AutoDock 4.2.6 Release Notes

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                    AutoDock Release Notes
                  Release 4.2.6 (July 2014)
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Supported computer platforms in 4.2.6:

Linux2 on Intel i86 (32-bit) and on Intel x86_64 (64-bit).
Linux3 on Intel x86_64 (64-bit).
Macintosh OS X 10.5 (Leopard) on PowerPC (32- and 64-bit),
  OS X 10.5-10.9 (Leopard, Snow Leopard, Lion, Mountain Lion,
 and Mavericks) on Intel i86 (32-bit) and Intel x86_64 (64-bit).
Solaris 8 (SunOS 5.8) on SPARC.
Windows 5-8.1 on Intel i86.

The executable binaries (autogrid4, autodock4) for Macintosh OS X
are built on Mac OS X 10.5 and tested on up to Mac OS X 10.9.
Each of the two binaries is "universal" and will run on any of
the supported Macs.

The executable binaries for Windows on Intel i86 are built on
Windows 5 (XP) and have been tested on Windows 6, Windows 7, and Windows 8.1.
Windows users do not need to install the CygWin environment,
but they may if they like.

To increase consistency across platforms, all executable programs (both
autogrid and autodock) are compiled using double-precision arithmetic.
The grid maps, as read by AutoDock, are stored internally in single-precision.

Multiple search methods are now possible in a single AutoDock job:
such as 20 runs using Simulated Annealing, 20 runs using the Genetic
Algorithm, and 20 runs using local-search-only.  The runs are
done serially and no results "carry over" from one method to another.
However, all results are ranked and clustered together in the
analysis step at the end of the entire job.

You can now use ADT (AutoDock Tools) to visualize results from AutoDock
jobs that use simulated annealing or local-search-only. You must download the
latest build of ADT from http://mgltools.scripps.edu/downloads/latest

Note a limitation in the 4.2.6 release: the "do_local_only" command
runs the pseudo-solis-wets algorithm, even if the solis-wets has been
specified using "set_local sw1".  This applies only to "do_local_only":
the "ga_run" command will use whichever local search has been specified.
(We recommend the pseudo-solis-wets for all local searches: "set psw1").

AutoDock calculations are performed as a series of independent
runs.  Users will occasionally need to repeat a run. For example,
they might want to repeat a particular run to examine the search space
and convergence of that run.  AutoDock now reports the specific random
number seeds used for each run. Any specific run can be repeated
exactly by using the random number seeds reported in the prior calculation.

The docking log file (.dlg) contents have been further standardized:
Regardless of 'outlev' setting, the host name, run date, working directory,
and names of input PDBQT files are reported at the beginning of the AutoDock
job.  Each 'run' (GA, LGA, local search, simulated annealing) reports its
initial random number seeds and its ending total energy and state
in a uniform format suitable for automated analysis.  At outlev setting
"BASIC" (0) or above, the initial PDBQT ligand (and flexres, if present)
coordinates are reported.  At outlev setting "ADT" (1) or above, the
final docked coordinates of each run are reported.
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Some advanced autodock users customize the program for
their own specific needs. We've improved and simplified building
AutoDock and AutoGrid from source files. We have documented the
process of compiling new atomic parameter tables into AutoDock and
AutoGrid in the README file included in this distribution.

We continue to improve AutoDock's robustness and stability. AutoDock
now verifies that all its input grid maps are the same size.
If AutoDock's standard input has not been redirected to come from a file
or from a pipe, you must specify a docking parameter file using
"-p <docking parameter file.dpf>". When the docking parameters are
read from standard input (e.g., "autodock4 -l mol.dlg < mol.dpf"),
the docking parameter file now appears in output PDBQT files as "stdin".
Reading and parsing the input PDBQT coordinate files has been made more robust.

Other changes since the 4.2.5.1 release (12/13/2012):
Improved error checking of command-line arguments.
Better checking of the atom numbers that define internal and "flexres" torsions.
Better cross-platform compatibility of the internal random number generator.
Running "autodock4 (or autogrid4) --version" reports compile-time configuration options.

==
                  AutoDock Release Notes
                Release 4.2.5.1 (December 13, 2012)
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The changes since the 4.2.5 release (11/02/2012):
#bug fix
4.2.5 incorrectly calculated part of the intermolecular desolvation
energy term; 4.2.5.1 corrects this. All 4.2.5 users should upgrade
to 4.2.5.1 and re-do any runs.

