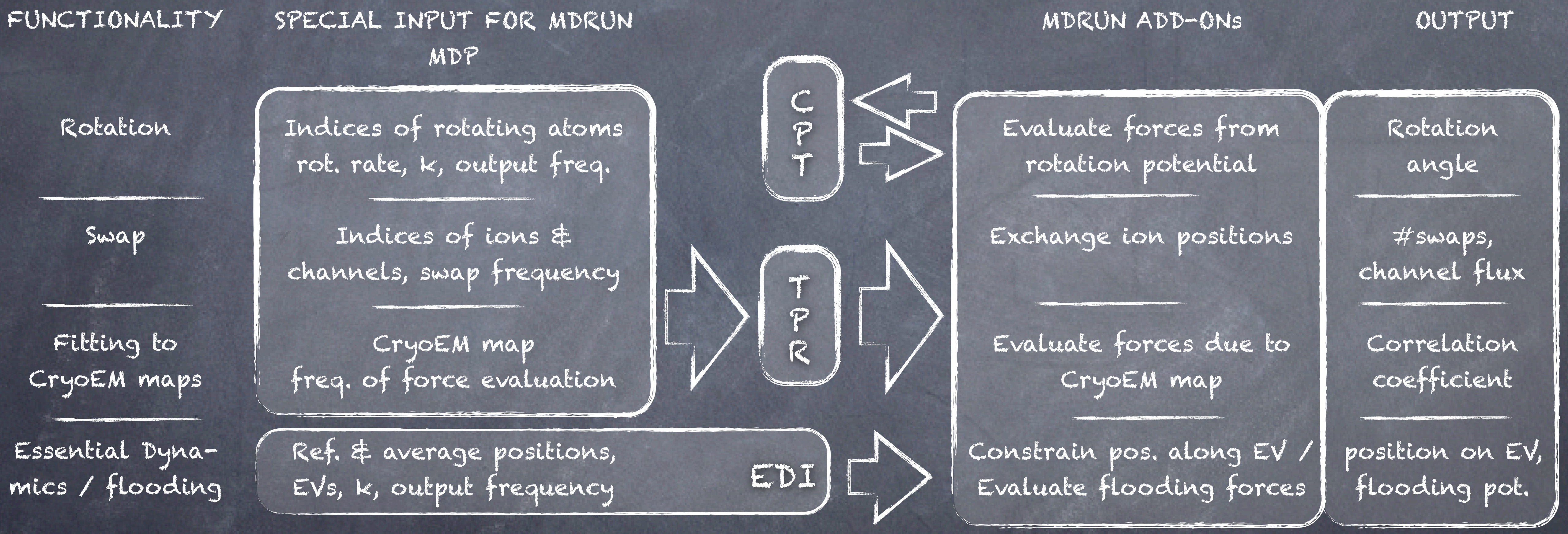
thread_mpi

nonbonded

#10 Hacking Gromacs examples

Implementing new core functionality

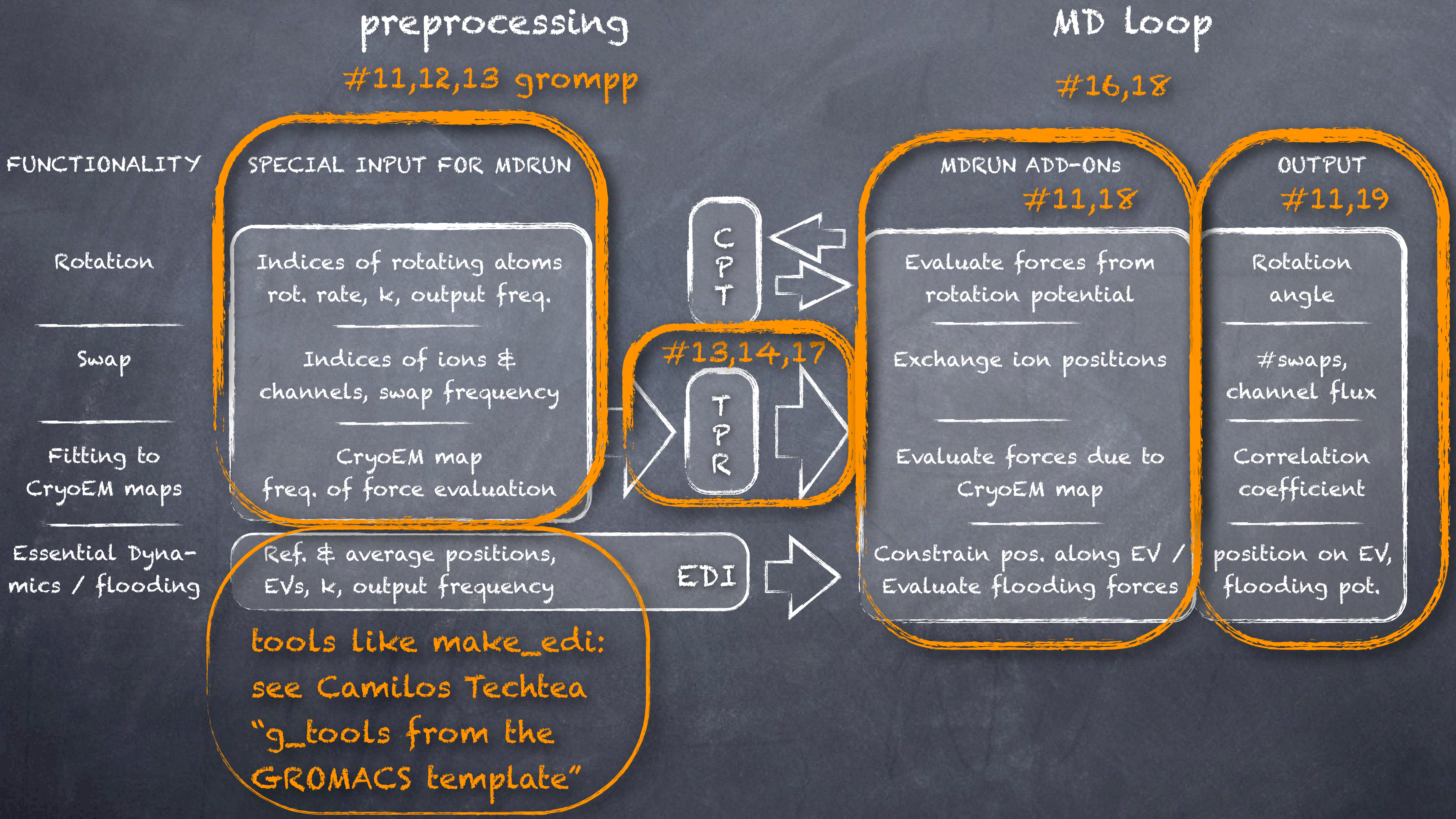
preprocessing | mdrun



FUNCTIONALITY	SPECIAL INPUT FOR MDRUN MDP	MDRUN ADD-ONs	OUTPUT
Rotation	Indices of rotating atoms rot. rate, k, output freq.	Evaluate forces from rotation potential	Rotation angle
Swap	Indices of ions & channels, swap frequency	Exchange ion positions	#swaps, channel flux
Fitting to CryoEM maps	CryoEM map freq. of force evaluation	Evaluate forces due to CryoEM map	Correlation coefficient
Essential Dynamics / flooding	Ref. & average positions, EVs, k, output frequency EDI	Constrain pos. along EV / Evaluate flooding forces	position on EV, flooding pot.

#10 Hacking Gromacs examples

Implementing new core functionality



preprocessing

#11,12,13 grompp

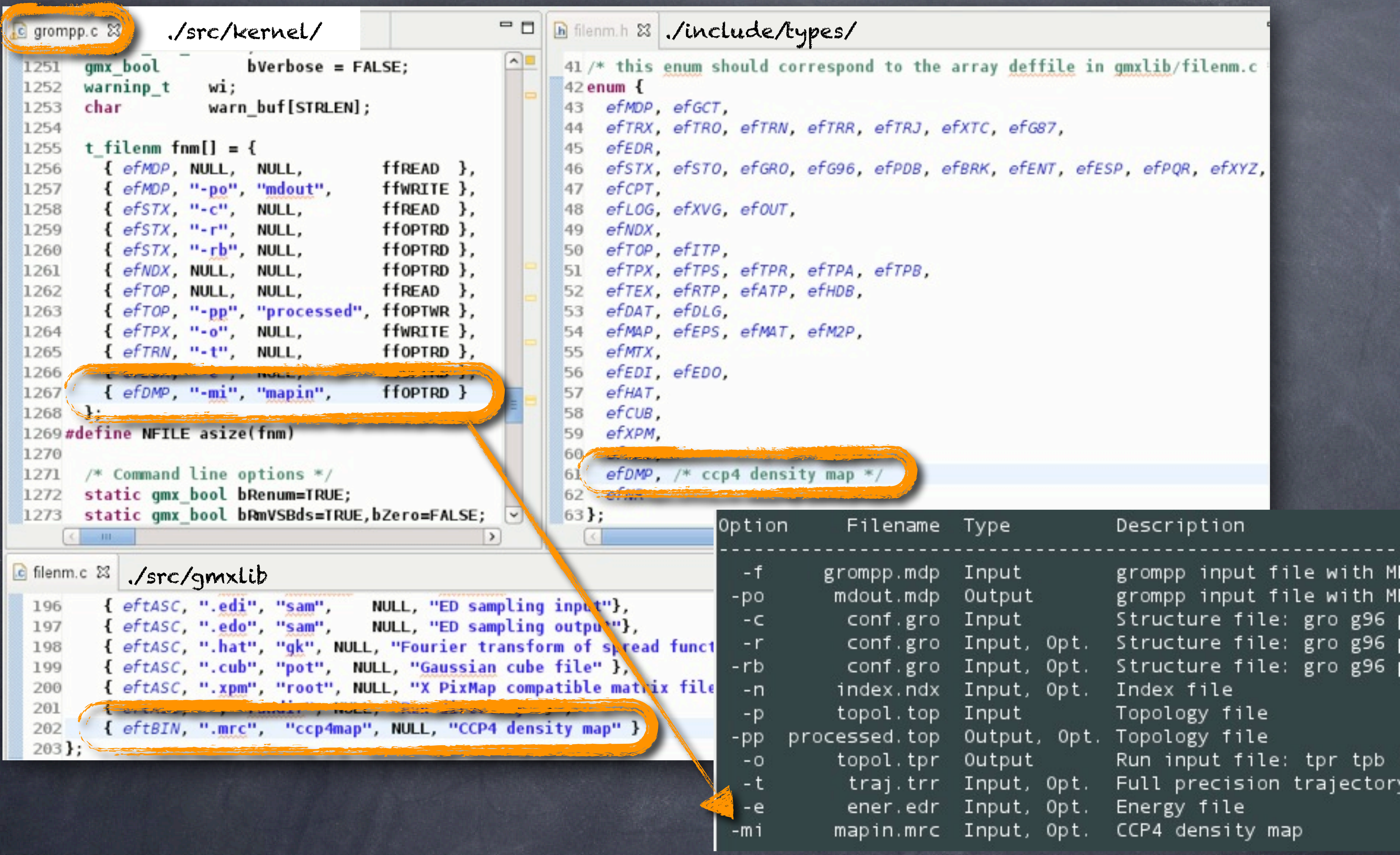
MD loop

#16,18

FUNCTIONALITY	SPECIAL INPUT FOR MDRUN	MDRUN ADD-ONs #11,18	OUTPUT #11,19
Rotation	Indices of rotating atoms rot. rate, k, output freq.	Evaluate forces from rotation potential	Rotation angle
Swap	Indices of ions & channels, swap frequency	Exchange ion positions	#swaps, channel flux
Fitting to CryoEM maps	CryoEM map freq. of force evaluation	Evaluate forces due to CryoEM map	Correlation coefficient
Essential Dynamics / flooding	Ref. & average positions, EVs, k, output frequency	Constrain pos. along EV / Evaluate flooding forces	position on EV, flooding pot.

