



MIDWEST INTEGRATED CENTER FOR COMPUTATIONAL MATERIALS

<http://miccom-center.org>

Topic: COPSS-Polarization Tutorial

Presenter: Xikai Jiang, The University of Chicago



Access COPSS-Polarization

- COPSS-Polarization repository on Bitbucket.

The screenshot shows the Bitbucket repository page for COPSS-Polarization-public. The page is organized into several sections:

- Navigation:** A sidebar on the left contains navigation links for Overview, Source, Commits, Branches, Pull requests, Pipelines (marked as NEW), Issues, Wiki, and Downloads.
- Repository Overview:** The main content area displays the repository name, a table of statistics, and a description of the software.
- Recent Activity:** A list of recent activity on the right side of the page, including file name changes and commits.

Last updated	2017-05-08	0	2
Language	C++	Open PRs	Watchers
Access level	Read	1	0
		Branch	Forks

COPSS

COPSS (Continuum Particle Simulation Suite) is an open source, **libMesh** based, software for continuum-particle simulations. The package is designed to be easy to use, extensible, and scalable. It currently includes two modules, **COPSS-Hydrodynamics** to solve hydrodynamic interactions in colloidal suspensions and **COPSS-Polarization** to solve electrostatic interactions in heterogeneous dielectric media. The algorithms beneath **COPSS** have been published or under-review, but the code framework, user-interface, etc., are still rough. We are working on improving **COPSS** and appreciate your contributions.

COPSS-Polarization

COPSS-Polarization solves the electrostatic interactions in charged systems that exhibit sharp discontinuous changes in dielectric permittivity. It is based on an efficient $\mathcal{O}(N)^2$ computational approach to model arbitrary-shaped sharp interfaces separating dielectrics with spatially different dielectric permittivities. A parallel boundary element Poisson solver is the center of the algorithm.

Installation

COPSS is written using **libMesh** framework. It also requires **PETSc** for parallel linear equation solvers and **ScalFMM** for fast multipole computations. Before installing **COPSS**, you need to install **PETSc**, **libMesh**, and **ScalFMM**. To achieve the best parallel performance of COPSS, we suggest install it on a Linux cluster environment.

0. System environment prep

Recent activity

- File names change**
Issue #1 updated in COPSS/copss-polarizati...
Xikai Jiang · 2017-05-16
- File names change**
Issue #1 commented on in COPSS/copss-pol...
Xikai Jiang · 2017-05-16
- 1 commit**
Pushed to COPSS/copss-polarization-public
e2ac050 New file names. Class name cha...
Xikai Jiang · 2017-05-08
- 1 commit**
Pushed to COPSS/copss-polarization-public
74e497b Readme.md edited online with Bi...
Xikai Jiang · 2017-05-08
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Issue #1 updated in COPSS/copss-polarizati...
Xikai Jiang · 2017-05-06
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Xikai Jiang · 2017-05-06
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Issue #1 created in COPSS/copss-polarizati...
Xikai Jiang · 2017-05-06
- 1 commit**



Access COPSS-Polarization

- Download (clone) COPSS-Polarization repository.

The screenshot shows the Bitbucket web interface for the repository 'COPSS-Polarization-public'. The browser address bar shows the URL 'https://bitbucket.org/COPSS/copss-polarization-public/overview'. The Bitbucket logo and navigation links are visible at the top. The repository name 'COPSS-Polarization-public' is displayed in the top left. The main content area shows the 'Overview' section with a 'Clone' button and a 'Clone in SourceTree' button. A table displays repository statistics: 0 Open PRs, 2 Watchers, 1 Branch, and 0 Forks. The 'Recent activity' section on the right lists several commits and file name changes by Xikai Jiang. The bottom of the page shows the URL 'https://bitbucket.org/COPSS/copss-polarization-public/overview#clone' and the text 'environment prep'.

Bitbucket Features Pricing Find a repository... English Sign up Log in

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Overview

Clone in SourceTree

Atlassian SourceTree is a free Git and Mercurial client for Mac.

0	2
Open PRs	Watchers
1	0
Branch	Forks

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environment prep



COPSS-Polarization Tutorial

- Directories in COPSS-Polarization repository.

The screenshot shows a Bitbucket repository page for 'COPSS-Polarization-public'. The browser address bar shows the URL 'https://bitbucket.org/COPSS/copss-polarization-public/src'. The page header includes the Bitbucket logo, navigation links for 'Features' and 'Pricing', a search bar, and user options for 'Sign up' and 'Log in'. The left sidebar contains navigation options: 'Clone', 'Compare', 'Fork', 'Overview', 'Source' (selected), 'Commits', 'Branches', 'Pull requests', 'Pipelines' (marked as NEW), 'Issues', 'Wiki', and 'Downloads'. The main content area shows the 'Source' view for the 'master' branch. It lists several directories: 'contrib/scalfmm', 'doxygen', 'examples', 'src', and 'tools'. Below these is a table of files:

File Name	Size	Last Modified	License
LICENSE	17.8 KB	2016-06-28	GNU GPL
Readme.md	8.1 KB	2017-05-08	New file names. Class name change from RigidParticles to DielectricInterfaces.

