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Topic: Continuum-Particle Simulation Software (COPSS)
Electrostatic Polarization

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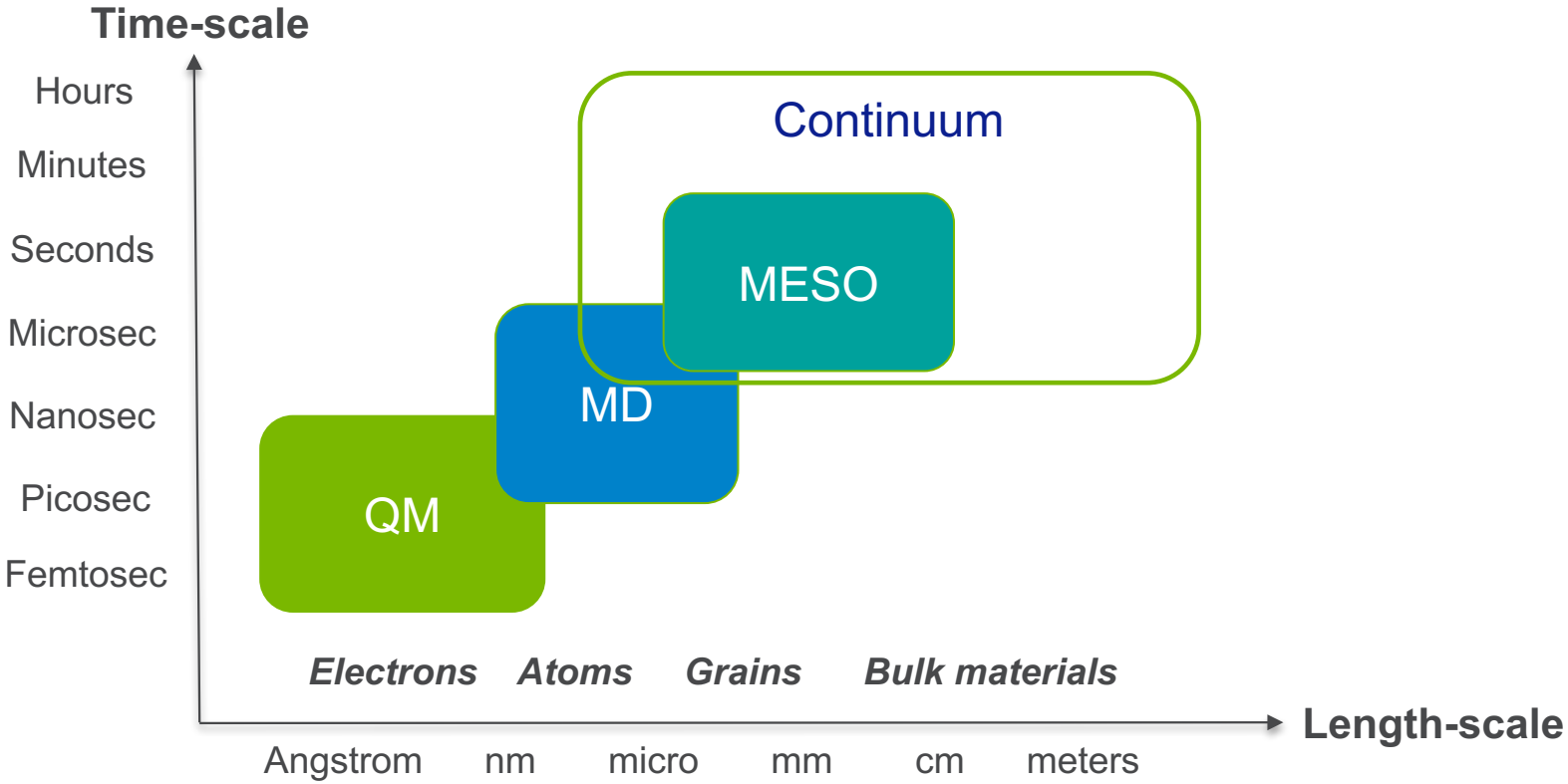
Continuum-Particle Simulation