tools like make_edi: see Camilos Techtea "g_tools from the GROMACS template"

#11 Add a file



grompp.c ./src/kernel/

```
  gmx_bool          bVerbose = FALSE;
  warninp_t     wi;
  char          warn_buf[STRLEN];

  t_filenm fnm[] = {
    { efMDP, NULL,   NULL,        ffREAD  },
    { efMDP, "-po", "mdout",      ffWRITE },
    { efSTX, "-c",  NULL,         ffREAD  },
    { efSTX, "-r",  NULL,         ffOPTRD },
    { efSTX, "-rb", NULL,         ffOPTRD },
    { efNDX, NULL,  NULL,         ffOPTRD },
    { efTOP, NULL,  NULL,         ffREAD  },
    { efTOP, "-pp", "processed",  ffOPTWR },
    { efTPX, "-o",  NULL,         ffWRITE },
    { efTRN, "-t",  NULL,         ffOPTRD },
    { [illegible], "-e", NULL,    [illegible] },
    { efDMP, "-mi", "mapin",      ffOPTRD }
  };
#define NFILE asize(fnm)

  /* Command line options */
  static gmx_bool bRenum=TRUE;
  static gmx_bool bRmVSBds=TRUE,bZero=FALSE;
```

filenm.h ./include/types/

```
/* this enum should correspond to the array deffile in gmxlib/filenm.c
enum {
  efMDP, efGCT,
  efTRX, efTRO, efTRN, efTRR, efTRJ, efXTC, efG87,
  efEDR,
  efSTX, efSTO, efGRO, efG96, efPDB, efBRK, efENT, efESP, efPQR, efXYZ,
  efCPT,
  efLOG, efXVG, efOUT,
  efNDX,
  efTOP, efITP,
  efTPX, efTPS, efTPR, efTPA, efTPB,
  efTEX, efRTP, efATP, efHDB,
  efDAT, efDLG,
  efMAP, efEPS, efMAT, efM2P,
  efMTX,
  efEDI, efEDO,
  efHAT,
  efCUB,
  efXPM,
  [illegible]
  efDMP, /* ccp4 density map */
  [illegible]
};
```

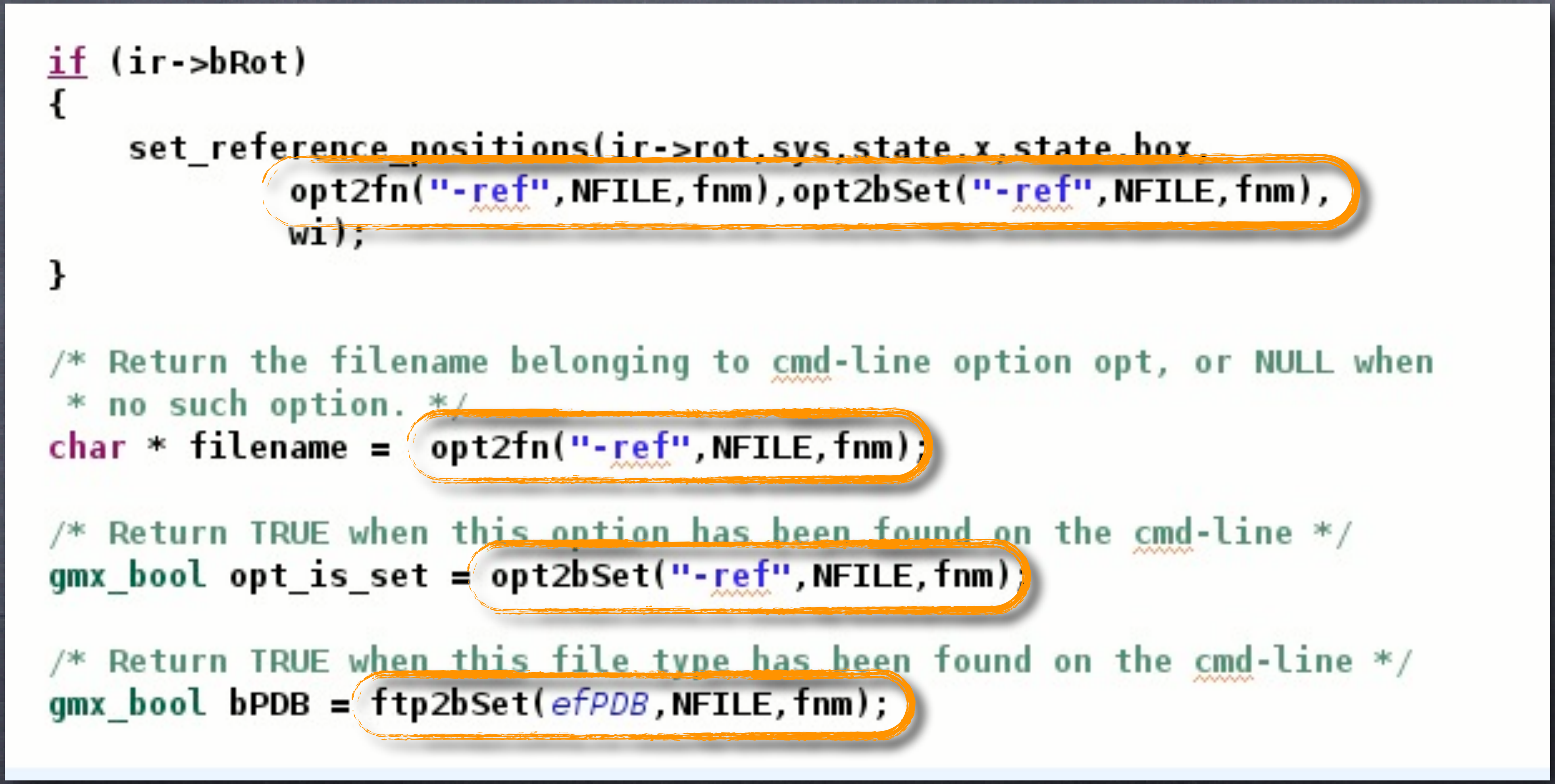
filenm.c ./src/gmxlib

```
    { eftASC, ".edi", "sam",    NULL, "ED sampling input"},
    { eftASC, ".edo", "sam",    NULL, "ED sampling output"},
    { eftASC, ".hat", "gk", NULL, "Fourier transform of spread funct
    { eftASC, ".cub", "pot",  NULL, "Gaussian cube file" },
    { eftASC, ".xpm", "root", NULL, "X PixMap compatible matrix file
    [illegible]
    { eftBIN, ".mrc",  "ccp4map", NULL, "CCP4 density map" }
};
```

```
Option     Filename  Type         Description
------------------------------------------------------------
  -f       grompp.mdp  Input        grompp input file with MI
 -po        mdout.mdp  Output       grompp input file with MI
  -c         conf.gro  Input        Structure file: gro g96 p
  -r         conf.gro  Input, Opt.  Structure file: gro g96 p
 -rb         conf.gro  Input, Opt.  Structure file: gro g96 p
  -n        index.ndx  Input, Opt.  Index file
  -p        topol.top  Input        Topology file
 -pp    processed.top  Output, Opt. Topology file
  -o        topol.tpr  Output       Run input file: tpr tpb
  -t        traj.trr   Input, Opt.  Full precision trajector
  -e        ener.edr   Input, Opt.  Energy file
 -mi       mapin.mrc   Input, Opt.  CCP4 density map
```

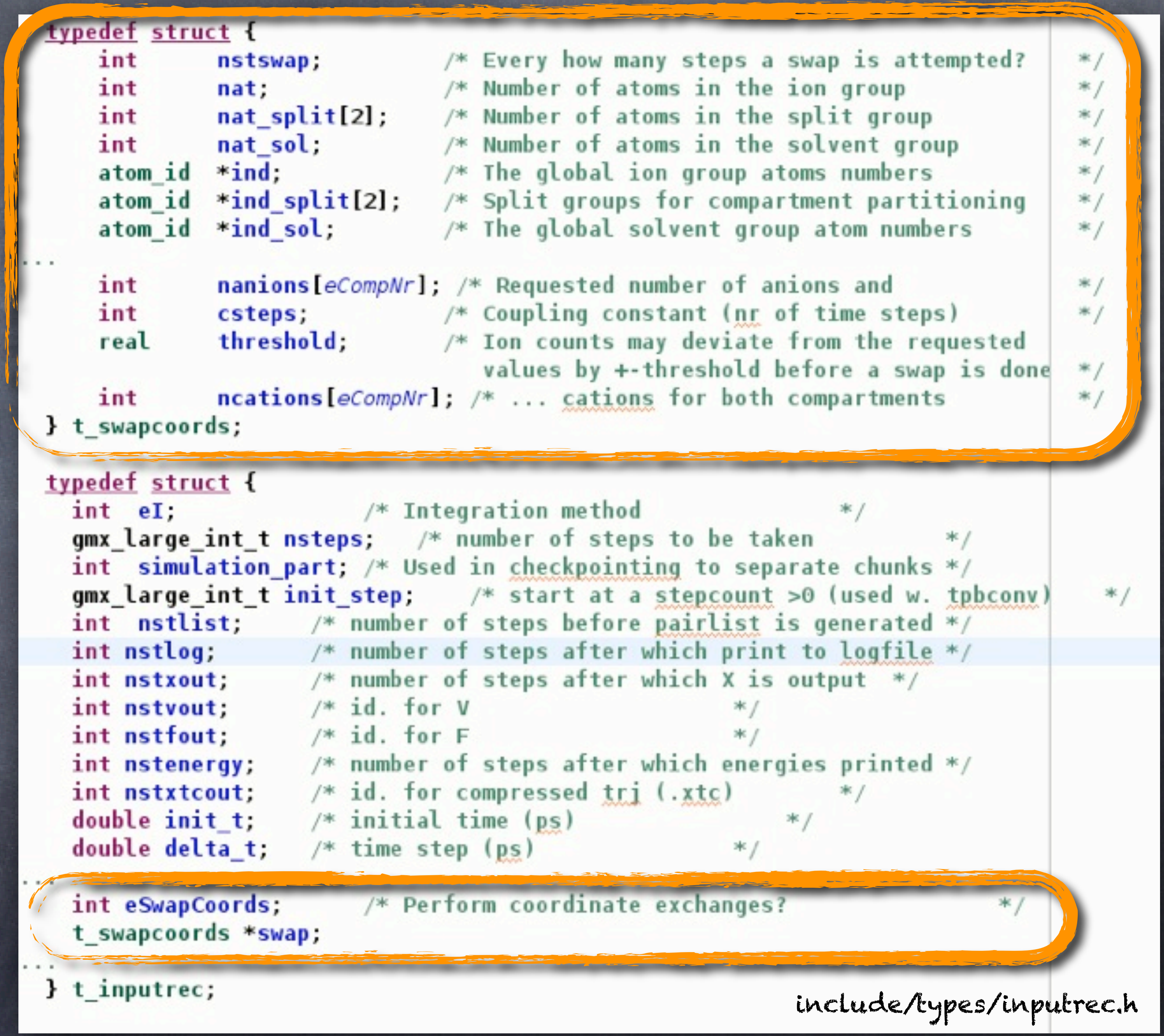
#11b File / option handling

Use routines in ./include/filenm.h



```
if (ir->bRot)
{
    set_reference_positions(ir->rot,sys,state.x,state.box,
            opt2fn("-ref",NFILE,fnm),opt2bSet("-ref",NFILE,fnm),
            wi);
}

/* Return the filename belonging to cmd-line option opt, or NULL when
 * no such option. */
char * filename = opt2fn("-ref",NFILE,fnm);

/* Return TRUE when this option has been found on the cmd-line */
gmx_bool opt_is_set = opt2bSet("-ref",NFILE,fnm);

/* Return TRUE when this file type has been found on the cmd-line */
gmx_bool bPDB = ftp2bSet(efPDB,NFILE,fnm);
```

