Using \texttt{g_mdmat} from GROMACS 4.5.4, the xvg output file formats the legend metadata in a way that \texttt{xmgrace} 5.1.22 does not understand, complaining of "Unallocated set: LEGEND STRING ..." for each legend entry.

Example \texttt{g_mdmat} command:

```bash
  g_mdmat
  -f testout/20110720-1614/trajectory.trr
  -s tpr/hasyn_0001.tpr
  -n gro/hasyn_0001.ndx
  -mean testout/20110720-1614/mdmat_mean.xpm
  -frames testout/20110720-1614/mdmat_frames.xpm
  -no testout/20110720-1614/mdmat_num.xvg
```

The xvg file produced formats the legend as:

```plaintext
@ legend string 0 "Total/mean"
@ legend string 1 "Total"
@ legend string 2 "Mean"
@ legend string 3 "# atoms"
@ legend string 4 "Mean/# atoms"
```

but \texttt{xmgrace} wants

```plaintext
@ s0 legend "Total/mean"
@ s1 legend "Total"
@ s2 legend "Mean"
@ s3 legend "# atoms"
@ s4 legend "Mean/# atoms"
```

... which is how the other \texttt{g_} utilities that I've used generate it.

I'm not confident enough to suggest a diff, but the string "legend string" appears in these files:

- `src/tools/gmx_analyze.c` lines 552 553
- `src/tools/gmx_enemat.c` lines 417 419 421
- `src/tools/gmx_mdmat.c` lines 324-328
- `src/tools/gmx_saltbr.c` line 252 -- this seems to only be output for \texttt{xmgr}, as (I think) is correct. Maybe that's the problem with \texttt{g_mdmat}?
- `src/gmxlib/xvgr.c` line 358 -- again, only for \texttt{xmgr}

My guess is that \texttt{g_analyze}, \texttt{g_enemat} and \texttt{g_mdmat} are producing \texttt{xmgr} format xvg files when they should output \texttt{xmgrace} files.
Moved heuristic neighbor-list code into mdlib

Moved iterated-constraints code into mdlib

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Moved various support functions for do_md into mdlib

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Make sure figure legends are adapted to xmgr/xmgrace

A few programs were not using the xvgr_legend call. g_mdmat has been modified to use it, and for g_analyse and g_enemat I at least fixed the existing direct-writing code by adding a conditional.

Fixes #783.

Change-Id: I782af539b93737b570f266ba744e718fbd846e5f

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Yes you are correct. Those tools should use the function xvgr_legend instead of printing directly. That way the format is correct for both programs. Could you please upload a patch to gerrit.gromacs.org?

- Priority changed from Normal to Low

Gerrit received a related patchset '1' for Issue #783.
Uploader: Erik Lindahl (erik@kth.se)
Change-Id: I782af539b93737b570f266ba744e718fbd846e5f
Gerrit URL: https://gerrit.gromacs.org/3583

- Status changed from New to Fix uploaded
- Affected version set to 4.6.x

- Status changed from Fix uploaded to Resolved
- % Done changed from 0 to 100

Applied in changeset 75f84652037affa3e28fcb651af8769c672f736a9.
- Status changed from Resolved to Closed