==
                  AutoDock Release Notes
                Release 4.2.5 (November 2, 2012)
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Please note that the previous general release was 4.2.3, 29 January 2010.
The 4.2.4 release (7 July 2010) was a specialized release for
"Fight Aids at Home" and other IBM World Community Grid projects.

Supported computer platforms in 4.2.5:

Linux2 on Intel x86 remains supported, as does Solaris 8 on SPARC.
Supported Macintosh platforms are OS X 10.4-10.5 (Tiger and Leopard) on
Intel x86 and PowerPC, and OS X 10.6-10.8 (Snow Leopard, Lion, and
Mountain Lion) on Intel x86. The executable binaries for Windows on
Intel x86 have been built on Windows 5 (XP) and have been tested on Windows 6
but they may if they like.

The changes since the 4.2.3 release (1/29/2010):

#new features
-: new support for specifying output verbosity ranging from low (-2) up to high (8)
   with symbolic settings for "outlev" defined in constants.h and used in main.cc
-: new automatic calculation of 'about' as the center of the ligand root group
-: new WIN32 MinGW portability - replacements for times() and getrusage()
-: new desolvation term separate from vdW+Hbond term in epdb
     "Per-atom Intermolecular Energy Analysis" table
-: now intelec is on by default; off if "intelec off" in DPF
-: Almost all AutoDock defaults now match defaults supplied by ADT, simplifying PDF files

#code inspection and internal interface self-documentation
-: We thank Steffen Moeller (steffen_moeller@gmx.de) for his enthusiastic
   and expert detailed inspection of all function and method calls,
   in particular identifying "constant" arguments and verifying
   data type compatibiliy.

#improvements
-: improved detailed output of Intermolecular Energy Analysis
-: increased MAX_RUNS from 256 to 2000
-: improved error detection and termination:

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      replaced exit() by EXIT_SUCCESS/EXIT_FAILURE(win32) or stop(msg)
-: increased precision of energy table
-: implemented EnergyComponent structures
-: integrated call_gs into call_glss
-: improved input checking with ga_run/gals_run
[Added checks to "ga_run/gals_run" for missing "set_ga" and missing "set_psw1" errors]
-: simplified logic so more of the FATAL errors are simply handed to "stop()"
-: now set random number seeds at beginning of simanneal execution; output reduced
-: new compile-time option to print energy terms for each atom [for debugging]
-: AutoDock intramolecular energy smoothing now matches that in AutoGrid
-: Consolidated the "side effects" of trilinterp that record per-atom energy components
   and total energy components into two sets of "EnergyComponent" structures instead
   of two Real arrays and two pointers to Real.
-: developed substitutes for WIN32 MinGW "times()" and "getpid()"
-: modified mkTorTree.cc to fill in the root atom information
-: Changed 'tlist' declaration to allow space for root atoms at end

#bug fixes
-: corrected energy breakdown report when using flexible residues
-: desolvation energy term is included even for distant pairs (r>nbc)
-: corrected eintcal side effects of "outlev" setting
-: removed support for unused DPF tokens

#autogrid
AutoGrid 4.2.5 has no functional changes from AutoGrid 4.2.3.
The only significant code changes were those required for porting to Windows.o
We added 'copyfilesfromAD', a maintenance script that copies key shared source files
from AutoDock to AutoGrid.

==========================================================================
                  AutoDock Release Notes
                 Release 4.2.3 (January 29 2010)
==========================================================================
The changes since the 4.2.2.1 release (9/16/2009):

Corrected printing of atom records whose element names are two characters
long (such as Br).  Our thanks to David Lancia for reporting this problem
and working with us on the correction.

Corrected genetic algorithm gene crossover flaw that slowed search progress
for ligands with many torsions. Our thanks to Garrett Morris and Sarnath for
reporting this problem and working with us on the correction.

AutoGrid 4.2.3 differs from AutoGrid 4.2.2 only in the version number.

