Corpuscles documentation

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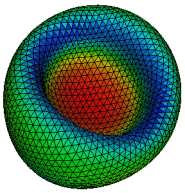


Corpuscles

Introduction

Corpuscles is a C library to resolve the elastic energy and force of a membrane surface, which is represented by an unstructured triangulated mesh. It also simulates transformations between different configurations/shapes of a closed membrane by a minimization procedure under various constraints.

Various components can be switched on/off at will, such as

1. Bending elasticity of lipip bilayer
2. Strain (both shear and strecth) elasticity of cytoskeleton
3. Viscosity of lipid membrane
4. Thermal fluctuations of lipid membrane
5. Constraint of reduced volume of a closed membrane surface
6. Constraint of total area of a closed membrane surface
7. Constratin of total volume of a closed membrane surface
8. Constratin of area difference between outer- and inner-surface

For different components, variations of model/law can be selected such as Helfrich/spontaneous curvature model for bending elasticity and Skalak law for strain elasticity.

For different models/laws, variations of schemes impelemented can also be choosen such as Gompper and Kroll scheme and Juelicher scheme for the bending model of spontaneous curvature. See more details in `https://cselab.github.io/corpuscles`

Install

Minimal dependencies are C and Fortran 90 compilers, GNU Scientific Library, and pkg-config.

Optional dependencies geomview, maxima, and pandoc.

Adjust conf.mk if you want to change defaults

```
$ cat conf.mk
CC = gcc
FC = gfortran

FCFLAGS = -O2 -g
FXFLAGS = -fallow-argument-mismatch

GSL_CFLAGS = " `gsl-config --cflags `"
GSL_LDFLAGS = " `gsl-config --libs `"

CFLAGS = -O2 -g
LDFLAGS =
PREFIX = $(HOME)/.local
DATAPATH = $(HOME)/.co
MAXIMA_HOME = $(HOME)/.maxima

# prefix for commands
P = co
```

`PREFIX/bin` should be on the path, for example

```
$ cat $HOME/.bashrc
PATH="$HOME/.local/bin:$PATH"
```

Library is installed under the path `PREFIX`. Run

```
$ MAKEFLAGS=-j4 ./install.sh
```

If you have atest you can run

```
$ make test
```

You can also use a docker containter.

Examples

Hello world

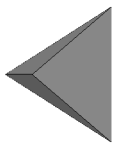
A program in example/hello computes area of a triangle.

```
$ cat main.c
#include <stdio.h>

#include <real.h>
#include <co/tri.h>

#define FMT CO_REAL_OUT

int
main(void)
{
    real A, a[] = { 0, 0, 0 }, b[] = { 2, 0, 0 }, c[] = { 0, 1, 0 };
    A = tri_area(a, b, c);
    printf("Area is of triangle: " FMT "\n", A);
}
```

```
$ cat Makefile
include ../../conf.mk
PREC = d
main: main.c
    $(CC) main.c $(CFLAGS)  `co.conf --cflags --libs $(PREC) ` $(LDFLAGS)
-o $@
clean:; rm -f main
```

Read mesh file

Corpuscles reads OFF files. Here is a file with triangular pyramid.



This program reads an OFF file from an input stream:

```
$ cat main.c
#include <stdio.h>

#include <real.h>
#include <co/array.h>
#include <co/he.h>
#include <co/y.h>

int
main(void)
{
    real *x, *y, *z, hi;
    He *he;
    int nv, nt;

    y_inif(stdin, &he, &x, &y, &z);
    nv = he_nv(he);
    nt = he_nt(he);
    hi = array_max(nv, x);
    printf("number of vertices is %d\n"
           "number of triangles is %d\n"
           "maximum x coordinate is " CO_REAL_OUT "\n", nv, nt, hi);
    y_fin(he, x, y, z);
}
```

```
$ make
$ ./main < `co.path`/regular/tetra.off
number of vertices is 4
number of triangles is 4
maximum x coordinate is 1
```

Write mesh file

Read off, compute area of every triangle, and output off file with colors (example/off/write/area)

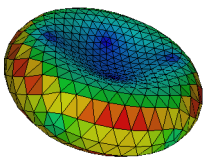
```
$ cat main.c
```

```
#include <stdio.h>

#include <real.h>
#include <co/area.h>
#include <co/err.h>
#include <co/off.h>
#include <co/he.h>
#include <co/memory.h>
#include <co/y.h>

int main(void) {
    int nt;
    real *x, *y, *z, *a;
    He *he;
    y_inif(stdin, &he, &x, &y, &z);
    nt = he_nt(he);
    CALLOC(nt, &a);
    he_area_tri(he, x, y, z, a);
    boff_tri_fwrite(he, x, y, z, a, stdout);
    y_fin(he, x, y, z);
    FREE(a);
}
```

```
$ ./main < $(co.path)/rbc/laplace/0.off > out.off
```