#12 Add MDP input parameters



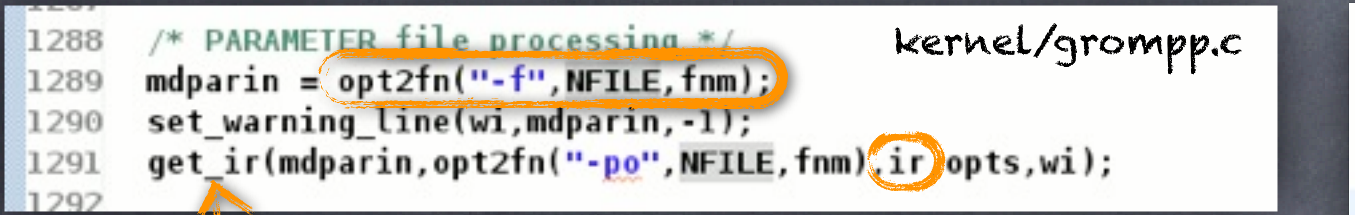
```
typedef struct {
    int       nstswap;          /* Every how many steps a swap is attempted?    */
    int       nat;              /* Number of atoms in the ion group             */
    int       nat_split[2];     /* Number of atoms in the split group           */
    int       nat_sol;          /* Number of atoms in the solvent group         */
    atom_id  *ind;              /* The global ion group atoms numbers           */
    atom_id  *ind_split[2];     /* Split groups for compartment partitioning    */
    atom_id  *ind_sol;          /* The global solvent group atom numbers        */
...
    int       nanions[eCompNr]; /* Requested number of anions and              */
    int       csteps;           /* Coupling constant (nr of time steps)         */
    real      threshold;        /* Ion counts may deviate from the requested
                                   values by +-threshold before a swap is done */
    int       ncations[eCompNr]; /* ... cations for both compartments           */
} t_swapcoords;

typedef struct {
  int  eI;                 /* Integration method                 */
  gmx_large_int_t nsteps;    /* number of steps to be taken           */
  int  simulation_part; /* Used in checkpointing to separate chunks */
  gmx_large_int_t init_step;    /* start at a stepcount >0 (used w. tpbconv)    */
  int  nstlist;        /* number of steps before pairlist is generated */
  int nstlog;          /* number of steps after which print to logfile */
  int nstxout;         /* number of steps after which X is output  */
  int nstvout;         /* id. for V                       */
  int nstfout;         /* id. for F                       */
  int nstenergy;       /* number of steps after which energies printed */
  int nstxtcout;       /* id. for compressed trj (.xtc)         */
  double init_t;       /* initial time (ps)               */
  double delta_t;      /* time step (ps)                  */
...
  int eSwapCoords;         /* Perform coordinate exchanges?                 */
  t_swapcoords *swap;
...
} t_inputrec;
```

include/types/inputrec.h

Start by adding your new variables to the t_inputrec structure

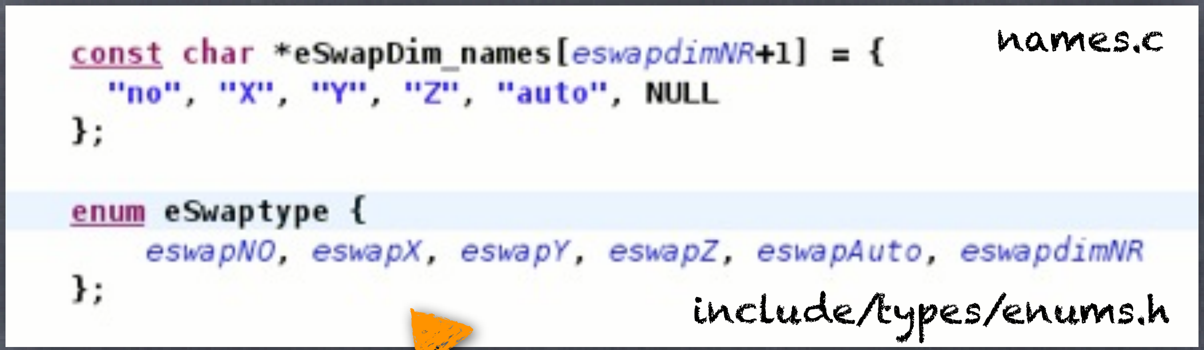
#12b Add MDP input parameters

- grompp parses MDP file



kernel/grompp.c

```
/* PARAMETER file processing */
mdparin = opt2fn("-f",NFILE,fnm);
set_warning_line(wi,mdparin,-1);
get_ir(mdparin,opt2fn("-po",NFILE,fnm),ir,opts,wi);
```



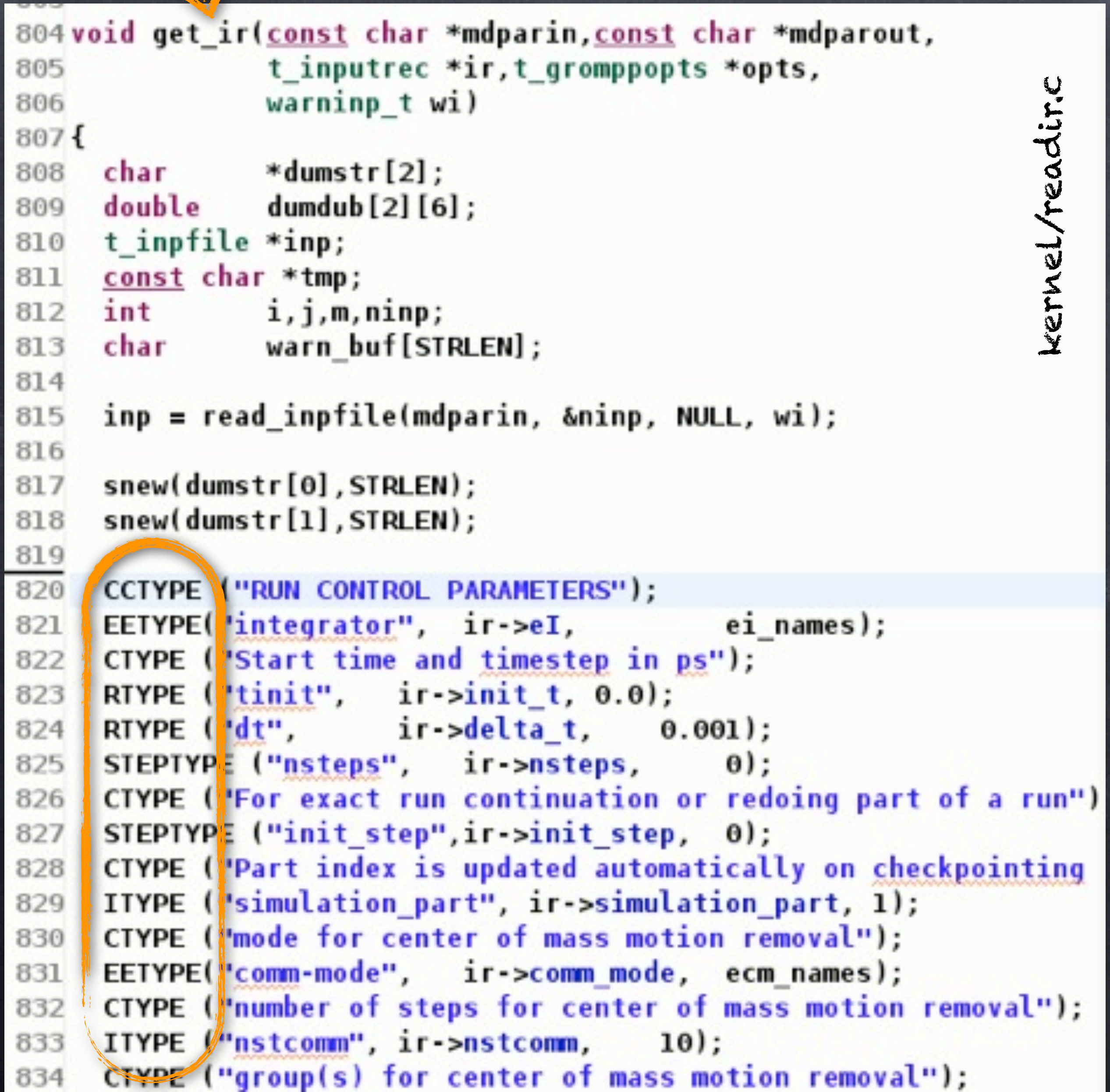
names.c

```
const char *eSwapDim_names[eswapdimNR+1] = {
  "no", "X", "Y", "Z", "auto", NULL
};
```

```
enum eSwaptype {
    eswapNO, eswapX, eswapY, eswapZ, eswapAuto, eswapdimNR
};
```

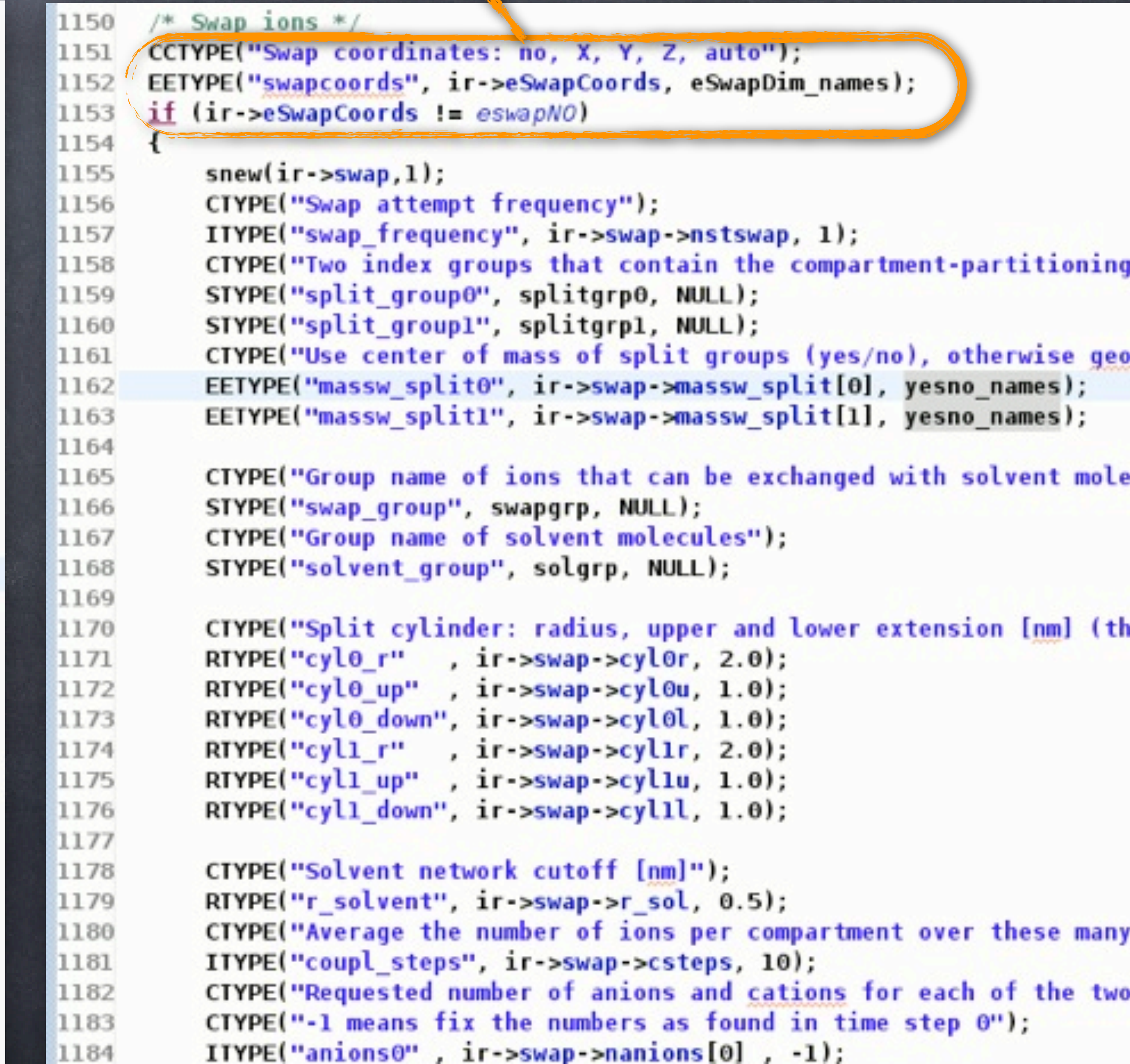
include/types/enums.h

- teach get_ir to parse the new entries:



kernel/readir.c

```
void get_ir(const char *mdparin,const char *mdparout,
            t_inputrec *ir,t_gromppopts *opts,
            warninp_t wi)
{
  char       *dumstr[2];
  double      dumdub[2][6];
  t_inpfile  *inp;
  const char *tmp;
  int         i,j,m,ninp;
  char        warn_buf[STRLEN];

  inp = read_inpfile(mdparin, &ninp, NULL, wi);

  snew(dumstr[0],STRLEN);
  snew(dumstr[1],STRLEN);

  CCTYPE ("RUN CONTROL PARAMETERS");
  EETYPE("integrator",   ir->eI,         ei_names);
  CTYPE ("Start time and timestep in ps");
  RTYPE ("tinit",     ir->init_t, 0.0);
  RTYPE ("dt",        ir->delta_t,    0.001);
  STEPTYPE ("nsteps",    ir->nsteps,      0);
  CTYPE ("For exact run continuation or redoing part of a run")
  STEPTYPE ("init_step",ir->init_step,  0);
  CTYPE ("Part index is updated automatically on checkpointing
  ITYPE ("simulation_part", ir->simulation_part, 1);
  CTYPE ("mode for center of mass motion removal");
  EETYPE("comm-mode",    ir->comm_mode,   ecm_names);
  CTYPE ("number of steps for center of mass motion removal");
  ITYPE ("nstcomm", ir->nstcomm,     10);
  CTYPE ("group(s) for center of mass motion removal");
```

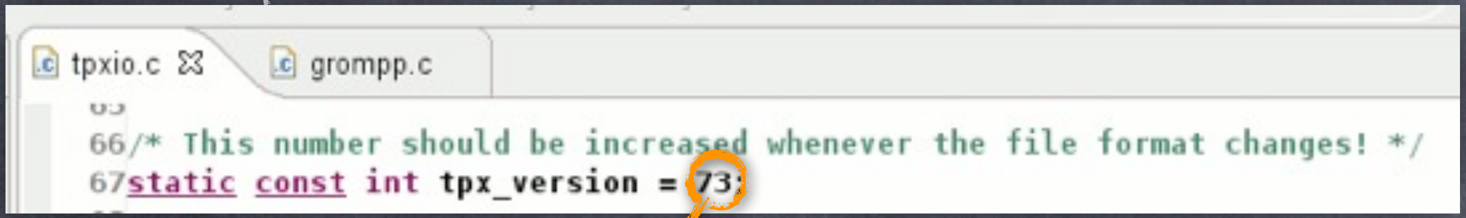


```
/* Swap ions */
CCTYPE("Swap coordinates: no, X, Y, Z, auto");
EETYPE("swapcoords", ir->eSwapCoords, eSwapDim_names);
if (ir->eSwapCoords != eswapNO)
{
    snew(ir->swap,1);
    CTYPE("Swap attempt frequency");
    ITYPE("swap_frequency", ir->swap->nstswap, 1);
    CTYPE("Two index groups that contain the compartment-partitioning
    STYPE("split_group0", splitgrp0, NULL);
    STYPE("split_group1", splitgrp1, NULL);
    CTYPE("Use center of mass of split groups (yes/no), otherwise geo
    EETYPE("massw_split0", ir->swap->massw_split[0], yesno_names);
    EETYPE("massw_split1", ir->swap->massw_split[1], yesno_names);

    CTYPE("Group name of ions that can be exchanged with solvent mole
    STYPE("swap_group", swapgrp, NULL);
    CTYPE("Group name of solvent molecules");
    STYPE("solvent_group", solgrp, NULL);

    CTYPE("Split cylinder: radius, upper and lower extension [nm] (th
    RTYPE("cyl0_r"    , ir->swap->cyl0r, 2.0);
    RTYPE("cyl0_up"   , ir->swap->cyl0u, 1.0);
    RTYPE("cyl0_down", ir->swap->cyl0l, 1.0);
    RTYPE("cyl1_r"    , ir->swap->cyl1r, 2.0);
    RTYPE("cyl1_up"   , ir->swap->cyl1u, 1.0);
    RTYPE("cyl1_down", ir->swap->cyl1l, 1.0);

    CTYPE("Solvent network cutoff [nm]");
    RTYPE("r_solvent", ir->swap->r_sol, 0.5);
    CTYPE("Average the number of ions per compartment over these many
    ITYPE("coupl_steps", ir->swap->csteps, 10);
    CTYPE("Requested number of anions and cations for each of the two
    CTYPE("-1 means fix the numbers as found in time step 0");
    ITYPE("anions0" , ir->swap->nanions[0] , -1);
```

#13 Write new parameters to tpr

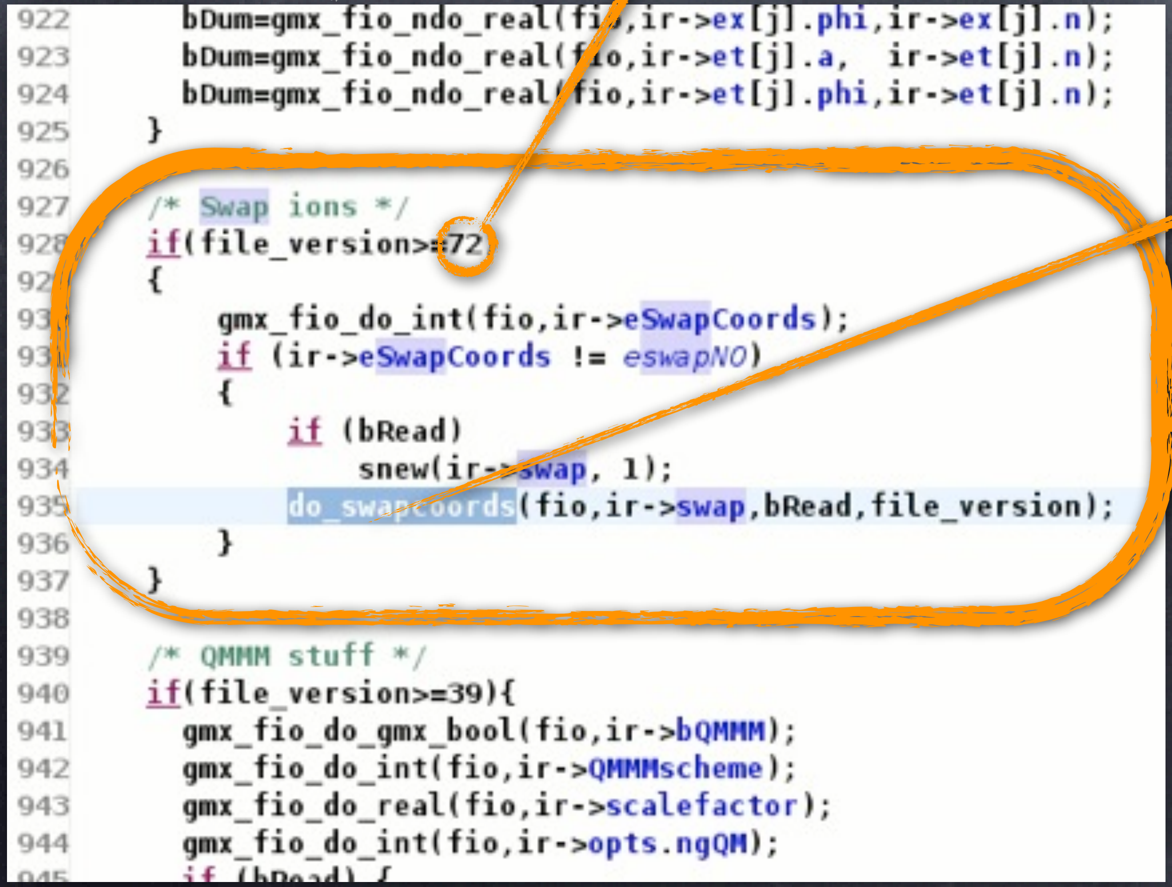
- grompp
  > write_tpx_state( )
  > do_tpx( )
  > do_inputrec( ) in gmxlib/tpxio.c writes ir to TPR

- increase tpx_version!

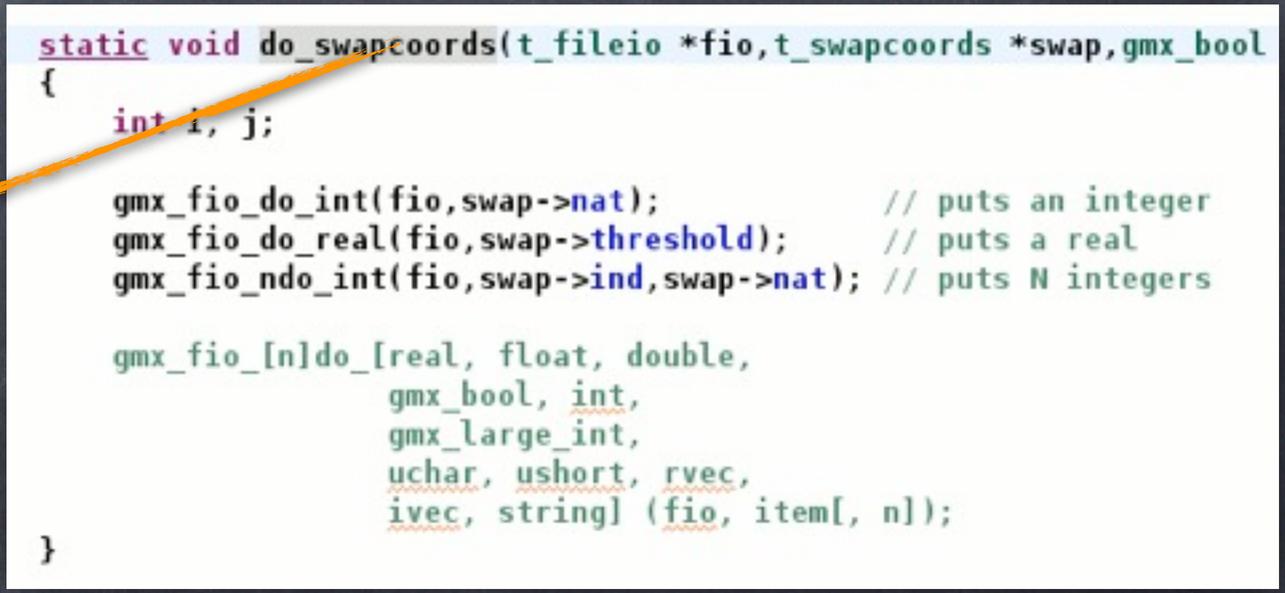


```
/* This number should be increased whenever the file format changes! */
static const int tpx_version = 73;
```