==========================================================================
                  AutoDock Release Notes
                Release 4.2.2.1 (September 16 2009)
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Please note that the current distribution's executable programs, autogrid and
autodock, were compiled for single precision arithmetic.  We believe
compiling with double-precision would increase consistency across platforms.
(See -DUSE_DOUBLE option in Makefile.am)

The changes since the 4.2.2 release (9/9/2009):

Updated printout of unbound system's energy when using "epdb" option
to correctly set unbound internal energy same_as_bound if appropriate.

==========================================================================
                  AutoDock Release Notes
                Release 4.2.2 (September 9 2009)
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The changes since the 4.2.1 release (6/2009):

Makefile.am
-in response to bug 1137 reported by Steffen Moeller@gmx.de added
Wno-write-strings to Makefile.am and strncpy to setflags.cc

calculateEnergies.cc
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-added setting the flexible residues internal energies to same_as_bound
(lines 262-265) after conversations with David, Mike and Garrett

eintcal.cc
-replaced missing backslash for newlines

readPDBQT.cc
-fixed bug in flexible residues overcounting number of pieces by changing
code so that ROOTs of all flexible residues are in the same rigid piece
-changed cut-off for nrigid_piece from MAX_TORS to MAX_TORS + nres
to compensate for (unfortunate) fact that each flexible residue has a ROOT

setflags.cc
-repaired copying argv[2] in param_file_fn
-modified lines 183-188 to check for filename length
-in response to bug 1137 reported by Steffen Moeller@gmx.de added
Wno-write-strings to Makefile.am and strncpy to setflags.cc

support.cc
-replaced missing backslash for newlines

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AutoDock Release Notes
Release 4.2.1 (June 9 2009)

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The key changes since the 4.0.1 release (5/2007):

1. Improved overall reliability and detection of input file errors.
2. Improved local search.

AD4.1_bound.dat
AD4_parameters.dat

NEW FEATURE:
-added parameters for G,GA,J and Q atom types used for ring-closure
-added parameters for the covalent atom type, "Z".

CHANGE:
-introduced new "parameter_file" .dat files for AutoDock 4.1 that
have the appropriate coefficients for the bound, compact and extended
models. The previous default parameter file for AutoDock 4.0 was
"AD4_parameters.dat"; the default parameter file for AutoDock 4.2
is "AD4.1_bound.dat".

AUTHORS

CHANGE:
-updated the authors list

INSTALL

CHANGE:
-copied current version from gnu

Makefile.am

CHANGE:
-removed superfluous VERSION_NUM line
-set cygwin stacksize and added possible extension for cygwin...
we don't really understand why the python-driven tests are not
working on cygwin although autodock appears to run ok

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    -changed version to 4.2.1
    -removed command mode
    -changed VERSION_NUM strings from 4.0 to 4.02 and from 4.1 to 4.1.1
    -removed summarizegrids[c,h]
    -added check for too many atom types in dpf 'ligand_types' command in
    parsetypes.
    -added map_declare.h so type of map (float or double) is
    independent of 'Real' and not affected by 'USE_DOUBLE' in Makefiles.
    -changed the target "check" to "test", since "make check" causes an
    error.  This means to test, the developer should use "make test", _not_
    "make check".  Also changed the "-o" argument to "test_autodock4.py",
    from "$$outputdir" to "$$outputdir/Tests".
    -Added the argument "AD4.1_bound.dat" to the new version of
    "paramdat2h.csh" to compile the "default_parameters.h".  Also added
    two new target, "BUILT_SOURCES", and "CLEANFILES", which depend on
    "default_parameters.h".
    -Added stack.{cc,h} to the dependencies required to make AutoDock.
    -Removed the -DDO_NOT_CROSSOVER_IN_QUAT flags and added -DASSERTQUATOK to "DBUG".
    -Changed default parameter file from AD4_parameters.dat to AD4.1_bound.dat,
    and added the new AD4.1 parameter files to EXTRA_DIST.
    -Rework of Coliny files to use the COLIN 3.0 code.
    -Fixed bug reported by Qing Zhong, so that "gs.cc" now uses the same
    compiler and flags as everything else except main.cc, i.e. $(CXXCOMPILE).
    This means that the option DO_NOT_CROSSOVER_IN_QUAT is now used in gs.cc,
    and thus ensures distorted geometries cannot be produced by wayward
    quaternions...  Now compiles without the spurious "-g -O2" generated by configure.


