http://miccom-center.org

Topic: COPSS-Polarization Tutorial

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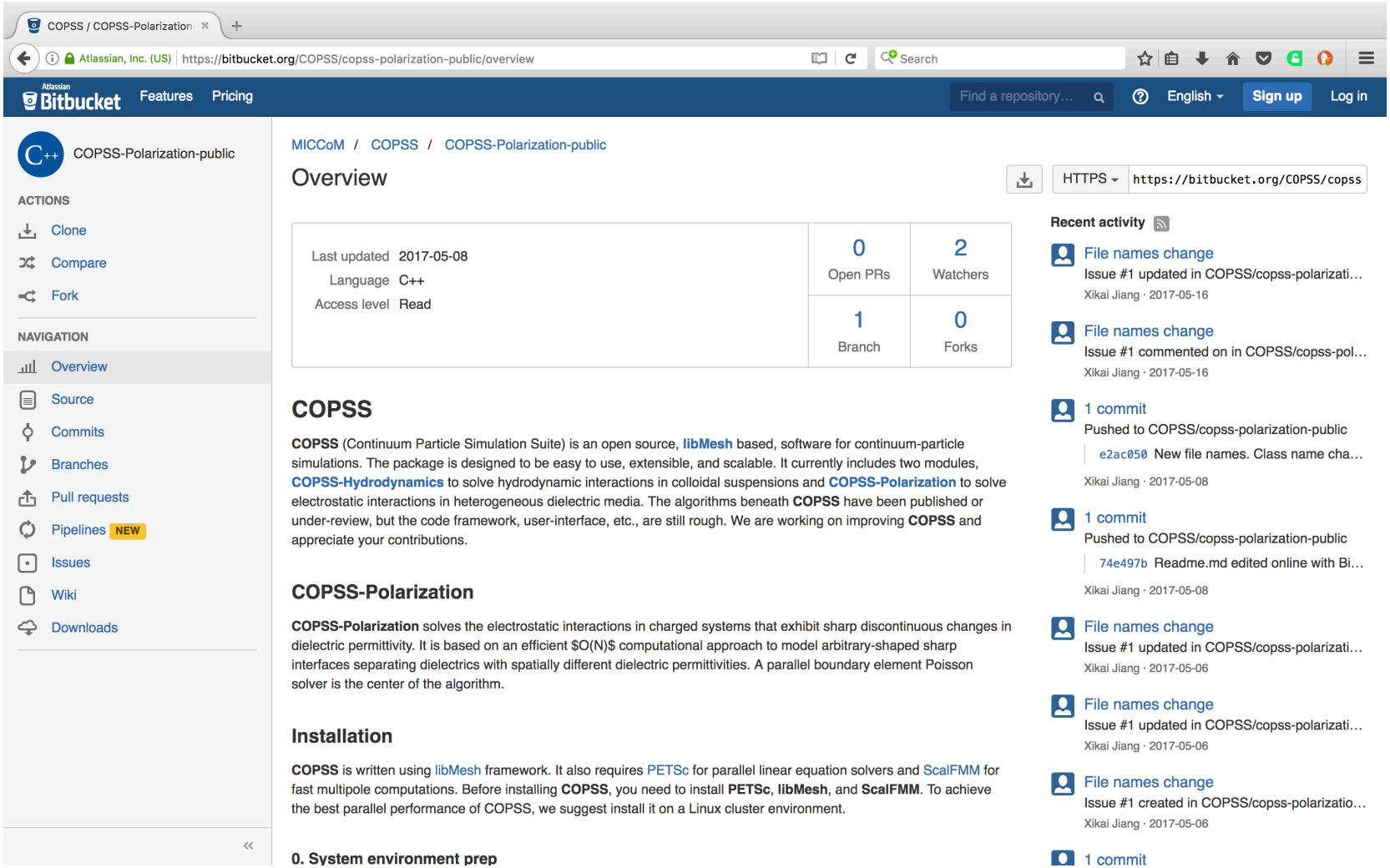