To see the results

```
$ co.geomview -r 55.9195 -13.672 8.69021 -f 25.0389 out.off
```

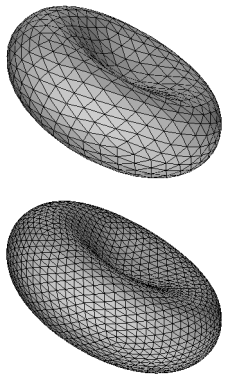


Refine mesh

Using sqrt(3)-subdivision scheme

```
$ co.geomview -r 60 -40 10 -f 22 `co.path`/rbc/icosahedron/0.off
```

```
$ co.sqrt3 < `co.path`/rbc/icosahedron/0.off > a.off
$ co.geomview -r 60 -40 10 -f 22 a.off
```



Visualization

We use a wrapper to geomview.

```
$ co.geomview -h
co.geomview [-t x y z] [-r x y z] [-a APPEARANCE] [-o FILE] [OFF]..
he geomview wrapper
-t x y z      translation
-r x y z      rotation in degree
-f zoom       field of view (default is 40)
-a APPEARANCE load appearance from a file
-o FILE       write FILE and exit
-O            write all PPM files and exit
-OO           write all oogl files and exit
-format ppmscreen|ppm|ps|ppmosmesa|ppmosglx
-p command    process every off file by running  'command ' < IN.off >
OUT.off
-n none|each|all|keep normalization status (see geomview manual)
-c command    run command on every file and write output to stderr, %f
is replaced by a file name
-e command    if keys  'e ' is pressed runs
               '<OFF command -t x y z -r x y z -f zoom -i [index of a
file] -n  [number of files]  ' or
               '<OFF command ' if -e  '|command ' is passed
```

```
-i command    run command on every image, %i replaced by input; %o --
by output; %b --- by basename

Keys:
    q: quit
    s: save snap.ppm
    S: save every snapshot
    e: run command on OFF file (see -e option)
    p: panel
    j/k: switch between off files
    J: dump file name
    [SPC]: dump orientation and field of view

Environment variables:
WX, WY: resolution of the snapshot (default: 800x600)
BACKGROUND: default ( '1 1 1 ')
GEOMVIEW_ARGS: pass to geomview

Examples:
co.geomview -t 0.25 0.25 0     data/rbc.off
co.geomview -a data/appearance data/rbc.off
co.geomview -o snap.ppm        data/rbc.off
co.geomview                    data/rbc.off data/sph.off
co.geomview -p co.orient       data/rbc.off data/sph.off
co.geomview -c off.volume      data/rbc.off data/sph.off
```

Library

Floating point precision

prec/s/real.h, prec/d/real.h, prec/l/real.h single, double, long double

Math

vec.h, edg.h, tri.h, dih.h, ten.h vector, edges, triangels, dihidrals, tensors

dvec.h, dedg.h, dtri.h, ddih.h derivatives of vector edges, triagels, dihidrals

ring.h operation on the first ring of neighbors

Utility

array.h array related functions

argv.h read from `argv` and shift

err.h error handling

endian.h deal with endianess

macro.h macros

sum.h Kahan summation

memory.h memory related

util.h uncategorazed

Surface properties

area.h area

volume.h volume

laplace.h Laplace operator of coordinates

normal.h normal

"Forces"

bending.h generic interface to several bending forces

forces.h generic interface to forces

stretch.h stretching force

Surface transformation

equiangulate.h equlatirate triangles

orient.h orient surface in a direction of eigen values of momentum tensor

restore.h restore a volume of the surface

transformation.h translate, rotate, and and scale surface

remesh.h "edit" surfaces

Half-edg related

read.h read half-edg to intermediate structure HeRead, used to initialize half-edg

he.h half edg data structure (provides half-edg API)

hash.h stores an integer for a pair of integers

IO

gts.h, obj.h, off.h, ply.h, punto.h, stl.h, stl.h, xdmf.h : read/write GTS, OBJ, OFF, PLY, punto, STL, VTK, and XDMF files.

X and Y

x.h simple interface for one surface

y.h not so simple interface

Documentation

git pages `docs/index.html` is generated from `README.md.m4`. To update run

```
$ make html
```

requires pandoc.

Publications

Bian, X., Litvinov, S., & Koumoutsakos, P. (2020). Bending models of lipid bilayer membranes: Spontaneous curvature and area-difference elasticity. Computer Methods in Applied Mechanics and Engineering, 359, 112758. doi:10.1016/j.cma.2019.112758