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 NEWS
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NEW FEATURE:
    -added DSG comment on new features


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 analysis.cc
 analysis.h
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CHANGE:
    -installed Debian compiler-compatibility patches from Stefan Moeller
    -Uses calculateBindingEnergies so that if AD4.1_Bound.dat is used,
    the internal energy of the unbound state can be set to that of the
    docked state.  No longer prints the "NEWDPF ndihe" line, since
    "ndihe" is deprecated in AutoDock 4.


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 atom_parameter_manager.cc
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CHANGE:
    -credit Michael Pique for helping to create this code which
    consist of changes to make it more readable.


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 autocomm.h
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CHANGE:
    -added a macro-version of assertQuatOK, so that when the assertion
    fails, the line number and file of where it failed is output,
    not the assertQuatOK function as it was before.


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autoglobal.h
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CHANGE:
    -moved AutoGridHelp into autogrid where it belongs
    - introduced initial "Unbound_Default" to detect multiple, inconsistent
    settings of ad4_unbound_model
    -updated command line arguments including --version
    -added a new global, ad4_unbound_model, which can take any of the
    enumerated values of Unbound_Model, namely,
    { Unbound_Same_As_Bound=0, Extended=1, Compact=2 }.


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 banner.cc
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CHANGE:
    -replaced version number in banner for ADT1.5.2 compatibility with 3 digits
    -added -C for copyright notice
    -changed format string for version_num, increasing it from 4s to 8s
    -updated banner output in the DLG such that the earlier copyright years
    matches the header comments (1989 instead of 1991), and the later year
    matches the current year (2008 instead of 2007).
    -installed Debian compiler-compatibility patches from Stefan Moeller


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 calculateEnergies.cc
 calculateEnergies.h
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CHANGE:
    -added Unbound_Default case
    -Added calculateBindingEnergies() and related functions, to support
    the ability to set the internal energy of the unbound state to that
    of the docked state.


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 call_glss.cc
 call_gs.cc
 gs.cc
 mapping.cc
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CHANGE:
    -correction of when genotype to phenotype mappings are done
    -changed so now Individual does mapping of its genotype into its
    phenotype and inverse_mapping of its phenotype into its genotype
    -changed argument to msort from 3 to 1
    -added an argument to the calling signature, "end_of_branch[]",
    which can be used to pass in the corresponding branch points for
    the new Branch Crossover Mode.  Added a call to
    "set_eob( end_of_branch )", a method of thisPop, which is a Population.
    -added a new integer, "max_numTries", set to 1000, that is used
    to prevent the generation of the initial population from getting
    stuck in an infinite loop.  The code prints a warning if this
    maximum number of tries is reached, while trying to create a
    population which does not have all energies equal.


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 cmdmode.cc
 cmdmode.h
 cmdtokens.h
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CHANGE:
    -removed command mode
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 coliny.cc
 coliny.h
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CHANGE:
    -rework of Coliny files to use the COLIN 3.0 code.
    -misc change to enable conditional compile of AutoDock with the
    new COLIN 3.0 mechanism.


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 configure.ac
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CHANGE:
    -changed version to 4.2.1
    -pass version_num to setflags
    -updated version to 4.1.0.
    -fixed bug reported by Qing Zhong, so that "gs.cc" now uses
    the same compiler and flags as everything else except main.cc,
    i.e. $(CXXCOMPILE).  This means that the option
    DO_NOT_CROSSOVER_IN_QUAT is now used in gs.cc, and thus ensures
    distorted geometries cannot be produced by wayward quaternions...
    Now compiles without the spurious "-g -O2" generated by configure.


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 configure_universal_Darwin8
 configure_universal_Darwin9
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NEW FEATURE:
    -new maintenance and distribution tools


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 conformation_sampler.cc
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CHANGE:
    -changed so now Individual does mapping of its genotype
    into its phenotype and inverse_mapping of its phenotype
    into its genotype


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 constants.h
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CHANGE:
    -introduced initial 'Unbound_Default' to be used to detect
    multiple, inconsistent settings of ad4_unbound_model
    -added a guard, using "#ifndef _UNBOUND_MODEL", around the
    definition of the enum "Unbound_Model", to prevent re-definition
    errors.
    -added "Unbound_Model", an enumerated variable, which can have
    the values { Unbound_Same_As_Bound=0, Extended=1, Compact=2 }


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 dpftoken.h
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CHANGE:
    -added psw rot scale and tor scale for rho values
    -added parsing of autodock_parameter_file version and unbound_model
    -made new token for obsolete token quat0 to give better error messages
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 getInitialState.cc
 getInitialState.h
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CHANGE:
    -Uses calculateBindingEnergies so that if AD4.1_Bound.dat is used,
    the internal energy of the unbound state can be set to that of the
    docked state.