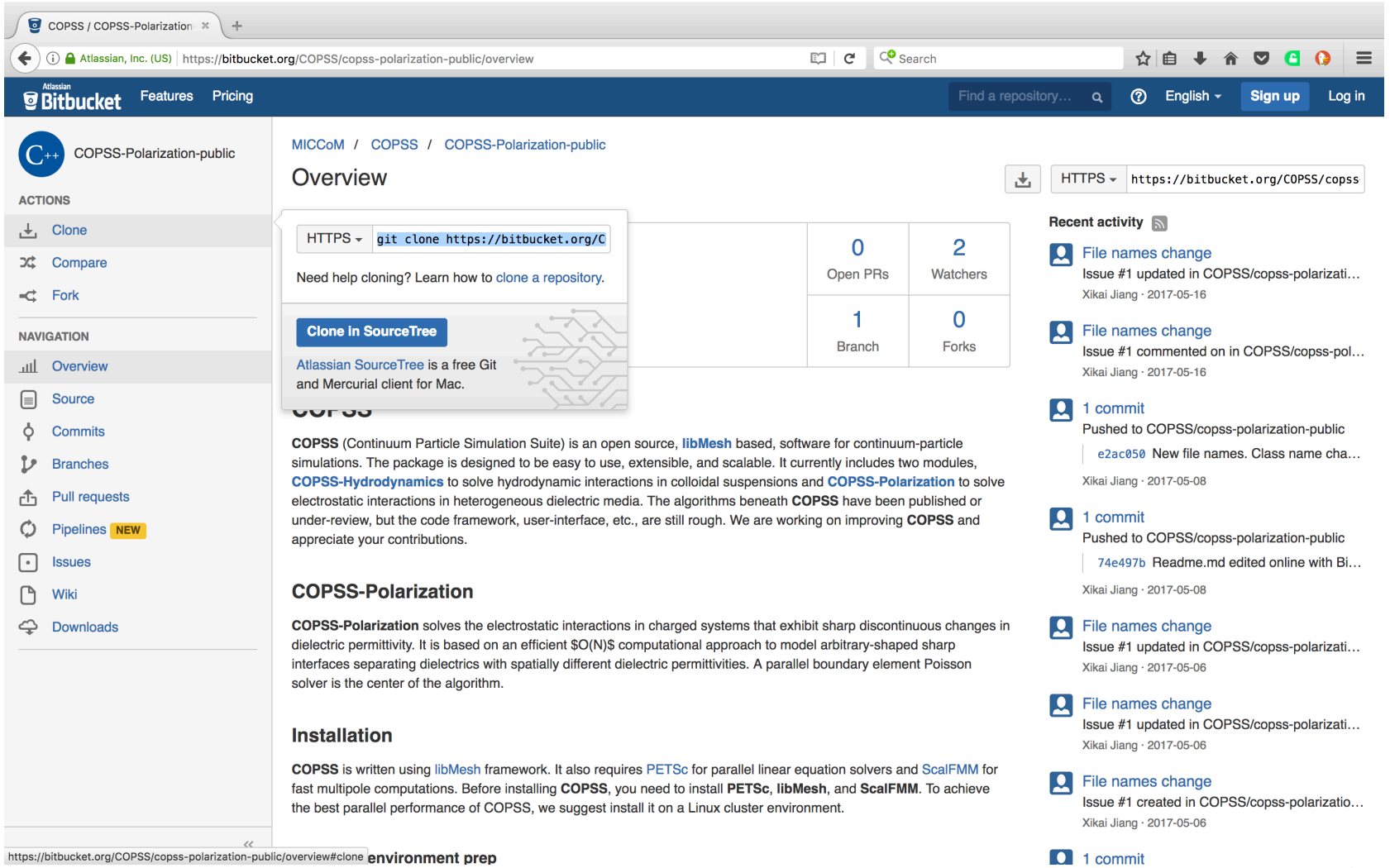
Access COPSS-Polarization

- COPSS-Polarization repository on Bitbucket.