- add i/o for your new stuff in do_inputrec( ):



```
      bDum=gmx_fio_ndo_real(fio,ir->ex[j].phi,ir->ex[j].n);
      bDum=gmx_fio_ndo_real(fio,ir->et[j].a,  ir->et[j].n);
      bDum=gmx_fio_ndo_real(fio,ir->et[j].phi,ir->et[j].n);
    }

    /* Swap ions */
    if(file_version>=72)
    {
        gmx_fio_do_int(fio,ir->eSwapCoords);
        if (ir->eSwapCoords != eswapNO)
        {
            if (bRead)
                snew(ir->swap, 1);
            do_swapcoords(fio,ir->swap,bRead,file_version);
        }
    }

    /* QMMM stuff */
    if(file_version>=39){
      gmx_fio_do_gmx_bool(fio,ir->bQMMM);
      gmx_fio_do_int(fio,ir->QMMMscheme);
      gmx_fio_do_real(fio,ir->scalefactor);
      gmx_fio_do_int(fio,ir->opts.ngQM);
      if (bRead) {
```

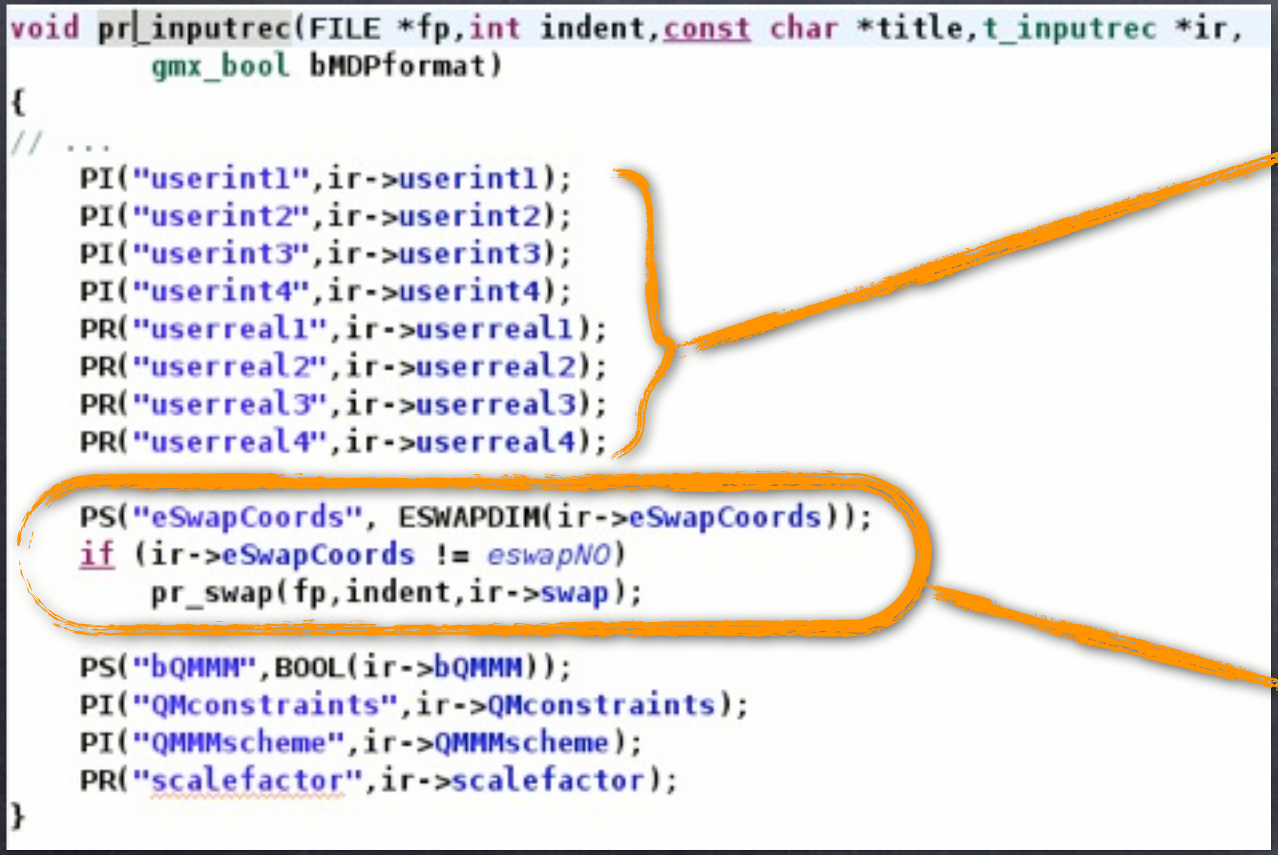


```
static void do_swapcoords(t_fileio *fio,t_swapcoords *swap,gmx_bool
{
    int i, j;

    gmx_fio_do_int(fio,swap->nat);                  // puts an integer
    gmx_fio_do_real(fio,swap->threshold);           // puts a real
    gmx_fio_ndo_int(fio,swap->ind,swap->nat); // puts N integers

    gmx_fio_[n]do_[real, float, double,
                   gmx_bool, int,
                   gmx_large_int,
                   uchar, ushort, rvec,
                   ivec, string] (fio, item[, n]);
}
```

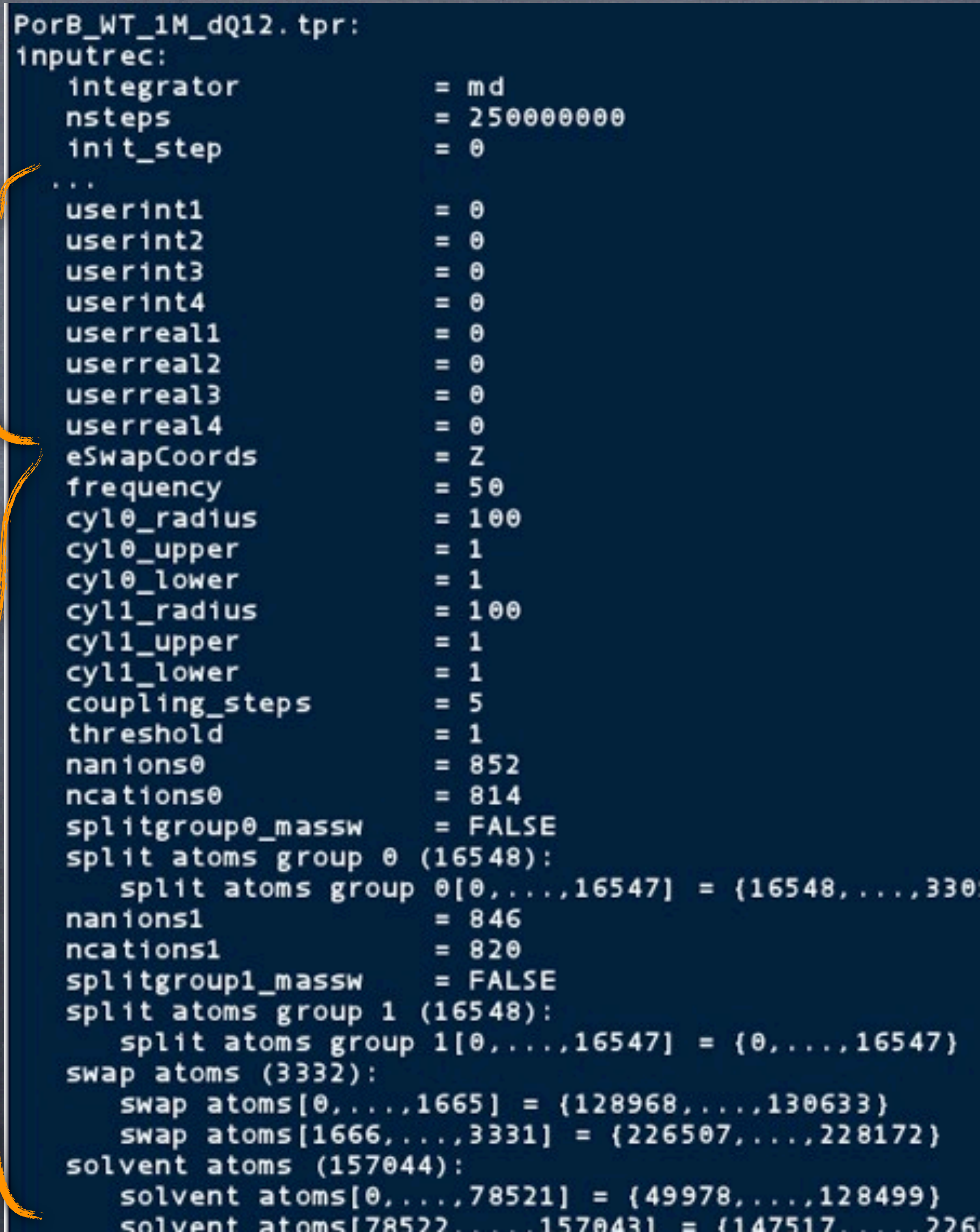
#14 Make gmxdump work

check whether new data made it to TPR

- gmxdump
  > list_tpx( )
  > pr_inputrec( ) in gmxlib/txtdump.c dumps ir



```
void pr_inputrec(FILE *fp,int indent,const char *title,t_inputrec *ir,
        gmx_bool bMDPformat)
{
// ...
    PI("userint1",ir->userint1);
    PI("userint2",ir->userint2);
    PI("userint3",ir->userint3);
    PI("userint4",ir->userint4);
    PR("userreal1",ir->userreal1);
    PR("userreal2",ir->userreal2);
    PR("userreal3",ir->userreal3);
    PR("userreal4",ir->userreal4);

    PS("eSwapCoords", ESWAPDIM(ir->eSwapCoords));
    if (ir->eSwapCoords != eswapNO)
        pr_swap(fp,indent,ir->swap);

    PS("bQMMM",BOOL(ir->bQMMM));
    PI("QMconstraints",ir->QMconstraints);
    PI("QMMMscheme",ir->QMMMscheme);
    PR("scalefactor",ir->scalefactor);
}
```