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 get_atom_type.cc
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CHANGE:
    -now allocate storage for message variable


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 gs.cc
 gs.h
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NEW FEATURE:
    -added a new enum to "Xover_Mode", namely "Branch", and added new
    code in the crossover method, to support the new "Branch Crossover
    Mode", where only torsion genes (if any) are recombined, and
    only those genes that lie within the sub-tree of the torsion
    tree affected by the first crossover point.  The Global Search
    Genetic Algorithm accesses the end_of_branch[] array using the
    accessor method get_eob() of the Population object,
    "original_population".
    -added slerp and alerp to arithmetic crossover to handle
    interpolation of rotations and torsion angles gracefully,
    and to preserve quaternion-magnitudes of 1.
    -added code to handle uniform crossover of the four genes
    describing the orientation.

CHANGE:
    -changed so now Individual does mapping of its genotype into its
    phenotype and inverse_mapping of its phenotype into its genotype
    -changed line 1091: now if avg==worst, alloc[i] is set to
    1/pop_size; added @@ to debug statements lines 1428,1440
    -added <stdlib.h> since MP & GMM added an exit(-1) as a bug check,
    to catch genes whose indices are not translation, rotation or
    conformation values.
    -added several debug statements; made change in translation
    alpha value, to make it consistent with slerp and alerp.
    -Modified 2-pt and 1-pt crossover to ensure every call does
    indeed perform some crossover.
    -Fixed uniform crossover such that it will not begin to crossover
    within the rotation genes.
    -added a "bug check" suggested by MP to catch invalid gene types.
    -removed the DO_NOT_CROSSOVER_IN_QUAT blocks.
    -added lines to uniform and arithmetic crossover to set the
    age of the crossed individuals to 0.


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 hybrids.h
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CHANGE:
    -added the argument, "int end_of_branch[MAX_TORS]", to the
    prototypes, call_glss() and call_gs().


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 ls.cc
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NEW FEATURE:
    -added psw rot scale and tor scale for rho values

CHANGE:
    -Changed so now Individual does mapping of its genotype
    into its phenotype and inverse_mapping of its phenotype
    into its genotype; added use of Boole modified to track
    whether mapping needs to be done


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 ls.h
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CHANGE:
    -changed return type of SW from void to Boole


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 main.cc
 main.h
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NEW FEATURE:
    -added psw rot scale and tor scale for rho values
    -added code provided by Stefano Forli which improves the warning
    message printed to the log file lines ~2108. The new code detects
    whether the custom rij+epsij values provided for DPF_INTNBP_REQM_EPS
    command are RING CLOSURE values or not
    -added named atom pairs to intnb_r_eps and intnb_coeffs to support
    ring-closing atom types
    -added exit early if number of maps is not equal to the number of
    ligand_atom_types plus 2 AND resetting num_maps when fld keyword is
    read so two sets of maps can be used
    -Added the "int end_of_branch[MAX_TORS]" array, and the parsing code to
    detect the new option, "branch", for the "ga_crossover_mode" keyword
    (in addition to "onept", "twopt", "uniform", and "arithmetic".  This
    is to support the new "Branch" crossover mode, which is designed to
    exchange only those torsion genes in the sub-tree descending from
    the first randomly-chosen torsion gene.
    -Modified the function that reads the ligand and flexible residue PDBQT
    files, "readPDBQT()", to count the number of non-hydrogen atoms, and
    return this value.  (Previously, the same argument position that this
    count of heavy atoms now occupies, was used to pass in "Htype", but
    Htype is no longer used inside "readPDBQT()".)