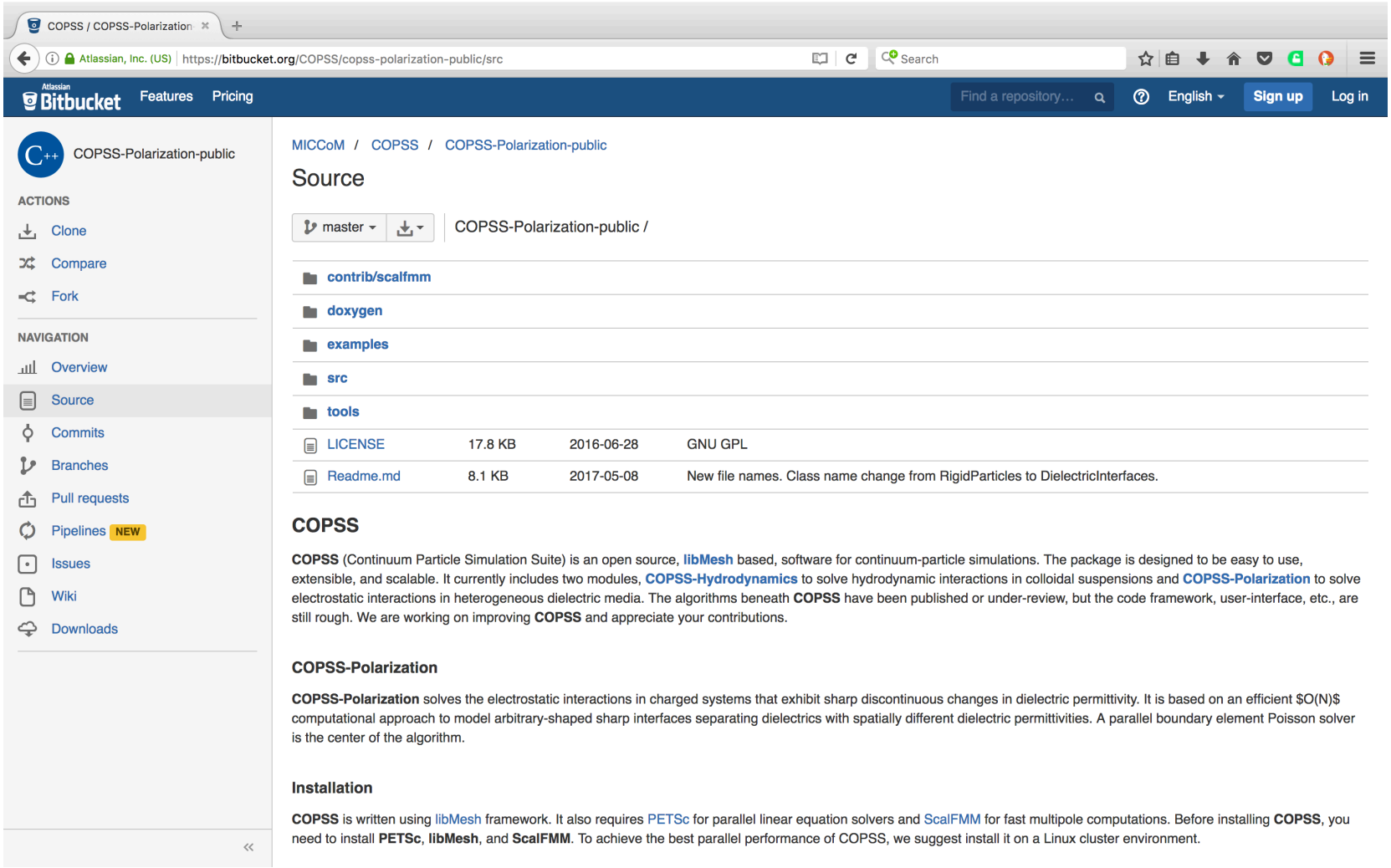
Access COPSS-Polarization

- Download (clone) COPSS-Polarization repository.