The 'COPSS' section describes it as an open source, libMesh based, software for continuum-particle simulations. It includes modules for hydrodynamics and polarization. The 'COPSS-Polarization' section explains it solves electrostatic interactions in charged systems. The 'Installation' section lists dependencies like PETSc, libMesh, and ScaFMm.



COPSS-Polarization Tutorial

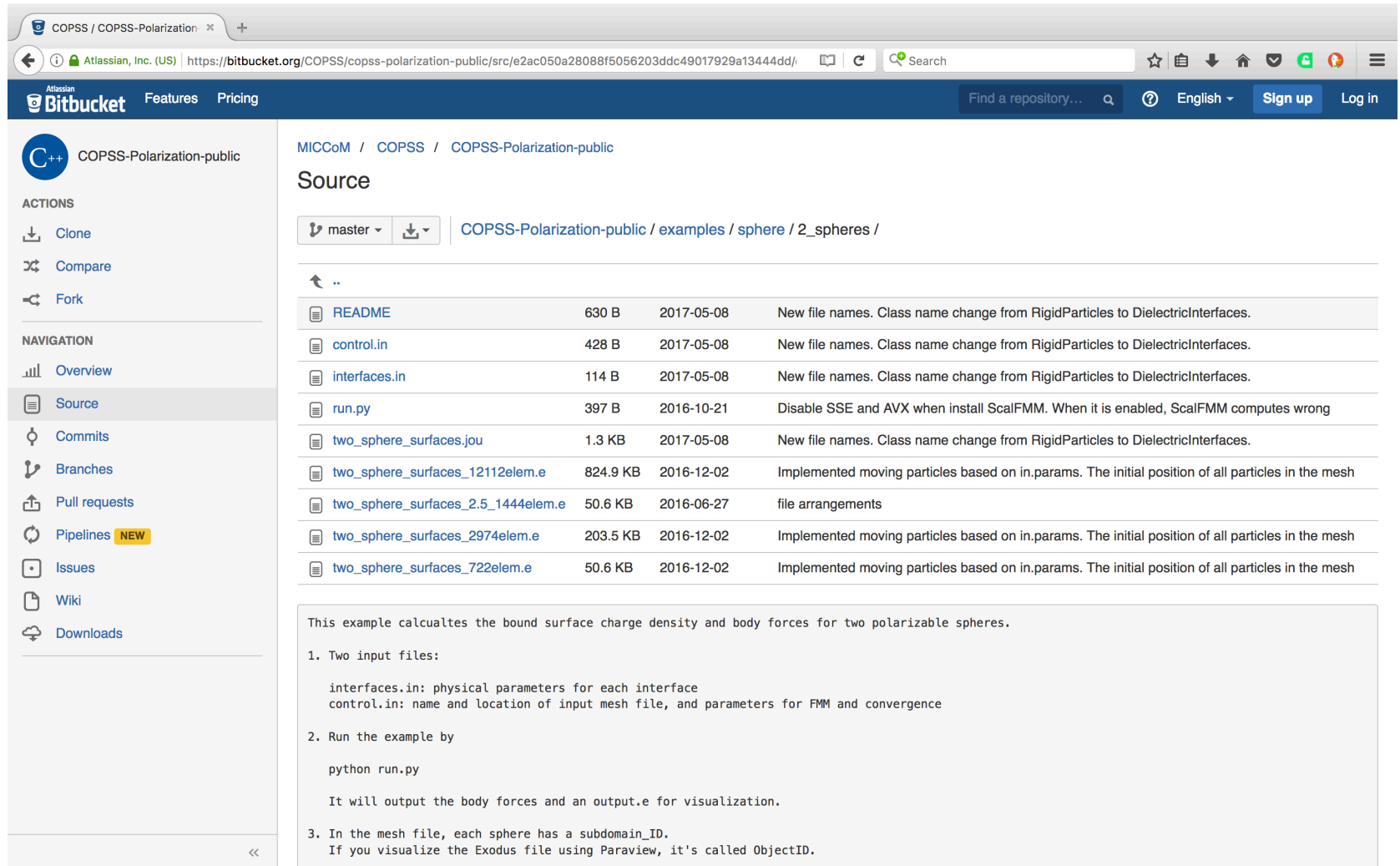
- Examples in COPSS-Polarization repository.