CHANGE:
    -installed Debian compiler-compatibility patches from Stefan Moeller
    -updated command line arguments including --version
    -updated syntax for unbound options following discussion with DSG
    -added reporting of which unbound model is used for each kind of search
    -changed interface to setup_parameter_library by adding ad4_unbound_model
    -added parsing of autodock_parameter_file version and unbound_model
    -pass version_num to setflags
    -removed command mode
    -added 'exit_if_missing_elecmap_desolvmap_about' method to check that
    these keywords have been found and exit if they are not all there
    -all filenames are dimensioned to PATH_MAX long, all strings read using
    sscanf are dimensioned to LINE_LEN
    -made new token for obsolete token quat0 to give better error messages
    -Updated the summations for the econf[] array that is used in the
    analysis() function, and which is reported in the clustering histogram.
    These summations needed to be updated to be able to handle the
    "ad4_unbound_model" properly; in this model, the unbound energy must be
    updated after each docking has finished, to match the internal energy
    at the end of the docking.
    -The "epdb" command now uses calculateBindingEnergies so that if
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AD4.1_Bound.dat is used, the internal energy of the unbound state can
be set to that of the docked state. * Also, added a check to see if
the number of values specified by the "dihe0" command matches the
number of torsions found in the ligand PDBQT (ntor), and prints a
warning if they do not match.
-Added extra variables and the function call to
"initialise_energy_breakdown()" to the DPF_MOVE-case to re-initialise
key variables before reading in a new ligand. ALSO: changed
version_num to 4.10 (from 4.00) and changed the comment from 4.0 to 4.1 beta.
-Changed sscanf from using %1s to %c, thanks to an email from Alexandre
Lebedev (alexmlebedev@mail.ru); this solves a bug in the simulated
annealing that appeared if the number of rejections, rejs<=255.
-Rework of Coliny files to use the COLIN 3.0 code.

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 mdist.h

NEW FEATURE:
-Introduced the "set_minmax(a1, a2, min, max)" macro, to set both
the [a1][a2] and [a2][a1] entries in the mindist[][] and maxdist[][]
arrays at the same time. Introduced the constant, "BOND_LENGTH_TOLERANCE",
with a default value of 0.1 Angstrom, to expand the allowed bond length
ranges. Entered an extensive list of values from the "Handbook of
Chemistry and Physics" specifying the lower and upper bounds for
acceptable bond lengths given the atom types of the two potentially-bonding
atoms. This new code is less permissive in creating bonds than the old
AutoDock 3 values, which consisted of 0.9 and 2.1 for most atom type
pairs. This modification was prompted by a compound with a C-bridged
cyclobutane, ZINC01557511, which caused "nonbonds.cc" to try to
access bonded[-1][]...

CHANGE:
-cleaned-up macro; corrected previous incorrect setting of diagonal values; removed 10% of code
-explicitly set values of enum

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 mkNewState.cc

TODO:
-TODO 5/1/2009: should call slerp to scale down by qtwStep"

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 mkTorTree.cc

CHANGE:
-moved error message for too many torsions earlier

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 mkdisttars

NEW FEATURE:
-new maintenance and distribution tools

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 nonbonds.cc

NEW FEATURE:
-Several changes have been made to improve the bond
and nonbond detection algorithm. Now, atoms that
can potentially form bonds are sorted by distance
first, so that the shortest candidate bonds are added

first. There is now a check to stop adding bonds when
the maximum number of bonds is reached. The bonded[][]
array values are now validated before they are used in
the for-l loop, to make sure they are not less than 0.
There are new debugging print statements that can be
triggered with the "-d" flag. The new algorithm, in
conjunction with the new bond length values in the file
"mdist.h", now correctly handles ZINC01557511, a compound
with a C-bridged cyclobutane that was previously causing
the code to attempt to access bonded[-1][].

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 paramdat2h.csh

NEW FEATURE:
    -compiles and builds both autodock4 and autodock4_0 with
    appropriate default parameter libraries. Reports which one is being
    used in dlg file.
    -changed paramdat2h.csh to now take one argument, the name of the
    parameter library.
    -changed the default parameter library file from "AD4_parameters.dat"
    to "AD4.1_bound.dat".

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 parameters.h

NEW FEATURE:
    -Introduced a new macro, "is_hydrogen_type(t)", that takes a
    found_parm->autogrid_type and returns true if the type is a
    hydrogen atom type, namely "H", "HD" or "HS".

---
 parse_PDBQT_line.cc

NEW FEATURE:
    -added detection of USER records, mapping to PDBQ_NULL.
    -now returns PDBQ_UNRECOGNIZED instead of PDBQ_NULL, when
    it cannot identify the token.