- Continuum simulation (Grid-based) solves Partial Differential Equations on discretized grids or meshes (Finite element method, Finite difference method, *etc.*)
- Particle simulation solves Equation of Motion, *e.g.,* Netwon's 2nd law, to evolve positions and velocities of discrete particles (Molecular dynamics, Dissipative particle dynamics, *etc.*)
- *Continuum-particle coupling* aims to bridge multiple length-scales for complex physics problems (e.g. part of the domain using continuum simulation, other parts use particle-simulation)

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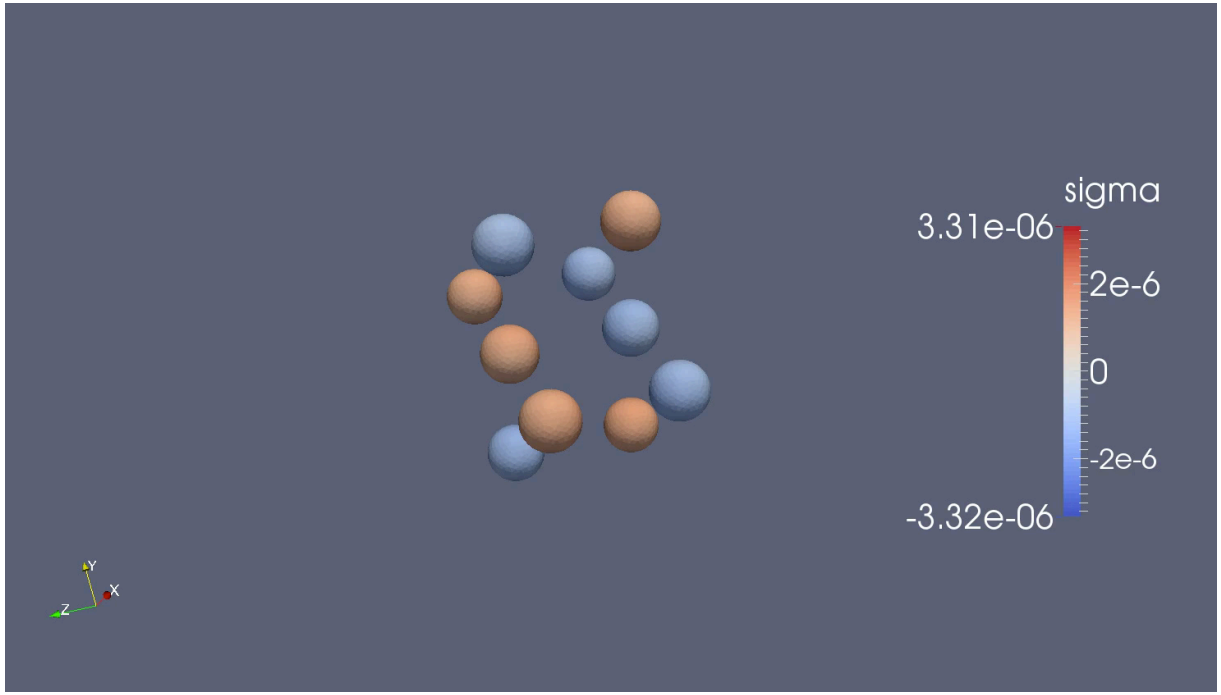
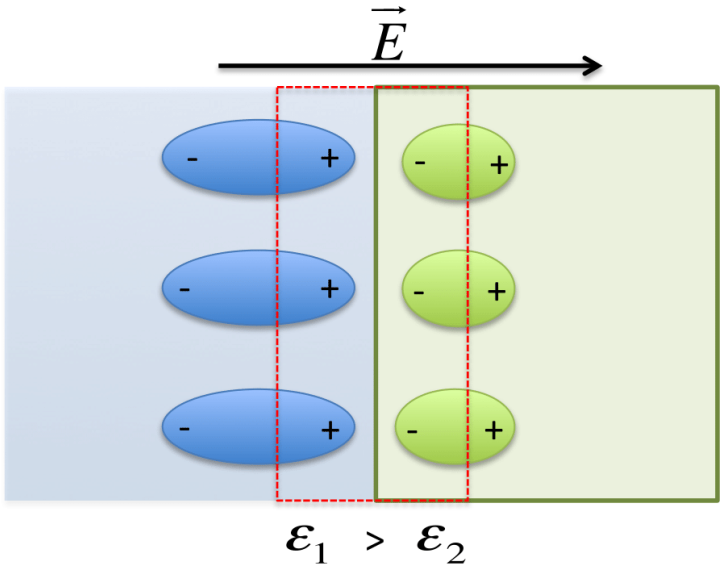
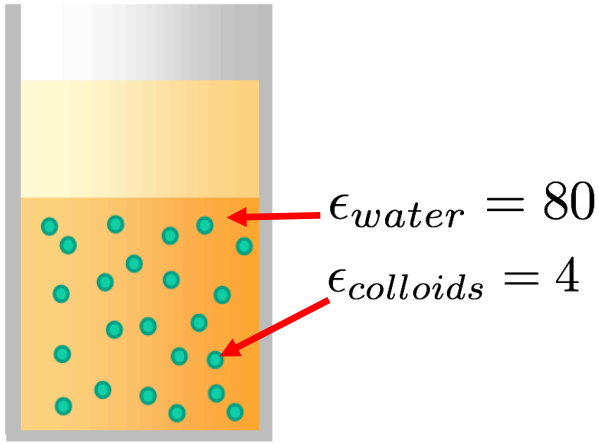
COPSS - Polarization