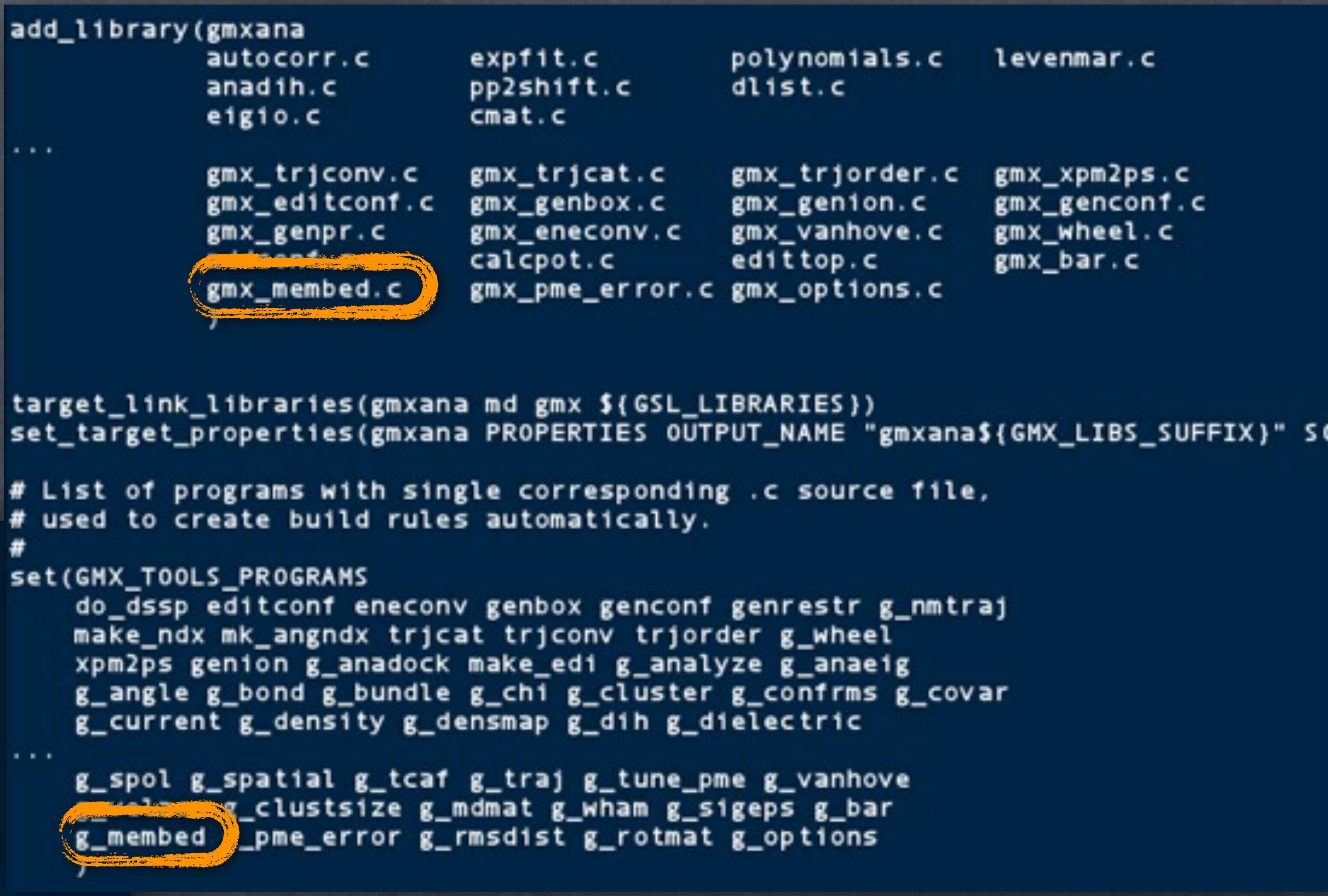
```
PorB_WT_1M_dQ12.tpr:
inputrec:
   integrator             = md
   nsteps                 = 250000000
   init_step              = 0
  ...
   userint1               = 0
   userint2               = 0
   userint3               = 0
   userint4               = 0
   userreal1              = 0
   userreal2              = 0
   userreal3              = 0
   userreal4              = 0
   eSwapCoords            = Z
   frequency              = 50
   cyl0_radius            = 100
   cyl0_upper             = 1
   cyl0_lower             = 1
   cyl1_radius            = 100
   cyl1_upper             = 1
   cyl1_lower             = 1
   coupling_steps         = 5
   threshold              = 1
   nanions0               = 852
   ncations0              = 814
   splitgroup0_massw      = FALSE
   split atoms group 0 (16548):
      split atoms group 0[0,...,16547] = {16548,...,330
   nanions1               = 846
   ncations1              = 820
   splitgroup1_massw      = FALSE
   split atoms group 1 (16548):
      split atoms group 1[0,...,16547] = {0,...,16547}
   swap atoms (3332):
      swap atoms[0,...,1665] = {128968,...,130633}
      swap atoms[1666,...,3331] = {226507,...,228172}
   solvent atoms (157044):
      solvent atoms[0,...,78521] = {49978,...,128499}
      solvent atoms[78522,...,157043] = {147517,...,226
```

- also mdrun prints this to md.log!
  mdrun
  > runner( )
  > pr_inputrec( )

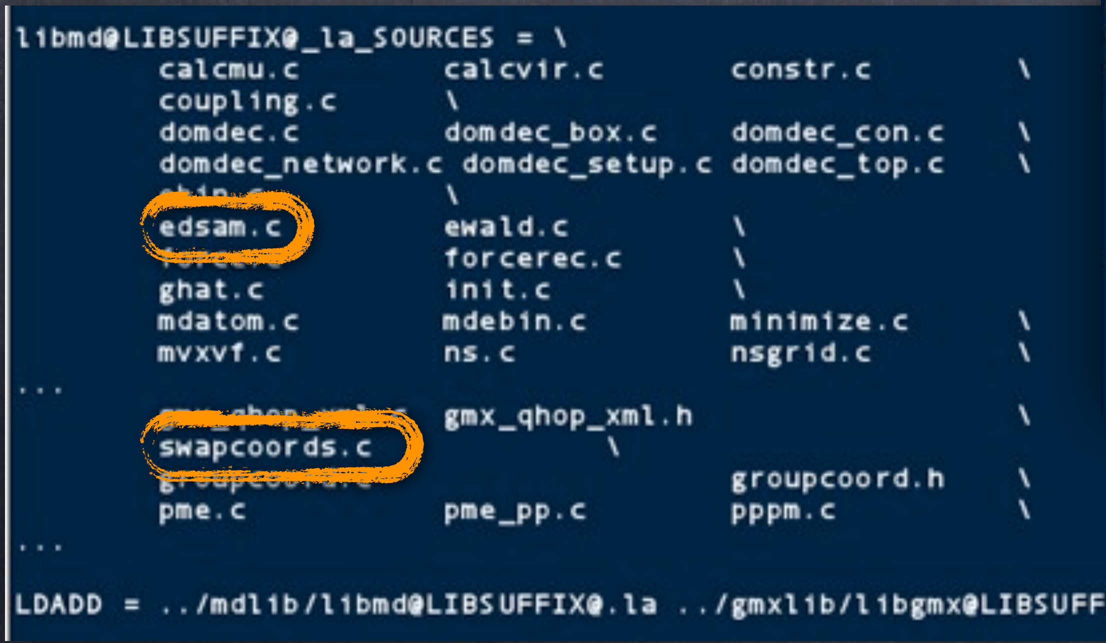
#15 Getting your module compiled

make yourfile.c part of gromacs

- Generally: make a new .c & .h file for new mdrun functionality, typically in src/mdlib, or src/tools
- keep your code together!
- add your source to Makefile.am and/or CMakeLists.txt



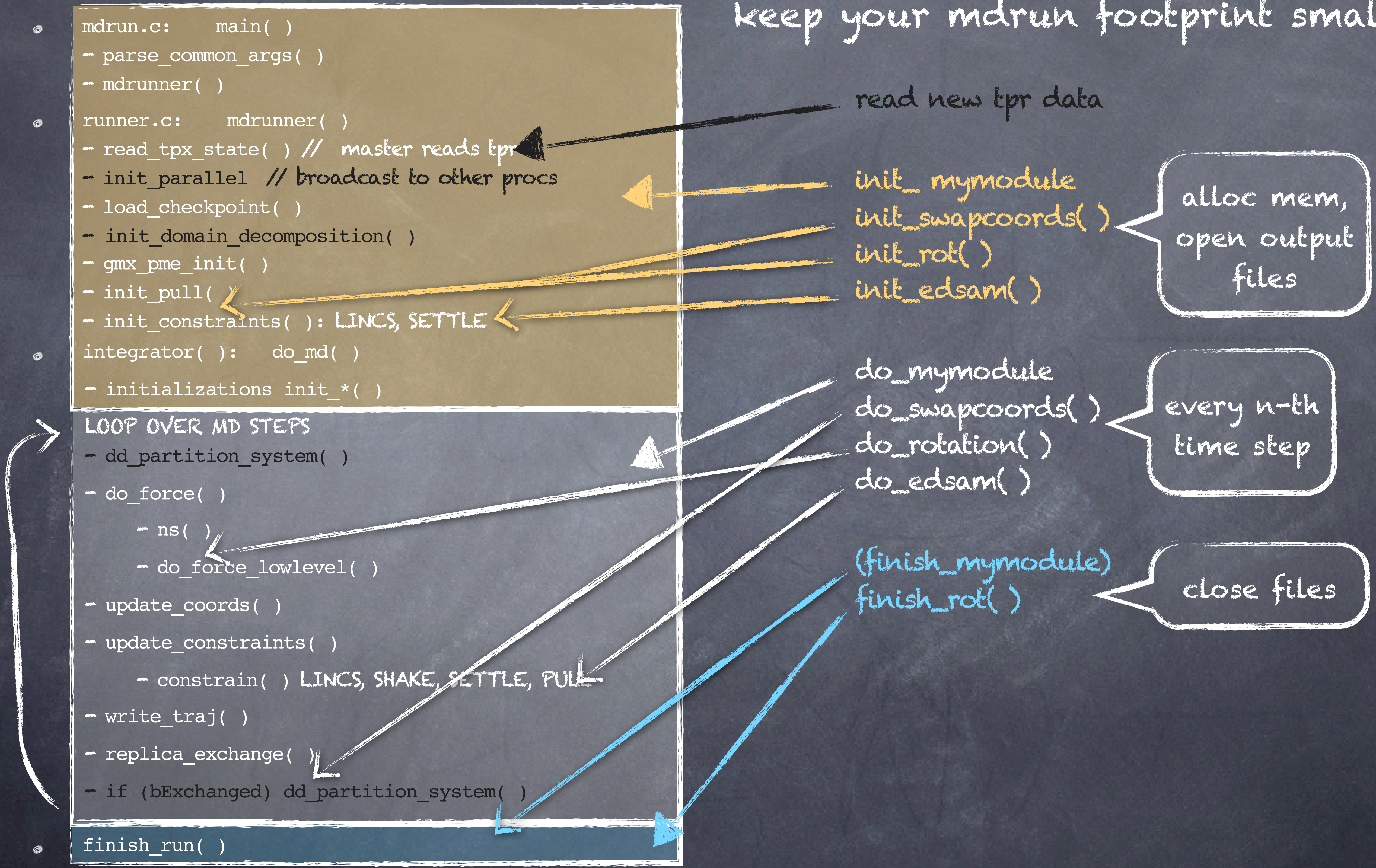
```
add_library(gmxana
            autocorr.c       expfit.c         polynomials.c    levenmar.c
            anadih.c         pp2shift.c       dlist.c
            eigio.c          cmat.c
...
            gmx_trjconv.c    gmx_trjcat.c     gmx_trjorder.c   gmx_xpm2ps.c
            gmx_editconf.c   gmx_genbox.c     gmx_genion.c     gmx_genconf.c
            gmx_genpr.c      gmx_eneconv.c    gmx_vanhove.c    gmx_wheel.c
            [illegible]      calcpot.c        edittop.c        gmx_bar.c
            gmx_membed.c     gmx_pme_error.c gmx_options.c
            )


target_link_libraries(gmxana md gmx ${GSL_LIBRARIES})
set_target_properties(gmxana PROPERTIES OUTPUT_NAME "gmxana${GMX_LIBS_SUFFIX}" S

# List of programs with single corresponding .c source file,
# used to create build rules automatically.
#
set(GMX_TOOLS_PROGRAMS
    do_dssp editconf eneconv genbox genconf genrestr g_nmtraj
    make_ndx mk_angndx trjcat trjconv trjorder g_wheel
    xpm2ps genion g_anadock make_edi g_analyze g_anaeig
    g_angle g_bond g_bundle g_chi g_cluster g_confrms g_covar
    g_current g_density g_densmap g_dih g_dielectric
...
    g_spol g_spatial g_tcaf g_traj g_tune_pme g_vanhove
    [illegible] g_clustsize g_mdmat g_wham g_sigeps g_bar
    g_membed g_pme_error g_rmsdist g_rotmat g_options
    )
```



```
libmd@LIBSUFFIX@_la_SOURCES = \
        calcmu.c          calcvir.c         constr.c          \
        coupling.c        \
        domdec.c          domdec_box.c      domdec_con.c      \
        domdec_network.c domdec_setup.c domdec_top.c      \
        [illegible]       \
        edsam.c           ewald.c           \
        force.c           forcerec.c        \
        ghat.c            init.c            \
        mdatom.c          mdebin.c          minimize.c        \
        mvxvf.c           ns.c              nsgrid.c          \
...
        [illegible]       gmx_qhop_xml.h                      \
        swapcoords.c                 \
        groupcoord.c                    groupcoord.h      \
        pme.c             pme_pp.c          pppm.c            \
...

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

#16 Decide where to interface mdrun

keep your mdrun footprint small