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 parse_com_line.cc
 parse_com_line.h

DEPRECATED:
    -removed command mode

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 parse_dpf_line.cc

CHANGE:
    -removed unnecessary numbering
    -added unbound_energy token; removed reminder about NUM_LEXEMES
    -added parsing of autodock_parameter_file version and unbound_model
    -made new token for obsolete token quat0 to give better error messages

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 parse_param_line.cc

CHANGE:
    -added the new keyword/token pair, {"FE_unbound_model", PAR_UNBOUND},
    to the parser.

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 parsetypes.cc

CHANGE:
    -Added check for too many atom types in dpf 'ligand_types' command in
    parsetypes. Added map_declare.h so type of map (float or double) is
    independent of 'Real' and not affected by 'USE_DOUBLE' in Makefiles.

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 partokens.h

CHANGE:
    -added a new token, PAR_UNBOUND.

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 printEnergies.cc

CHANGE:
    -installed Debian compiler-compatibility patches from Stefan Moeller
    -changed printout of receptor internal energy: previously only the
    total was reported. Now the moving-fixed and moving-moving components
    of the internal energy of the receptor are printed

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 qmultiply.cc

NEW FEATURE:
    -added quatDifferenceToAngle and quatDifferenceToAngleDeg methods;
    modified assert line 203 increasing 1 to 1.001
    -Introduced a new slerp function adapted from an implementation
    by John Ratcliff to replace the previous slerp by Martin Baker;
    the previous slerp caused problems with arithmetic-crossover-based
    dockings that used typical numbers of energy evaluations, but not
    with our "unit" tests which are extremely short dockings. The
    slerp based on the implementation from Martin Baker has been renamed
    "slerp1".
    -Added two new functions, alerp(a,b,fract) and a_range_reduction(a),
    which are used to interpolate (torsion) angles, such that the
    interpolation gives a if fract=0, b if fract=1, and some fraction
    of the smaller difference between a and b (note that the difference
    between two range-reduced angles can be either greater than 180 or
    less than 180 degrees, and we want to interpolate along the delta
    that is smaller than 180 degrees. E.g. the average, i.e. fract=0.5,
    of 1 and 359 degrees should be 0 deg, not 180 deg.) There is a test
    in one of the added comments, note, of alerp for a wide range of a
    and b values.

CHANGE:
    -commented out the assertQuatOK function, since the macro version
    was introduced in autocomm.h, to permit better reporting of where
    the assertion failed. Added a warning for the DEBUG_MUTATION
    directive in slerp(), to alert if theta is 180 degrees when the
    two quaternions are opposite. Added a comment to clarify that
    when fract==0, alerp returns a.

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 qmultiply.h

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NEW FEATURE:
    -added quatDifferenceToAngle and quatDifferenceToAngleDeg declarations
    -Introduced a new slerp function adapted from an implementation by John
    Ratcliff to replace the previous slerp by Martin Baker; the previous
    slerp caused problems with arithmetic-crossover-based dockings that
    used typical numbers of energy evaluations, but not with our "unit"
    tests which are extremely short dockings.  The slerp based on the
    implementation from Martin Baker has been renamed "slerp1".

CHANGE:
    -commented out the prototype for assertQuatOK().  Better to use the
    macro version in autocomm.h.
    -added prototypes for alerp(a,b,fract) and a_range_reduction(a),
    which are for interpolating angles and "mod"-ing angles.


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 readPDBQT.cc
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NEW FEATURE:
    -added new code that uses stacks, in particular stack_push(int)
    and stack_pop(), to build up the "end_of_branch[]" array, which
    is used in the new "Branch Crossover Mode" offered in the GA and
    Lamarckian GA search methods.  The intention of the branch crossover
    mode is to exchange only those torsion genes in the sub-tree
    descending from the first crossover point.
    -modified the function that reads the ligand and flexible residue PDBQT
    files, "readPDBQT()", to count the number of non-hydrogen atoms, and
    return this value.  (Previously, the same argument position that this
    count of heavy atoms now occupies, was used to pass in "Htype", but
    Htype is no longer used inside "readPDBQT()".)
    other PDBQT_ tokens.