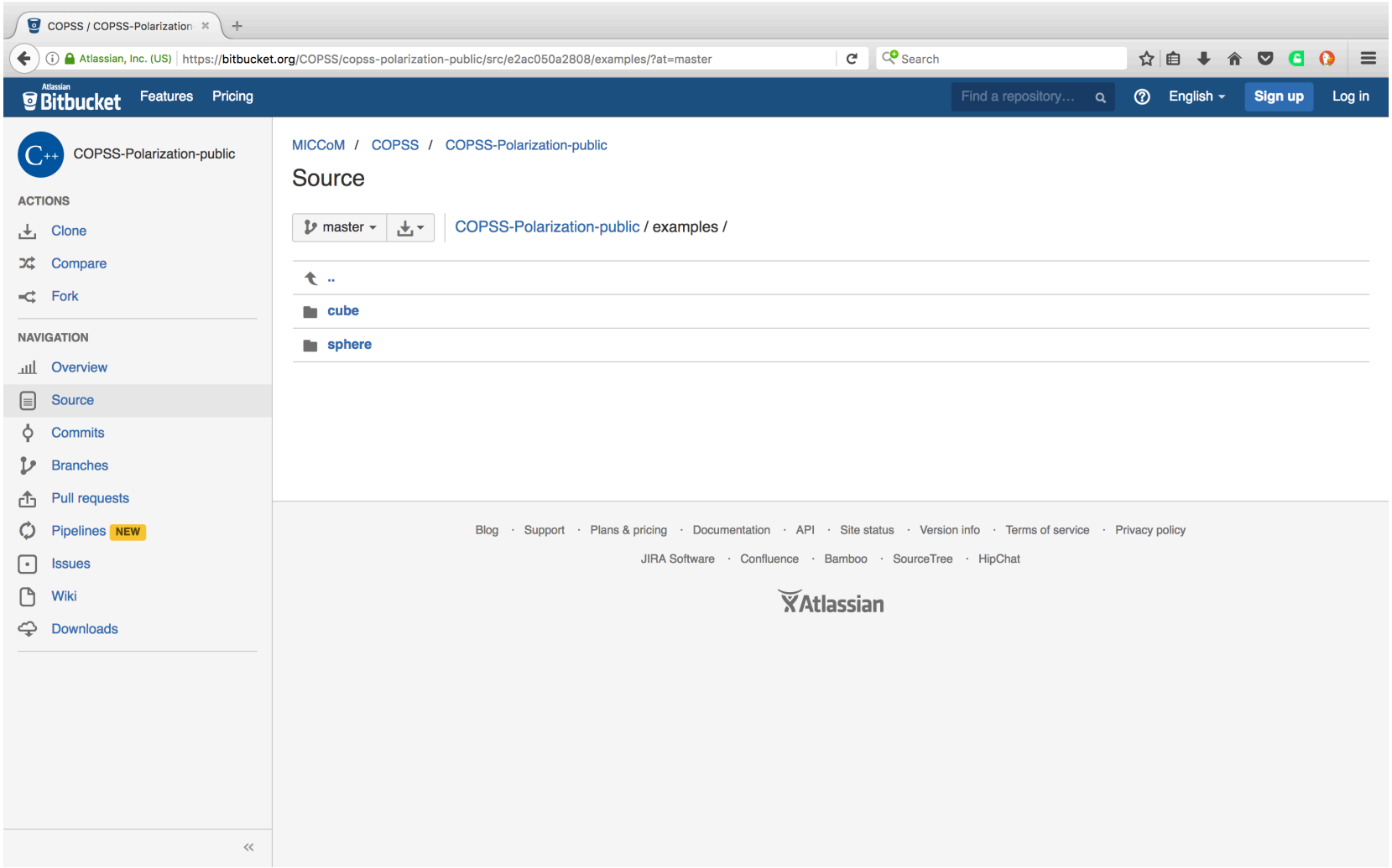
COPSS-Polarization Tutorial

- Directories in COPSS-Polarization repository.