```
mdrun.c:    main( )
- parse_common_args( )
- mdrunner( )

runner.c:    mdrunner( )
- read_tpx_state( ) // master reads tpr
- init_parallel // broadcast to other procs
- load_checkpoint( )
- init_domain_decomposition( )
- gmx_pme_init( )
- init_pull( )
- init_constraints( ): LINCS, SETTLE

integrator( ):    do_md( )
- initializations init_*( )

LOOP OVER MD STEPS
- dd_partition_system( )
- do_force( )
      - ns( )
      - do_force_lowlevel( )
- update_coords( )
- update_constraints( )
      - constrain( ) LINCS, SHAKE, SETTLE, PULL
- write_traj( )
- replica_exchange( )
- if (bExchanged) dd_partition_system( )

finish_run( )
```

read new tpr data

init_ mymodule
init_swapcoords( )
init_rot( )
init_edsam( )

alloc mem, open output files

do_mymodule
do_swapcoords( )
do_rotation( )
do_edsam( )

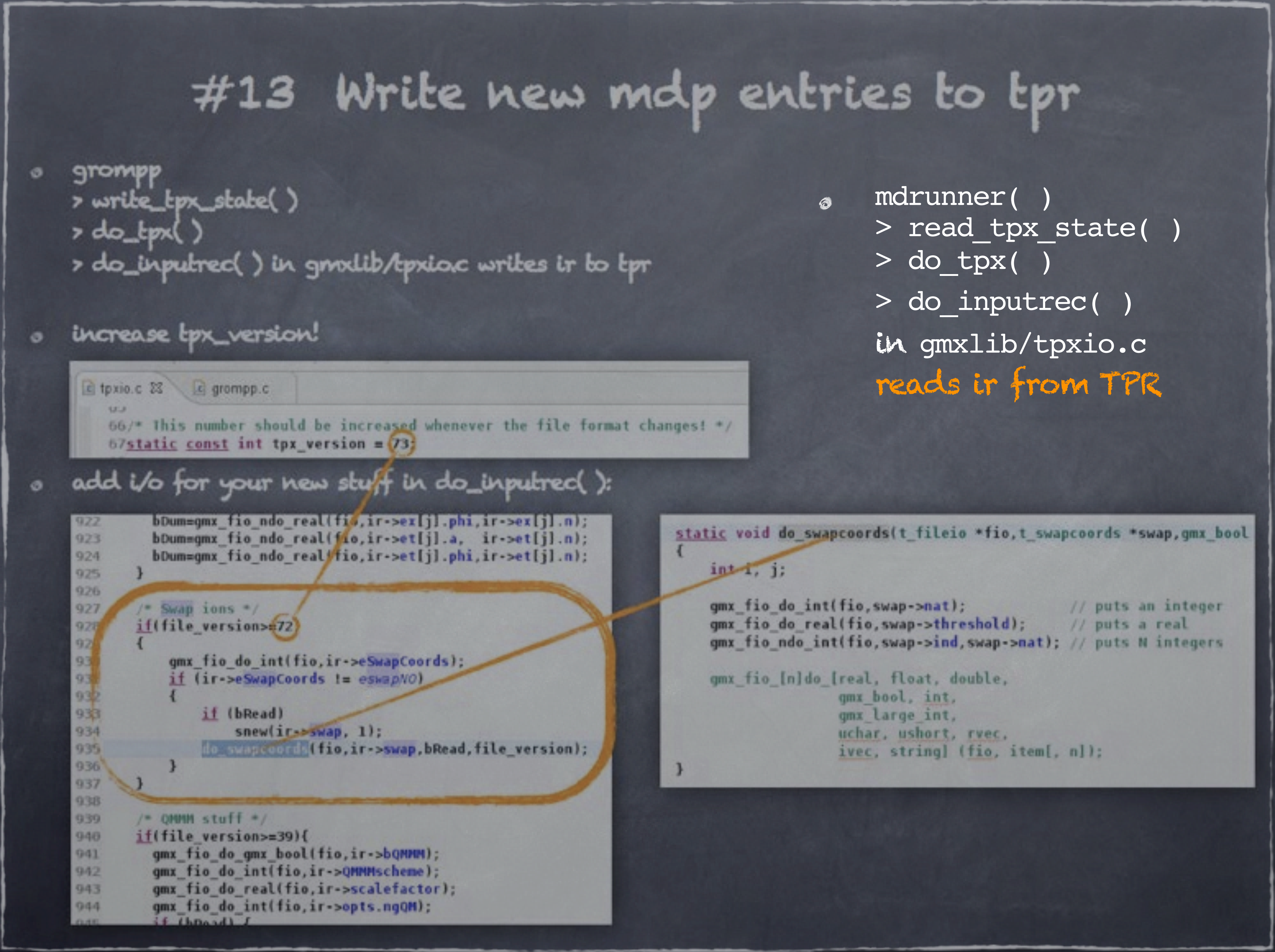
every n-th time step

(finish_mymodule)
finish_rot( )

close files

#17 Let mdrun read your TPR entries

already done!



#13 Write new mdp entries to tpr

- grompp
  > write_tpx_state( )
  > do_tpx( )
  > do_inputrec( ) in gmxlib/tpxio.c writes ir to tpr
- increase tpx_version!

```
/* This number should be increased whenever the file format changes! */
static const int tpx_version = 73;
```

- add i/o for your new stuff in do_inputrec( ):

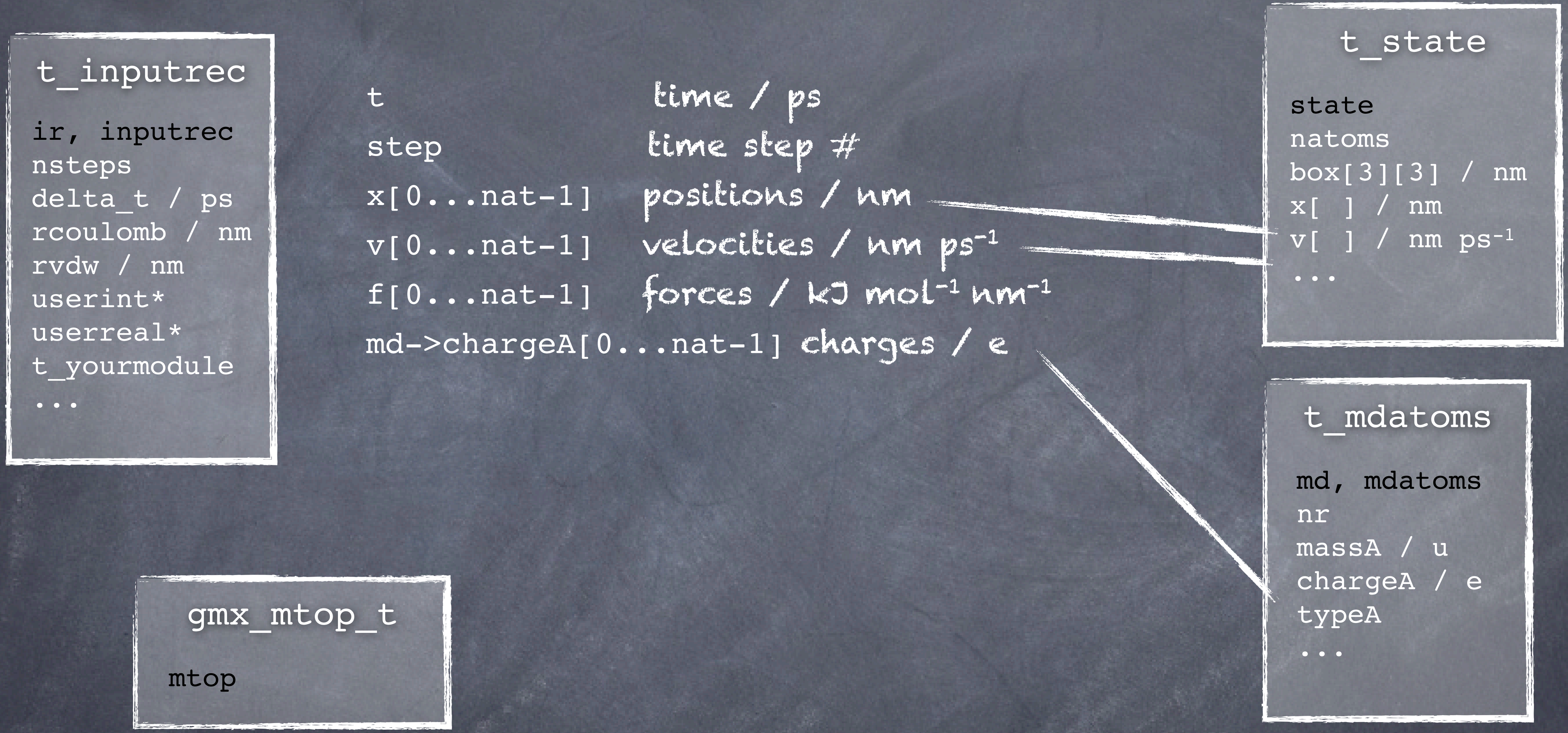
```
    bDum=gmx_fio_ndo_real(fio,ir->ex[j].phi,ir->ex[j].n);
    bDum=gmx_fio_ndo_real(fio,ir->et[j].a,  ir->et[j].n);
    bDum=gmx_fio_ndo_real(fio,ir->et[j].phi,ir->et[j].n);
  }

  /* Swap ions */
  if(file_version>=72)
  {
      gmx_fio_do_int(fio,ir->eSwapCoords);
      if (ir->eSwapCoords != eswapNO)
      {
          if (bRead)
              snew(ir->swap, 1);
          do_swapcoords(fio,ir->swap,bRead,file_version);
      }
  }

  /* QMMM stuff */
  if(file_version>=39){
    gmx_fio_do_gmx_bool(fio,ir->bQMMM);
    gmx_fio_do_int(fio,ir->QMMMscheme);
    gmx_fio_do_real(fio,ir->scalefactor);
    gmx_fio_do_int(fio,ir->opts.ngQM);
    if (bRead) {
```