- Continuum simulation (Grid-based) solves Poisson equation on discretized meshes using Boundary Element Method on the surfaces of colloidal particles
- Particle simulation solves Equation of Motion, *i.e.,* Netwon's 2nd law, to evolve positions and velocities of colloidal particles
- *Continuum-particle coupling:* continuum simulation provides force fields, particle simulation uses the force fields to evolve particles' motion

Dielectric Polarization





en.wikipedia.org/wiki/Colloid

- Dielectric materials (insulator) undergo electric polarization under the influence of applied electric fields
- The charges in dielectric materials don't move freely but only shift slightly from their equilibrium positions in applied electric fields
- Bound charges (induced charges) accumulate on the boundary of the dielectric materials, which ultimately affect force fields acting on dielectric materials and their motions

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Dielectric Polarization

4.2.2 Physical Interpretation of Bound Charge

In the last section we found that the field of a polarized object is identical to the field that would be produced by a certain distribution of "bound charges," σ_b and ρ_b. But this conclusion emerged in the course of abstract manipulations on the integral (4.9) and left us with no clue as to the physical meaning of these bound charges. Indeed, some authors give you the impression that bound charges are in some sense "fictitious"—mere bookkeeping devices used to facilitate the calculation of fields. Nothing could be farther from the truth; ρ_b and σ_b represent *perfectly genuine accumulations of charge*. In this section I'll show you how polarization leads to such accumulations of charge.

The basic idea is very simple: Suppose we have a long string of dipoles, as shown in Fig. 4.11. Along the line, the head of one effectively cancels the tail of its neighbor, but at the ends there are two charges left over: plus at the right end and

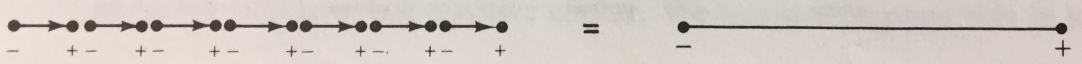


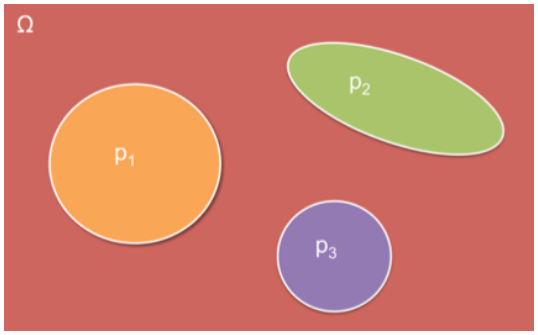
Figure 4.11

minus at the left. It is as if we had peeled off an electron at one end and carried it all the way down to the other end, though in fact no single electron made the whole trip—a lot of tiny displacements add up to one large one. We call the net charge at the ends *bound* charge to remind ourselves that it cannot be removed; in a dielectric every electron is permanently attached to a specific atom or molecule. But apart from that, bound charge is no different from any other kind.