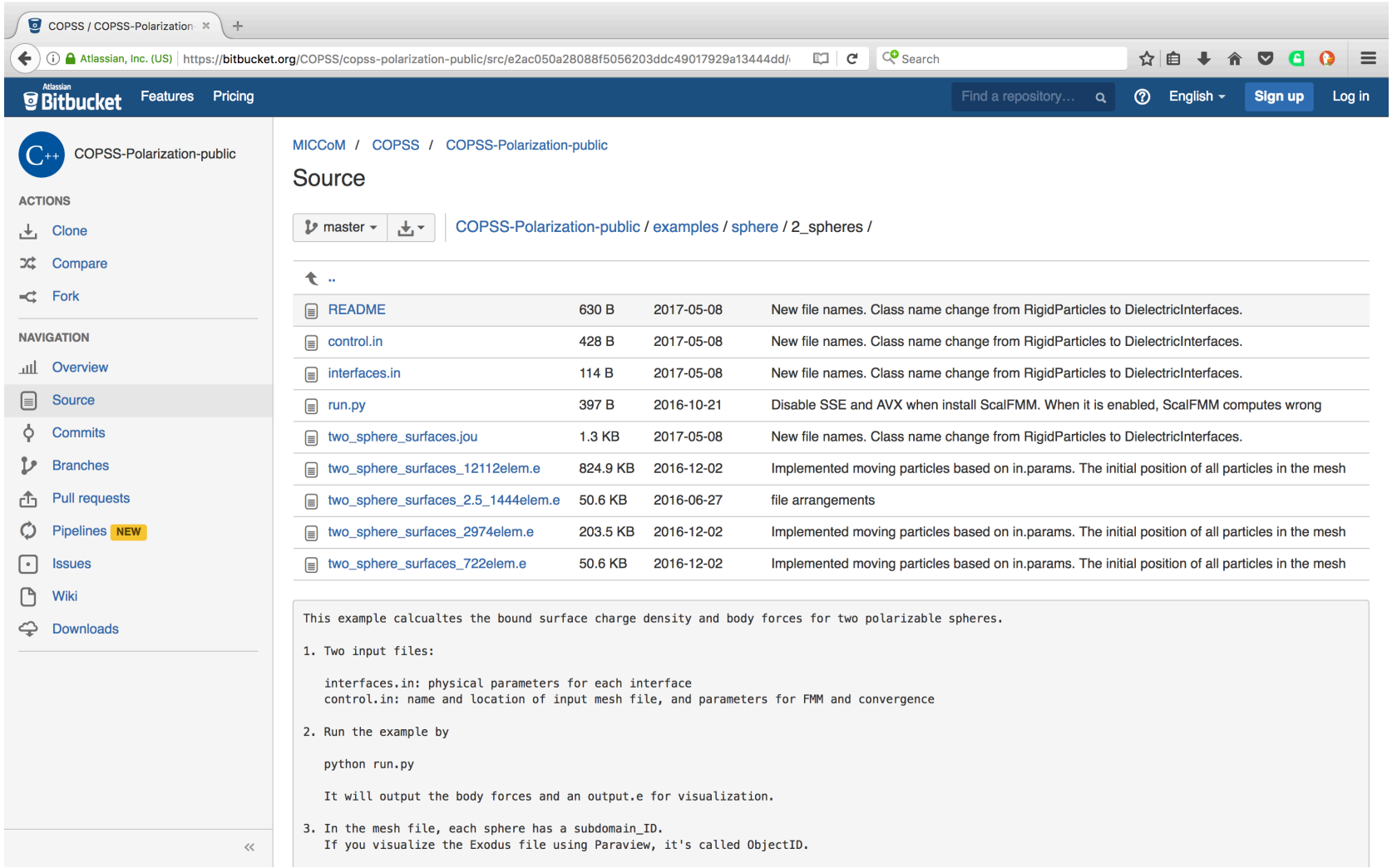
COPSS-Polarization Tutorial

- Examples in COPSS-Polarization repository.