The screenshot shows a Bitbucket web interface. The browser address bar displays the URL: <https://bitbucket.org/COPSS/copss-polarization-public/src/e2ac050a2808/examples/?at=master>. The Bitbucket header includes navigation links for Features and Pricing, a search bar, and user options for English, Sign up, and Log in. The left sidebar shows the repository name 'COPSS-Polarization-public' and a list of actions: Clone, Compare, Fork, Overview, Source (selected), Commits, Branches, Pull requests, Pipelines (NEW), Issues, Wiki, and Downloads. The main content area shows the 'Source' view for the 'examples' directory, listing subdirectories 'cube' and 'sphere'. The footer contains links for Blog, Support, Plans & pricing, Documentation, API, Site status, Version info, Terms of service, Privacy policy, and a list of Atlassian products: JIRA Software, Confluence, Bamboo, SourceTree, and HipChat. The Atlassian logo is centered at the bottom.



COPSS-Polarization Tutorial

- Run examples in COPSS-Polarization repository.



The screenshot shows a Bitbucket repository page for 'COPSS-Polarization-public'. The page is viewed in a browser with the URL <https://bitbucket.org/COPSS/copss-polarization-public/src/e2ac050a28088f5056203ddc49017929a13444dd/>. The repository is a C++ project. The left sidebar shows navigation options: Overview, Source (selected), Commits, Branches, Pull requests, Pipelines (NEW), Issues, Wiki, and Downloads. The main content area shows the 'Source' view for the path 'COPSS-Polarization-public / examples / sphere / 2_spheres /'. A table lists the files in the directory:

File Name	Size	Last Modified	Description
README	630 B	2017-05-08	New file names. Class name change from RigidParticles to DielectricInterfaces.
control.in	428 B	2017-05-08	New file names. Class name change from RigidParticles to DielectricInterfaces.
interfaces.in	114 B	2017-05-08	New file names. Class name change from RigidParticles to DielectricInterfaces.
run.py	397 B	2016-10-21	Disable SSE and AVX when install ScalFMM. When it is enabled, ScalFMM computes wrong
two_sphere_surfaces.jou	1.3 KB	2017-05-08	New file names. Class name change from RigidParticles to DielectricInterfaces.
two_sphere_surfaces_12112elem.e	824.9 KB	2016-12-02	Implemented moving particles based on in.params. The initial position of all particles in the mesh
two_sphere_surfaces_2.5_1444elem.e	50.6 KB	2016-06-27	file arrangements
two_sphere_surfaces_2974elem.e	203.5 KB	2016-12-02	Implemented moving particles based on in.params. The initial position of all particles in the mesh
two_sphere_surfaces_722elem.e	50.6 KB	2016-12-02	Implemented moving particles based on in.params. The initial position of all particles in the mesh

Below the table, there is a text block explaining the example:

This example calculates the bound surface charge density and body forces for two polarizable spheres.

- Two input files:
`interfaces.in`: physical parameters for each interface
`control.in`: name and location of input mesh file, and parameters for FMM and convergence
- Run the example by

```
python run.py
```


It will output the body forces and an `output.e` for visualization.
- In the mesh file, each sphere has a `subdomain_ID`.
If you visualize the Exodus file using Paraview, it's called `ObjectID`.



COPSS-Polarization Tutorial

- Input files for COPSS-Polarization.

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Source

master | [COPSS-Polarization-public / examples / sphere / 2_spheres / control.in](#)

e2ac050 2017-05-08 | Full commit

```
1  ##### mesh file
2  meshin = two_sphere_surfaces_722elem.e
3
4  with_fmm = true
5  ##with_self_correction = false
6
7  ##### mesh refinement level
8  r_steps = 0
9
10 ##### GMREs convergence criteria
11 eps = 1e-12
12
13 ##### medium dielectric constant
14 medium_dielectric = 1.0
15
16 ##### Fast Multipole control parameter
17 TreeHeight = 3
18 SubTreeHeight = 1
19
20 ##### number of interfaces
21 num_tot = 2
22
23 ##### shape (sphere or flat) for all interfaces
24 interface_shape = sphere
```



COPSS-Polarization Tutorial

- Input files for COPSS-Polarization.

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Source

master | [COPSS-Polarization-public / examples / sphere / 2_spheres / interfaces.in](#)

e2ac050 2017-05-08 Full commit

```
1 interface1 radius 1 charge 1 epsilon 15 position 0 0 0
2 interface2 radius 1 charge 10 epsilon 15 position 2.5 0 0
```




COPSS-Polarization Tutorial

■ Simulation outputs.

```

anlxtwls026-070:2_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:     anlxtwls026-070.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

```
anlxtwls026-070:2_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.