To calculate the actual amount of bound charge resulting from a given uniform polarization, examine a "tube" of dielectric parallel to **P**. The dipole moment of the tiny chunk shown in Fig. 4.12 is $P(As)$, where A is the cross-sectional area of the tube and s is the length of the chunk. In terms of the charge at the end, this same dipole moment can be written as. The bound charge that piles up at the [illegible]

Induced Charge Computation (ICC)

- A numerical method to solve dielectric polarization problem



- It starts with the Poisson equation for electrostatics subject to boundary conditions for dielectric polarization

$$-\varepsilon_0 \nabla \cdot [\varepsilon(\mathbf{r}) \nabla \psi(\mathbf{r})] = \rho(\mathbf{r})$$

- Poisson equation is transformed to a set of linear system of equations by using boundary-integral theories

$$A\sigma_b = b$$

- Induced charge densities on the dielectric interfaces/boundaries are the unknowns

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Induced Charge Computation (ICC)

- Mathematical details on the matrix equation

$$A\sigma_b = b$$

- Matrix-vector multiplication

$$A\sigma_b \equiv \bar{\epsilon}_i \sigma_b + \epsilon_0 \Delta\epsilon_i \mathbf{E}_b \cdot \mathbf{n}$$

ϵ_0 vacuum permittivity

$$\bar{\epsilon}_i = (\epsilon_i + \epsilon_m)/2$$

$$\Delta\epsilon_i = \epsilon_m - \epsilon_i$$

- Electric field from bound (induced) charges

$$\mathbf{E}_b = \frac{1}{4\pi\epsilon_0} \int_{\partial\Gamma} \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \sigma_b(\mathbf{r}')\, d^2\mathbf{r}'$$

- Right-hand-side $b = (1 - \bar{\epsilon}_i)\sigma_f - \epsilon_0 \Delta\epsilon_i \mathbf{E}_f \cdot \mathbf{n}$

- Electric field from free charges

$$\mathbf{E}_f = \frac{1}{4\pi\epsilon_0} \left(\int_{\partial\Gamma} \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \sigma_f(\mathbf{r}')\, d^2\mathbf{r}' + \int_{\Omega} \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \frac{\rho_f(\mathbf{r}')}{\epsilon_m}\, d^3\mathbf{r}' \right)$$

Reference: X. Jiang, et al J. Chem. Phys. 145, 064309, 2016

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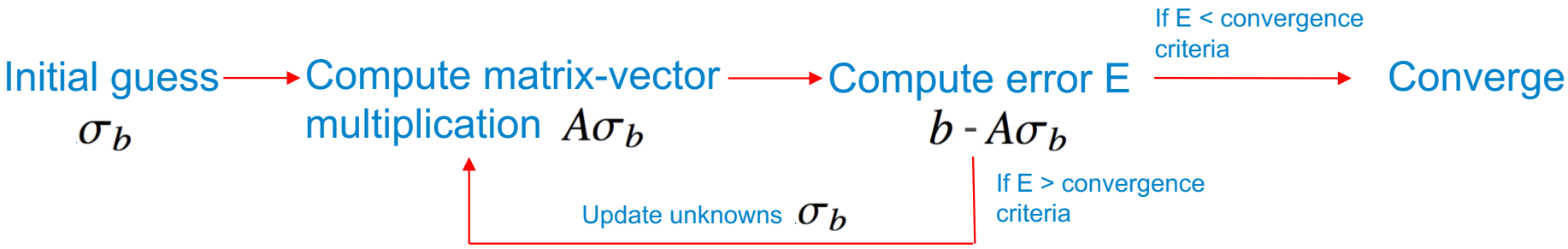
Solve the ICC Problem

- To solve the matrix equation $A\sigma_b = b$
- We use Iterative solver GMRES (Generalized Minimal Residual Method)



- Matrix-vector multiplication is the most expensive part in solving the problem

$$A\sigma_b \equiv \bar{\epsilon}_i \sigma_b + \epsilon_0 \Delta\epsilon_i \mathbf{E}_b \cdot \mathbf{n}$$

$$\mathbf{E}_b = \frac{1}{4\pi\epsilon_0} \int_{\partial\Gamma} \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^3} \sigma_b(\mathbf{r}')\, d^2\mathbf{r}'$$