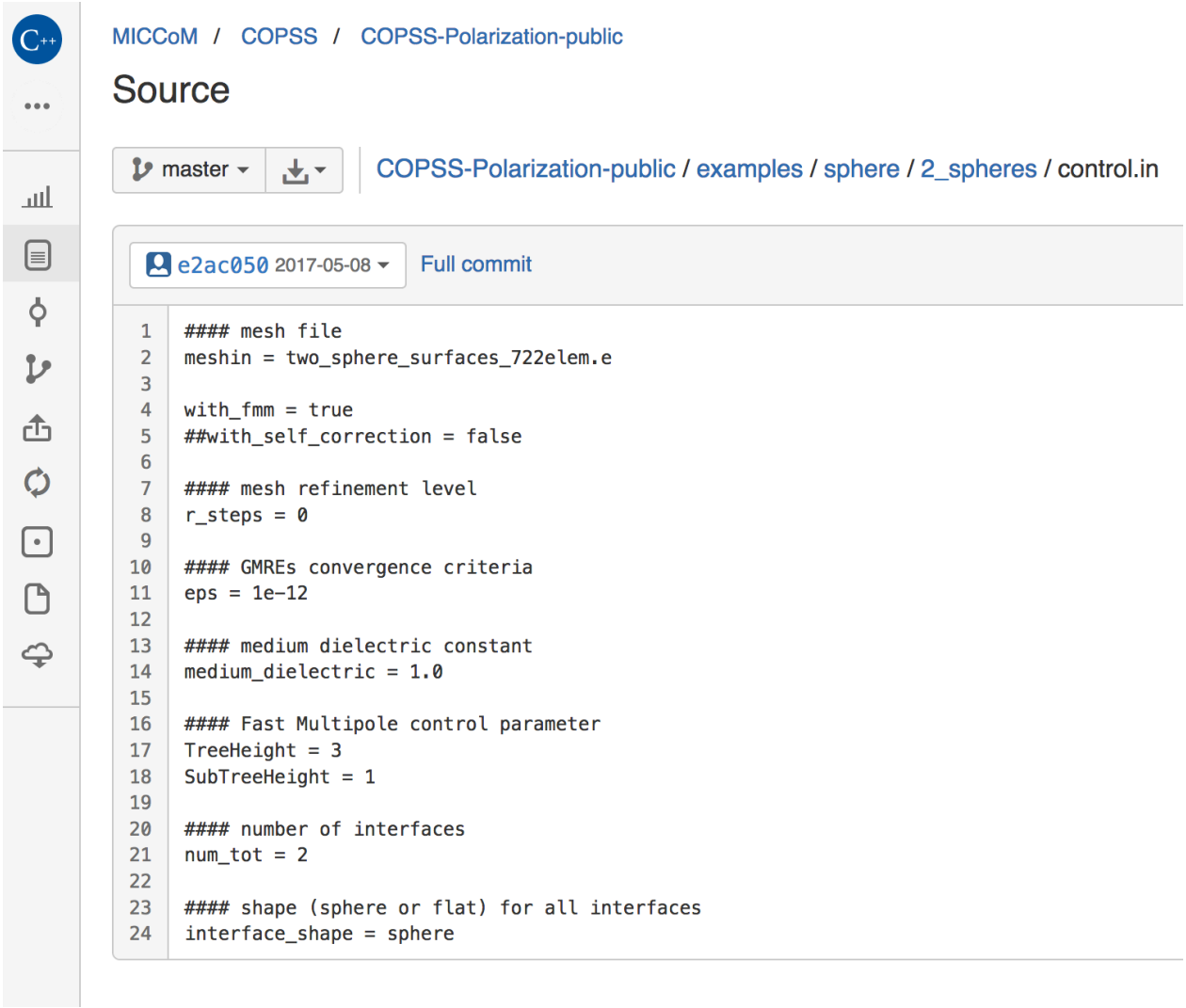
COPSS-Polarization Tutorial

- Run examples in COPSS-Polarization repository.



