ESPResSo

Mesoscopic Molecular Modeling

Analysis, Checkpointing, and the TestSuite

What do you want to sim today?

BASF

The Chemical Company

Analysis

What do you want to sim today?

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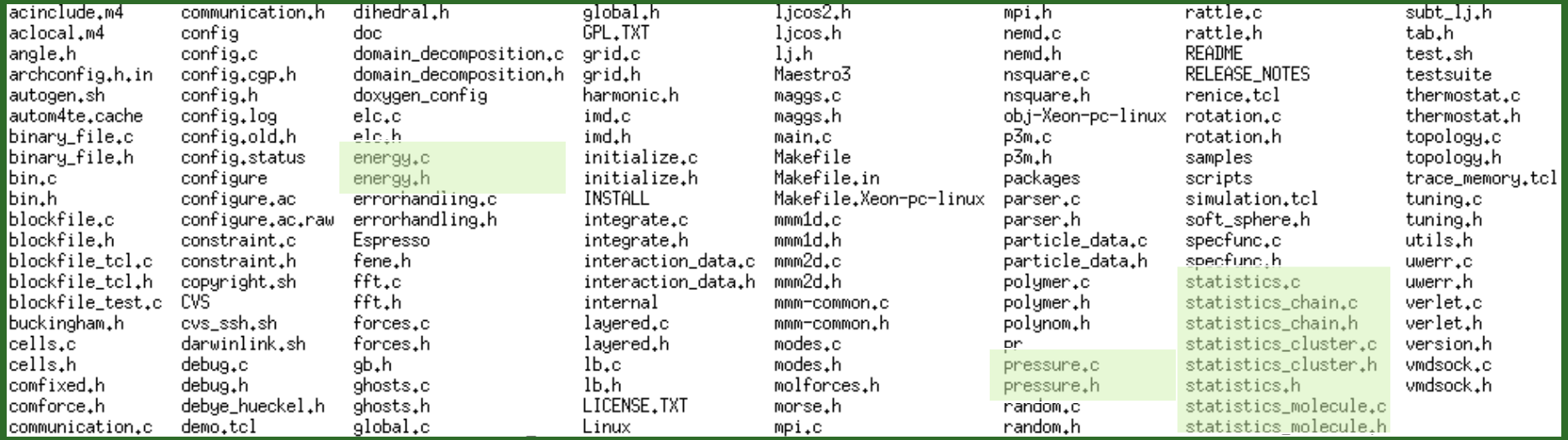

- access using `analyze <what> [<options>]` from the Tcl-Level, or by invoking the corresponding C-function from within the C-Level
- each feature shall consist of two parts:
  - parser `parse_NAME(interp,argc-2,argv+2)` for I/O to Tcl
  - main function `NAME(<arguments>)` to perform actual analysis, returning results as argument, pointer, or directly

Analysis

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- enter here in `statistics.c` from Tcl:

```
/*****************************************************************************************
 *                                main parser for analyze
 *****************************************************************************************/

int analyze(ClientData data, Tcl_Interp *interp, int argc, char **argv)
{
  int err = TCL_OK;
  if (argc < 2) {
    Tcl_AppendResult(interp, "Wrong # of args! Usage: analyze <what> ...", (char *)NULL);
    return (TCL_ERROR);
  }

  if (ARG1_IS_S("set"))
    err = parse_analyze_set_topology(interp, argc - 2, argv + 2);
  else if (ARG1_IS_S("get_folded_positions"))
    err = parse_get_folded_positions(interp, argc - 2, argv + 2);
  else if (ARG1_IS_S("configs"))
    err = parse_configs(interp, argc - 2, argv + 2);
  else {
    /* the default */
    /***************/
    Tcl_ResetResult(interp);
    Tcl_AppendResult(interp, "The operation \"", argv[1],
                     "\" you requested is not implemented.", (char *)NULL);
    err = (TCL_ERROR);
  }
```

Analysis

- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`:
    - `double mindist(IntList *set1, IntList *set2)`
    - `int aggregation(...)`
    - `void centermass(int type, double *com)`
    - `void  momentofinertiamatrix(...)`
    - `void nbhood(..., IntList *il, int planedims[3] )`
    - `double distto(double p[3], int pid)`
    - `void calc_cell_gpb(..., double *result)`
    - `void calc_part_distribution(..., double *dist)`
    - `void calc_rdf(..., double *rdf)`
    - `void calc_rdf_av(..., double *rdf, ...)`
    - `void calc_rdf_intermol_av(...)`
    - `void analyze_structurefactor(..., double **_ff)`
    - `int analyze_radial_density_map (...)`

Analysis

- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`
  - file `statistics_chain.c`:
    - `void calc_re{_av}(double **re);`
    - `void calc_rg{_av}(double **rg);`
    - `void calc_rh{_av}(double **rh);`
    - `void calc_internal_dist{_av}(double **idf);`
    - `void calc_bond_l{_av}(double **bond_l);`
    - `void calc_bond_dist{_av}(double **bdf, int ind_n);`
    - `void calc_g123(double *g1, double *g2, double *g3);`
    - `void calc_g{1|2|3}{_av}(double **g{1|2|3})`
    - `void analyze_formfactor{_av}(..., double **_ff);`
    - `void analyze_rdfchain(..., double **_rdf, ...);`