CHANGE:
    -increased QTOL from .005 to .05; softened warning message
    -corrected ROOT logic for flexible residues
    -repaired and clarified detection of end_of_branch entries by
    adding a separate array 'branch_last_piece': now the root is
    numbered piece one and the rigid pieces moved by torsions are
    numbered starting at two; removed 'stack_size' (which should
    have been stack_depth anyway) and 'top' from debug statements;
    updated DEBUG: indicies; added code to catch error and exit if
    parent <0
    -added code to check that each of the fields is read correctly in
    readPDBQLine.  Now checks that each ATOM/HETATM line in the PDBQT
    file is at least 78 characters long; if not, the parser now exits
    with a fatal error.   The warning if an atom type is not found is now
    much more informative, now advising the user to check the
    "ligand_types" line and to add a "map" line to the DPF.  The parser
    now explicitly handles all the tokens that can be returned by the
    parse_PDBQT_line function.  There is now a warning if an unrecognised
    token is found in the PDBQT file.  The code that handled BEGIN_RES
    records has now been mostly moved into a case block, alongside the


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 read_parameter_library.cc
 read_parameter_library.h
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CHANGE:
    -installed Debian compiler-compatibility patches from Stefan Moeller
    -removed unused extern variable
    -added warning to PAR_UNBOUND in setup_parameter_library
    -added reporting of which unbound model is used for each kind of search
    -changed interface to setup_parameter_library by adding ad4_unbound_model
    -replaced determining version number using 'strcmp' with
    'string_begins_with' to support the new longer version number format: #.#.3
    -added a print statement to record the error message in the logFile,
```

    if the FN_parameter_library cannot be opened.

---
 rep.cc

CHANGE:
    -added lines to set low and high from init_low and init_high,
    supplied in the constructor form ConstrainedRealVector::
    ConstrainedRealVector(int num_els, double init_low, double init_high).

---
 rep_constants.h

CHANGE:
    -added definitions for Y_TRANSLATION_INDEX, is_first_rotation_index(i)
    and is_within_rotation_index(i).
    -added a macro to determine if the index of a gene is part of the
    conformation, i.e. a torsion gene. (is_conformation_index(i))

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 setflags.cc
 setflags.h

CHANGE:
    -added include banner to get to show_warranty and show_copyright
    -added -C for copyright notice
    -updated command line arguments including --version
    -pass version_num to setflags
    -removed command mode
    -added setlinebuf to ensure output even if program crashes

---
 simanneal.cc

CHANGE:
    -updated the summations for the econf[] array that is used in the
    analysis() function, and which is reported in the clustering
    histogram. These summations needed to be updated to be able to
    handle the "ad4_unbound_model" properly; in this model, the
    unbound energy must be updated after each docking has finished,
    to match the internal energy at the end of the docking.

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 stack.cc

NEW FEATURE:
    -Added new code to handle integer stacks, kindly contributed by
    Mike Pique. Added new code to test the stack code.

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 support.cc
 support.h

NEW FEATURE:
    -changed so now Individual does mapping of its genotype into
    its phenotype and inverse_mapping of its phenotype into its
    genotype; in both cases returns a reference to itself;
    added a check for self-assignment

-improved bounds checking in heap sort (Population::msort)
-added <stdlib.h> for exit(), which needs to be included on some(?)
systems.
-added "end_of_branch[MAX_TORS]" to the Population class, the
logic being that every Individual in the Population is the same,
so rather than add the overhead to all the Individuals, we added
it to the Population. Also introducted two new methods, set_eob()
and get_eob(), to set the end_of_branch[] array, and get values
given a key torsion number. These changes are to support the
new "Branch Crossover mode".

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 usage.cc

CHANGE:
-updated command line arguments including --version

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 version.h

CHANGE:
-pass version_num to setflags
-version numbers changed to match autoconf version numbers.

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 writePDBQT.cc

CHANGE:
-correction to handling of 2 letter atom names provided by Stefano Forli
-uses calculateBindingEnergies so that if AD4.1_Bound.dat is
used, the internal energy of the unbound state can be set to
that of the docked state.
-to accommodate writing names of atoms with 2 character elements
correctly, increased by one indicies on lines 114: 14->15,
9->10; 132 and 133: 14->15, 9->10;280 and 281:13->14;lines
288 and 289:13->12, 8->9; line 326:14->15; lines 328 and 329:13->14