COPSS-Polarization Tutorial

- Input files for COPSS-Polarization.



MICCoM / COPSS / COPSS-Polarization-public

Source

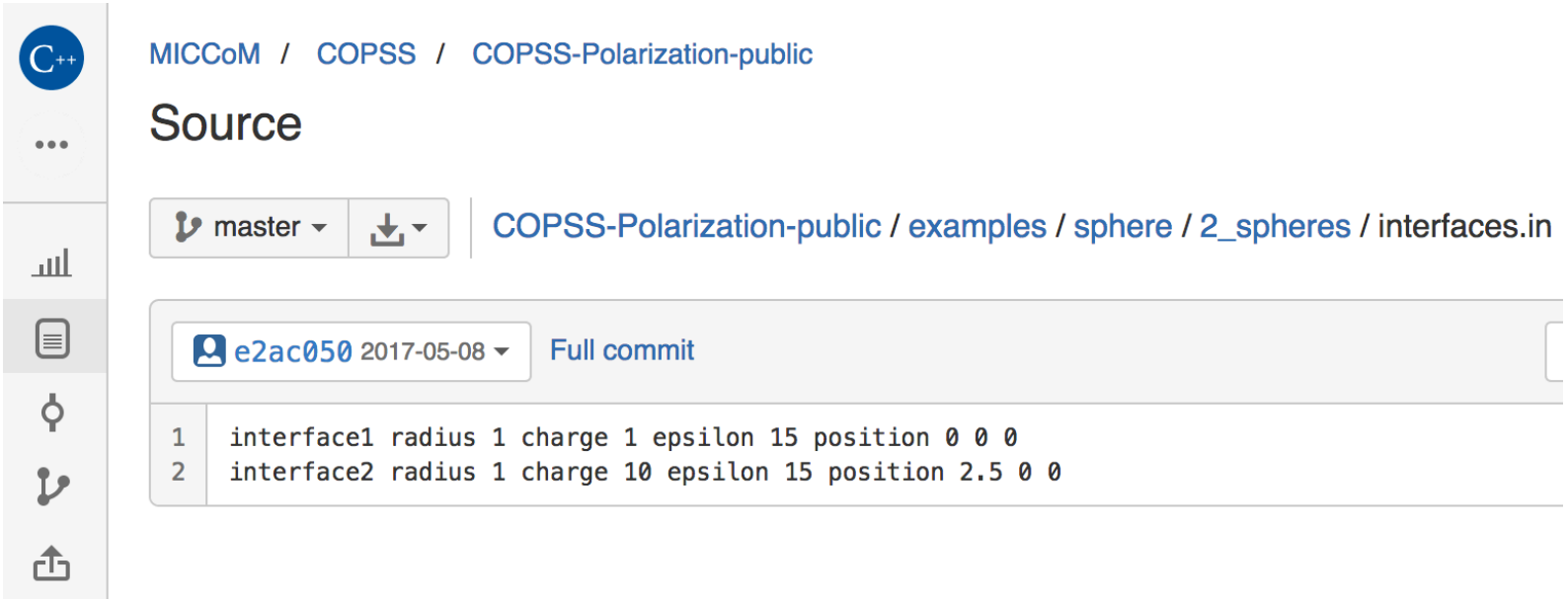
master | COPSS-Polarization-public / examples / sphere / 2_spheres / control.in

e2ac050 2017-05-08 | Full commit

```
#### mesh file
meshin = two_sphere_surfaces_722elem.e

with_fmm = true
##with_self_correction = false

#### mesh refinement level
r_steps = 0

#### GMREs convergence criteria
eps = 1e-12

#### medium dielectric constant
medium_dielectric = 1.0

#### Fast Multipole control parameter
TreeHeight = 3
SubTreeHeight = 1

#### number of interfaces
num_tot = 2

#### shape (sphere or flat) for all interfaces
interface_shape = sphere
```

COPSS-Polarization Tutorial

- Input files for COPSS-Polarization.