Analysis

- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`:
  - file `statistics_chain.c`,
    which require chain information / topology to be set via
    `analyze set chain <chain_start> <n_chains> <chain_length>`:
    - `int print_chain_structure_info(...);`
    - `int parse_chain_structure_info(...);`
    - `void update_mol_ids_setchains();`
    - `int check_and_parse_chain_structure_info(...);`
  - in the long run, chain information should instead use `mol_id` of particles

Analysis

- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`:
  - file `statistics_chain.c`
  - file `statistics_molecule.c`:
    - `int analyze_fold_molecules(...);`
    - `void calc_mol_center_of_mass(Molecule mol, ...);`
    - `void mol_center_of_mass_(Molecule mol, ...);`

Analysis

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- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`:
  - file `statistics_chain.c`
  - file `statistics_molecule.c`
  - file `statistics_cluster.c`:
    - `int parse_necklace_analyzation(...)`

Analysis

- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`:
  - file `statistics_chain.c`
  - file `statistics_molecule.c`
  - file `statistics_cluster.c`
  - file `pressure.c`:
    - `void pressure_calc(double *result, int v_comp)`
    - `void add_non_bonded_pair_virials(...)`
    - `void add_bonded_virials(Particle *p1)`
    - `void add_kinetic_virials(Particle *p1,int v_comp)`
    - `int parse_and_print_pressure(..., int v_comp)`

    - `int parse_bins(...);`
    - `int parse_and_print_p_IK1(...);`

Analysis

- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`:
  - file `statistics_chain.c`
  - file `statistics_molecule.c`
  - file `statistics_cluster.c`
  - file `pressure.c`
  - file `energy.c`:
    - (same as for the pressure)

Analysis

- enter here in `statistics.c` from Tcl
- continue to parser / functions in
  - file `statistics.c`:
  - file `statistics_chain.c`
  - file `statistics_molecule.c`
  - file `statistics_cluster.c`

  → master-node, copy of particle data (RAM!)
  - file `pressure.c`
  - file `energy.c`

  → parallel (→ `integrate 0`)
- advantages of current implementation:
  - easy access from Tcl and from C
  - very straightforward to enhance
  - simple structures allow convenient processing of particle data
- disadvantages:
  - non-parallel code is slow
  - double data storage can quickly become big problem (e.g. trajectories)
  - only partial particle informations available

Checkpointing

- want to be able to restart at any point, reproducing uninterrupted trajectory
- use Tcl-functions in `scripts/auxiliary.tcl`, i.e.:
  - `checkpoint_set { destination { cnt "all" } { tclvar "all" } { ia "all" } { var "all" } { ran "all" } { COMPACT_CHK 0 } ... }`
  - `checkpoint_read { origin { read_all_chks 1 } { write 0 } { name "anim" } { pdb_sfx 5 }`
- current state being saved using `polyBlockWriteAll` with everything on
- simple textfile contains consecutive list of blockfiles building the trajectory, where suffix of given filename is removed to construct its name
  - e.g. use `checkpoint_set my_sim.[format %03d $i].gz` to get list of (gzipped) blockfiles `my_sim.000.gz, my_sim.001.gz,...` and blockfile list `my_sim.chk` in same path
  - simply use `checkpoint_read my_sim.chk` to read all stuff back in
- *everything* can be saved, incl. *internal* state of random number generator
- particle distribution to nodes depends on communication → possible problem

TestSuite

- built-in self-consistency check for basic functionality
- supposed to be easily usable to ensure frequent employment:
  - `gmake test`
- therefore, output should be self-explanatory
- the following tests are currently implemented
  - `madelung.tcl, kinetic.tcl, thermostat.tcl`
  - `nve_pe.tcl, npt.tcl, intpbc.tcl, intppbc.tcl`
  - `layered.tcl, nsquare.tcl`
  - `lj.tcl, lj-cos.tcl, fene.tcl, harm.tcl, gb.tcl`
  - `dh.tcl, p3m.tcl, mmm1d.tcl, el2d.tcl,`
  - `comfixed.tcl, comforce.tcl, tabulated.tcl`
  - `analysis.tcl, pe_micelle.tcl`
  - `constraints.tcl, rotation.tcl, uwerr_test.tcl`
- tests are automatically blacklisted if unapplicable due to compilation state
- if all tests succeed, ESPResSo is not necessarily bug-free,
  but if just one of them fails, it's definitely having a problem

SampleSuite

- set of “real” test scenarios, preferably reproducing well-known “real” systems (e.g. published long ago, heavily cited, never doubted) with automated analysis for simple comparison to original data
- also serves as set of examples and system showcase

- difference TestSuite ↔ SampleSuite:
  - running time (seconds *vs.* hours / days / weeks)
  - background (artificial and purely technical setup *vs.* “real” experiment)
  - employment (use as little as possible *vs.* use whatever you like)
  - coverage (check few features *vs.* evaluate entire scenarios)

- if a test case fails, you know exactly where to look *(well, almost always)*, if a sample case fails, you just know that *something*’s wrong; but: since sample cases aren’t artificial, you’re more likely to find errors!