```
static void do_swapcoords(t_fileio *fio,t_swapcoords *swap,gmx_bool
{
    int i, j;

    gmx_fio_do_int(fio,swap->nat);                // puts an integer
    gmx_fio_do_real(fio,swap->threshold);         // puts a real
    gmx_fio_ndo_int(fio,swap->ind,swap->nat); // puts N integers

    gmx_fio_[n]do_[real, float, double,
                   gmx_bool, int,
                   gmx_large_int,
                   uchar, ushort, rvec,
                   ivec, string] (fio, item[, n]);
}
```

- mdrunner( )
  > read_tpx_state( )
  > do_tpx( )
  > do_inputrec( )
  in gmxlib/tpxio.c
  reads ir from TPR

#18 In the MD loop

Variables you might need



t	time / ps
step	time step #
x[0...nat-1]	positions / nm
v[0...nat-1]	velocities / nm ps^{-1}
f[0...nat-1]	forces / kJ mol^{-1} nm^{-1}
md->chargeA[0...nat-1]	charges / e

t_inputrec

ir, inputrec
nsteps
delta_t / ps
rcoulomb / nm
rvdw / nm
userint*
userreal*
t_yourmodule
...

t_state

state
natoms
box[3][3] / nm
x[ ] / nm
v[ ] / nm ps^{-1}
...

t_mdatoms

md, mdatoms
nr
massA / u
chargeA / e
typeA
...

gmx_mtop_t

mtop

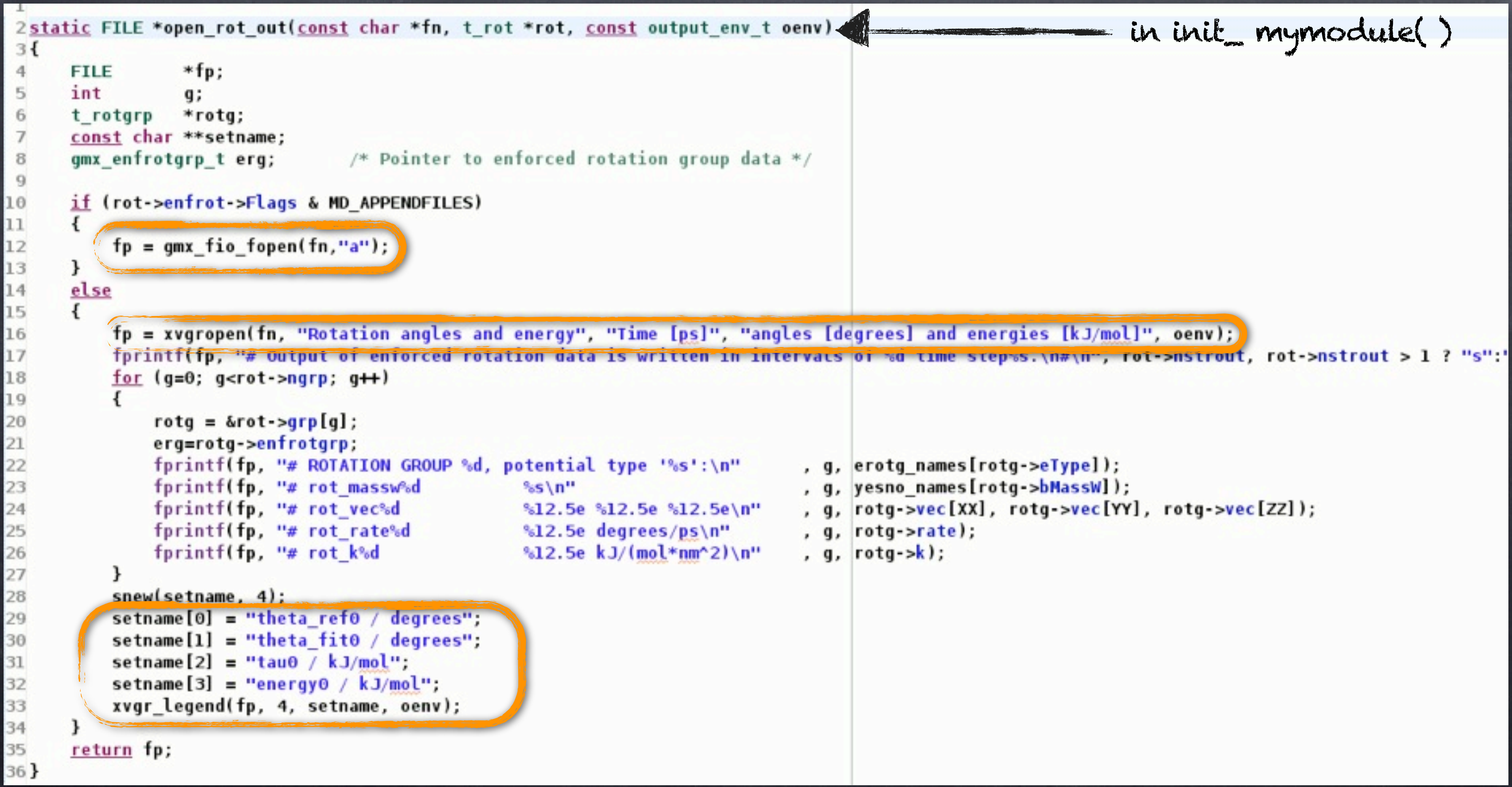
gmx_mtop_atomnr_to_atom(gmx_mtop_t, int nr, t_atom atom)

atom -> m, q, type

gmx_mtop_atominfo_global -> atomname, resname

#19 Output

Why not write an XVG file?

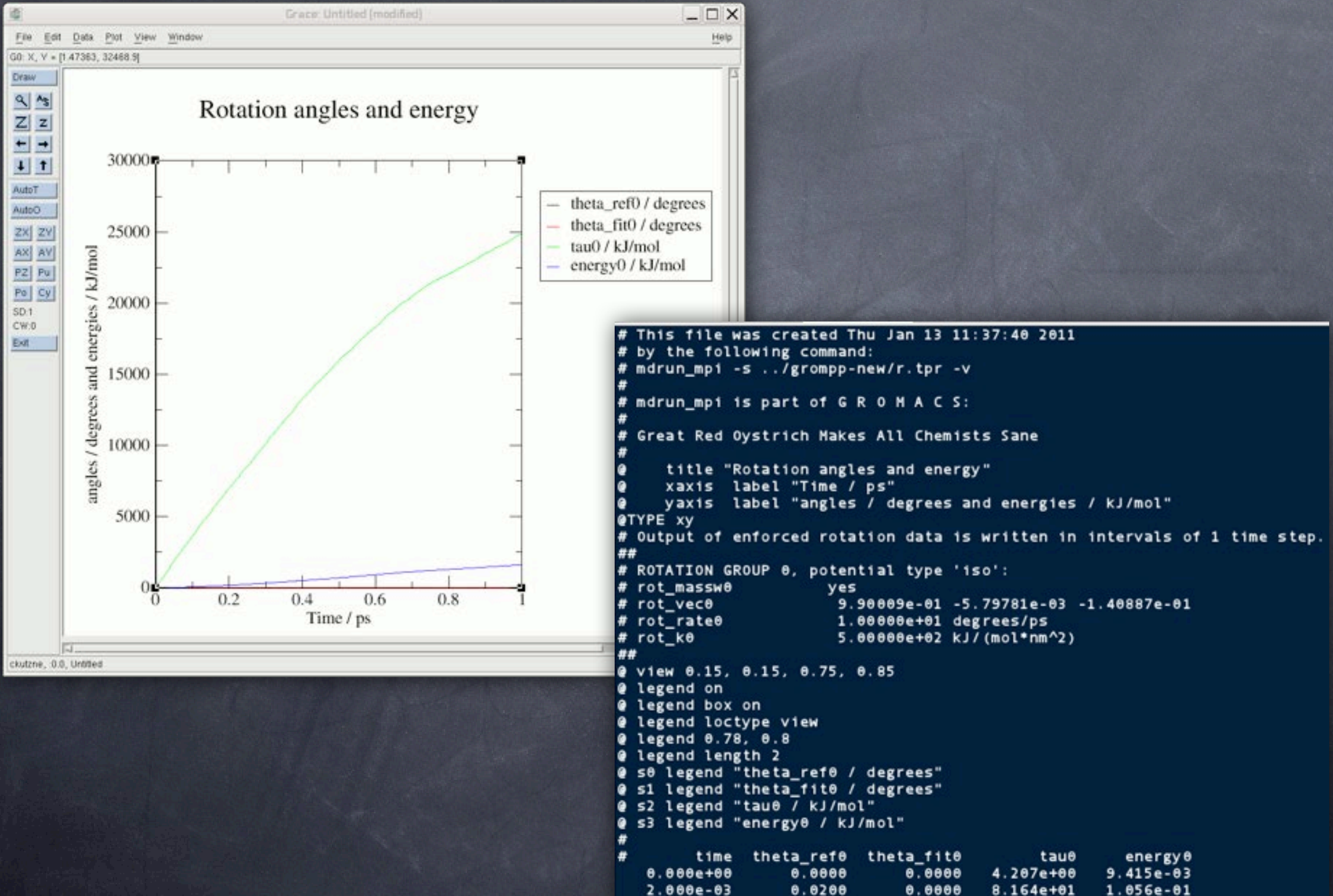


```
static FILE *open_rot_out(const char *fn, t_rot *rot, const output_env_t oenv)
{
    FILE       *fp;
    int         g;
    t_rotgrp   *rotg;
    const char **setname;
    gmx_enfrotgrp_t erg;       /* Pointer to enforced rotation group data */

    if (rot->enfrot->Flags & MD_APPENDFILES)
    {
        fp = gmx_fio_fopen(fn,"a");
    }
    else
    {
        fp = xvgropen(fn, "Rotation angles and energy", "Time [ps]", "angles [degrees] and energies [kJ/mol]", oenv);
        fprintf(fp, "# Output of enforced rotation data is written in intervals of %d time step%s.\n#\n", rot->nstrout, rot->nstrout > 1 ? "s":"
        for (g=0; g<rot->ngrp; g++)
        {
            rotg = &rot->grp[g];
            erg=rotg->enfrotgrp;
            fprintf(fp, "# ROTATION GROUP %d, potential type '%s':\n"      , g, erotg_names[rotg->eType]);
            fprintf(fp, "# rot_massw%d          %s\n"                      , g, yesno_names[rotg->bMassW]);
            fprintf(fp, "# rot_vec%d            %12.5e %12.5e %12.5e\n"    , g, rotg->vec[XX], rotg->vec[YY], rotg->vec[ZZ]);
            fprintf(fp, "# rot_rate%d           %12.5e degrees/ps\n"       , g, rotg->rate);
            fprintf(fp, "# rot_k%d              %12.5e kJ/(mol*nm^2)\n"    , g, rotg->k);
        }
        snew(setname, 4);
        setname[0] = "theta_ref0 / degrees";
        setname[1] = "theta_fit0 / degrees";
        setname[2] = "tau0 / kJ/mol";
        setname[3] = "energy0 / kJ/mol";
        xvgr_legend(fp, 4, setname, oenv);
    }
    return fp;
}
```

in init_ mymodule( )

#19b Output

Why not write an XVG file?



```
# This file was created Thu Jan 13 11:37:40 2011
# by the following command:
# mdrun_mpi -s ../grompp-new/r.tpr -v
#
# mdrun_mpi is part of G R O M A C S:
#
# Great Red Oystrich Makes All Chemists Sane
#
@    title "Rotation angles and energy"
@    xaxis  label "Time / ps"
@    yaxis  label "angles / degrees and energies / kJ/mol"
@TYPE xy
# Output of enforced rotation data is written in intervals of 1 time step.
##
# ROTATION GROUP 0, potential type 'iso':
# rot_massw0          yes
# rot_vec0             9.90009e-01 -5.79781e-03 -1.40887e-01
# rot_rate0            1.00000e+01 degrees/ps
# rot_k0               5.00000e+02 kJ/(mol*nm^2)
##
@ view 0.15, 0.15, 0.75, 0.85
@ legend on
@ legend box on
@ legend loctype view
@ legend 0.78, 0.8
@ legend length 2
@ s0 legend "theta_ref0 / degrees"
@ s1 legend "theta_fit0 / degrees"
@ s2 legend "tau0 / kJ/mol"
@ s3 legend "energy0 / kJ/mol"
#
#       time  theta_ref0  theta_fit0        tau0     energy0
  0.000e+00      0.0000      0.0000   4.207e+00   9.415e-03
  2.000e-03      0.0200      0.0000   8.164e+01   1.056e-01
```

#20 Want more?

topics not covered

- actually write your module! homework :)
- writing to checkpoint file
- parallelism / domain decomposition
- best practices C coding
- g_something is not working correctly. What can I do?
- ?