Solve the ICC Problem

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$$\mathbf{E}_b = \frac{1}{4\pi\epsilon_0}\int_{\partial\Gamma}\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|^3}\sigma_b(\mathbf{r}')\,d^2\mathbf{r}'$$

(N) (N)

- Direct evaluation requires $O(N^2)$ operations: N discretized nodal points on the boundary mesh, $\boldsymbol{E}_b$ needs to be evaluated on every nodal points

- Fast Multipole Method (FMM) is used to the computational cost to be in $O(N)$ operations

$$f(\mathbf{r}_i) = \sum_{j=1}^{N} K(\mathbf{r}_i, \mathbf{r}_j)\sigma_j$$

Reference: W. Fong et. al.,The black-box fast multipole method, J. Compt. Phys., 228, 8712-8725, 2009

- COPSS-Polarization is written on top of ScalFMM (FMM library) and libMesh (parallel finite element and mesh management library)

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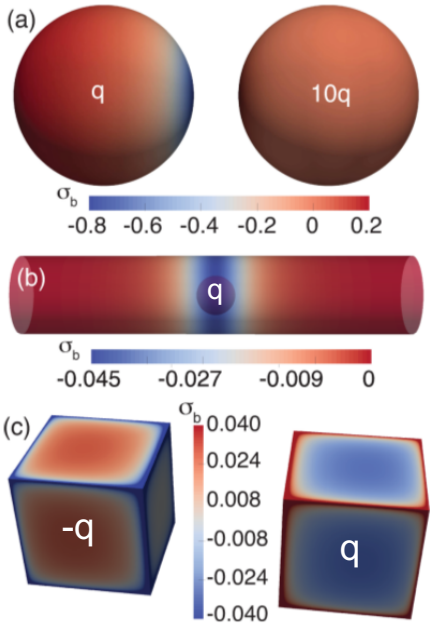
COPSS-Polarization

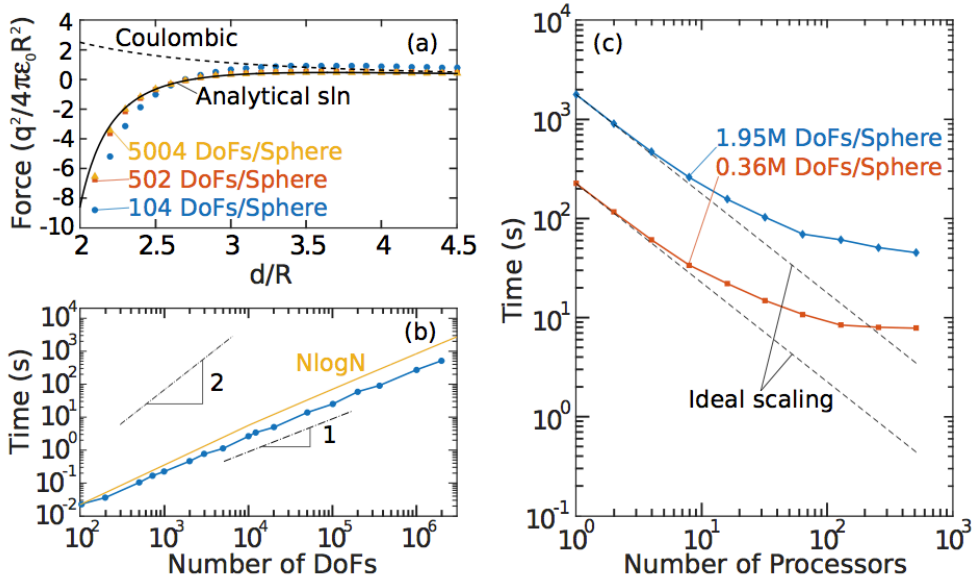


$\epsilon_{sphere} = 15$
$\epsilon_{out} = 1$

$\epsilon_{sphere} = \epsilon_{cavity} = 1$
$\epsilon_{cylinder} = 2$

$\epsilon_{cube} = 15$
$\epsilon_{out} = 1$

Distribution of induced bound surface charge densities for (a) spherical particles, (b) a spherical particle in a confined geometry, and (c) non-spherical particles.