COPSS-Polarization Tutorial

- Simulation outputs.

```
anlextwls026-070:2_spheres xikai$ ../../../src/polarization-opt
Compressed M2L operators (104) read from binary file m2l_kONE_OVER_R_d_o6_e1e-06.bin in 0.0166562sec.
Solved linear system in 15 iterations, residual norm is 3.11048e-10.

 ---------------------------------------------------------------------------------------------------------
| Time:           Thu Jul 13 15:18:10 2017                                                                |
| OS:             Darwin                                                                                  |
| HostName:       anlextwls026-070.wl.anl-external.org                                                    |
| OS Release:     16.6.0                                                                                  |
| OS Version:     Darwin Kernel Version 16.6.0: Fri Apr 14 16:21:16 PDT 2017; root:xnu-3789.60.24~6/RELEASE_X86_64 |
| Machine:        x86_64                                                                                  |
| Username:       xikai                                                                                   |
| Configuration:  ../source/configure  '--prefix=/Users/xikai/Softwares/libmesh/build'                    |
|  '--with-methods=opt'                                                                                   |
|  '--enable-silent-rules'                                                                                |
|  '--enable-unique-id'                                                                                   |
|  '--disable-warnings'                                                                                   |
|  '--enable-unique-ptr'                                                                                  |
|  '--enable-openmp'                                                                                      |
|  '--disable-maintainer-mode'                                                                            |
|  '--enable-petsc-required'                                                                              |
|  '--disable-timestamps'                                                                                 |
|  'CXX=mpicxx'                                                                                           |
|  'CC=mpicc'                                                                                             |
|  'FC=mpif90'                                                                                            |
|  'F77=mpif77'                                                                                           |
|  'PETSC_DIR=/Users/xikai/Softwares/petsc-3.7.4'                                                         |
|  'PETSC_ARCH=arch-darwin-c-opt'                                                                         |
|  'SLEPC_DIR=/Users/xikai/Softwares/slepc-3.7.3'                                                         |
 ---------------------------------------------------------------------------------------------------------
 ---------------------------------------------------------------------------------------------------
| Polarization Performance: Alive time=0.341899, Active time=0.282607                               |
 ---------------------------------------------------------------------------------------------------
| Event                        nCalls     Total Time  Avg Time    Total Time  Avg Time    % of Active Time  |
|                                         w/o Sub     w/o Sub     With Sub    With Sub    w/o S    With S   |
|---------------------------------------------------------------------------------------------------|
|                                                                                                   |
| output                       1          0.0024      0.002407    0.0024      0.002407    0.85     0.85     |
| read-in-mesh                 1          0.0030      0.003027    0.0030      0.003027    1.07     1.07     |
| solve                        1          0.2772      0.277173    0.2772      0.277173    98.08    98.08    |
 ---------------------------------------------------------------------------------------------------
| Totals:                      3          0.2826                                100.00              |
```

COPSS-Polarization Tutorial

- Simulation outputs

```
anlextwls026-070:2_spheres xikai$ ls
README                          m2l_kONE_OVER_R_d_o6_e1e-06.bin    two_sphere_surfaces_12112elem.e
control.in                      output.e                           two_sphere_surfaces_2.5_1444elem.e
forces_energy.dat               run.py                             two_sphere_surfaces_2974elem.e
interfaces.in                   two_sphere_surfaces.jou            two_sphere_surfaces_722elem.e
```

Output files:

- output.e (open it using Paraview, visualize surface charge densities)
- forces_energy.dat (contains forces acting on every sphere)

Thanks for your attention.

Q & A.

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