Performance of Induced Charge Computation. (a) Accuracy, (b) efficiency – the *O(N)* scaling, and (c) parallel scalability.

- COPSS-Polarization houses parallel and efficient solver for electrostatic polarization problem involving multiple dielectric interfaces

MICCoM codes: http://miccomcodes.org/

COPSS-Polarization codes: https://bitbucket.org/COPSS/copss-polarization-public.git

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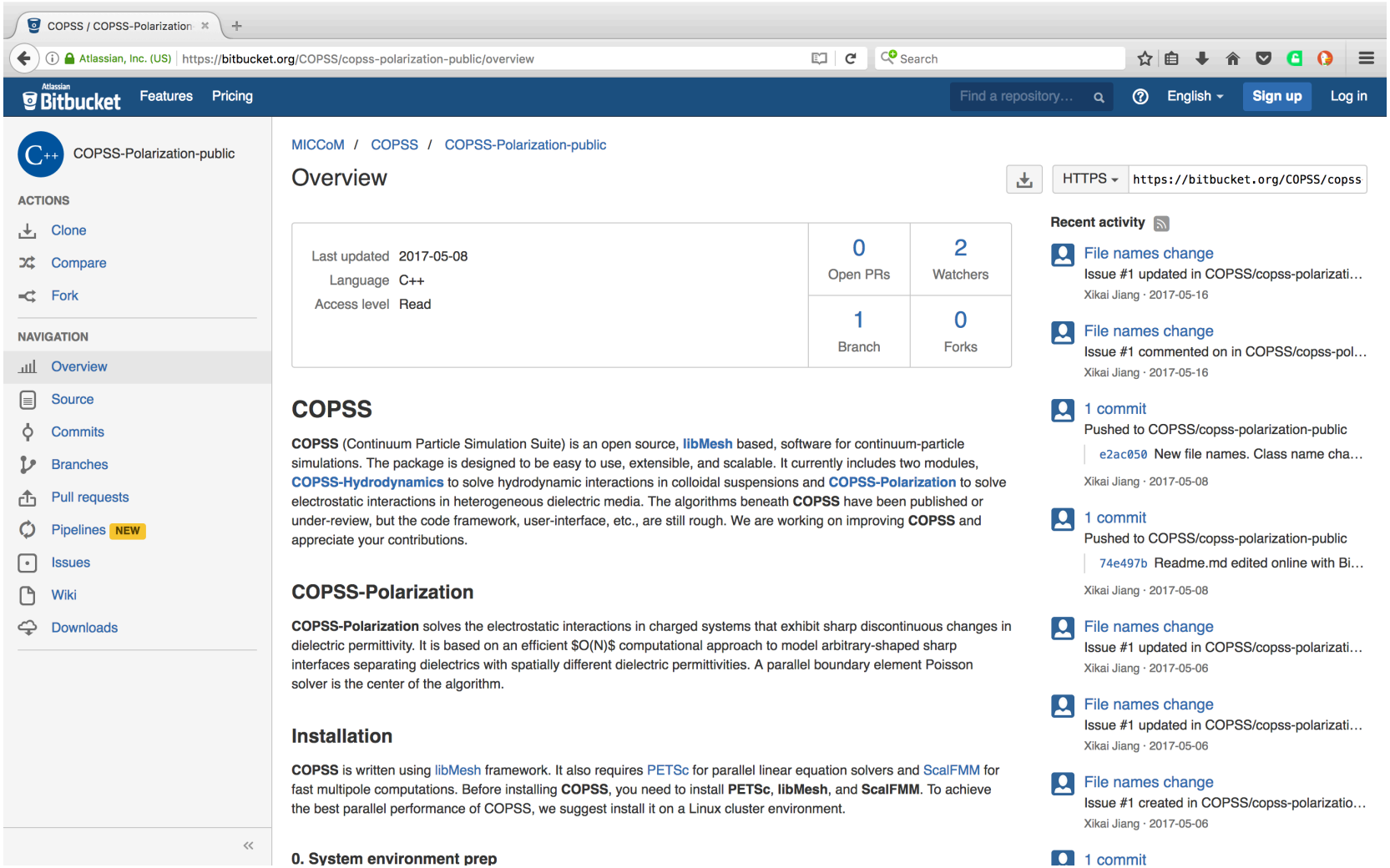
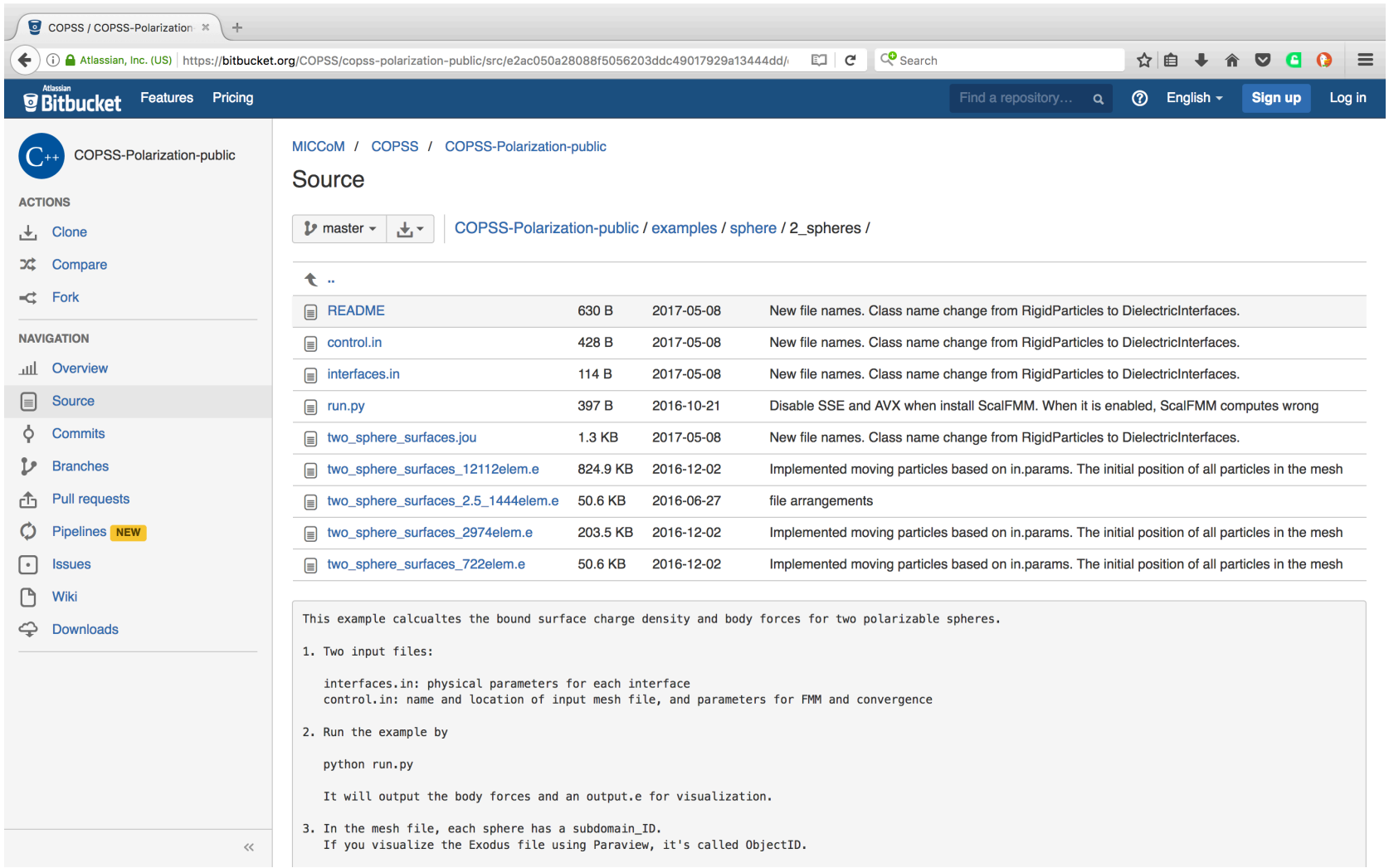
Access COPSS-Polarization

- COPSS-Polarization repository on Bitbucket.



Access COPSS-Polarization

- Run examples in COPSS-Polarization repository.



Thanks for your attention.

Q & A.

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