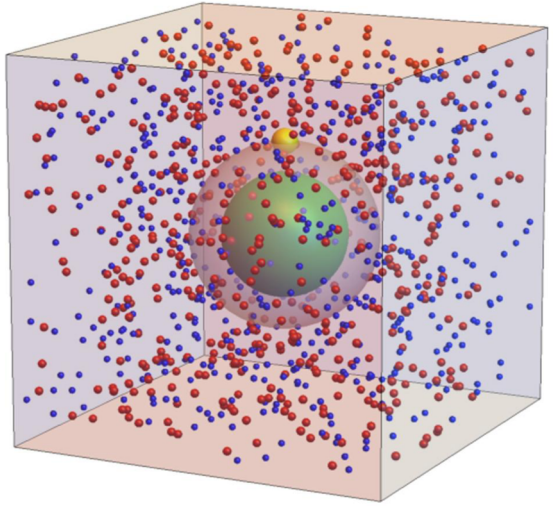
Nanosphere Electrostatics Lab

By Kadupitiya Kadupitige, Nicholas Brunk, Sohile Ali, Fox, Geoffrey C., Vikram Jadhao



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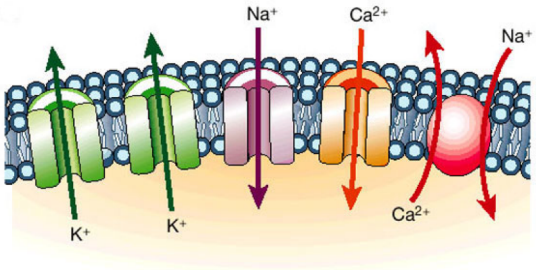
Introduction

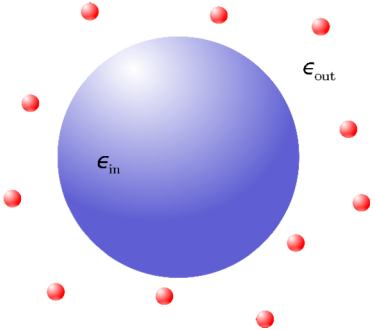
- Accurate knowledge of ***ionic structure & dynamics*** is critical to study nanoparticle dynamics

Ion channels

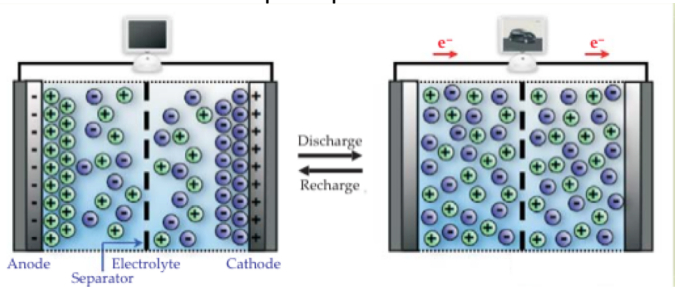


Marbán, E. Nature 415, 213-218 (2002)

Stabilization of colloids



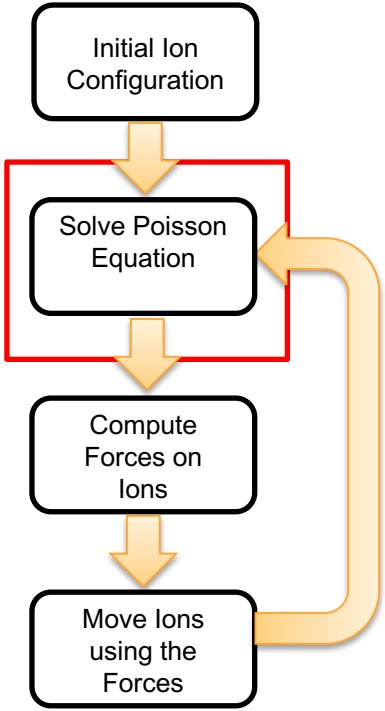
Supercapacitors



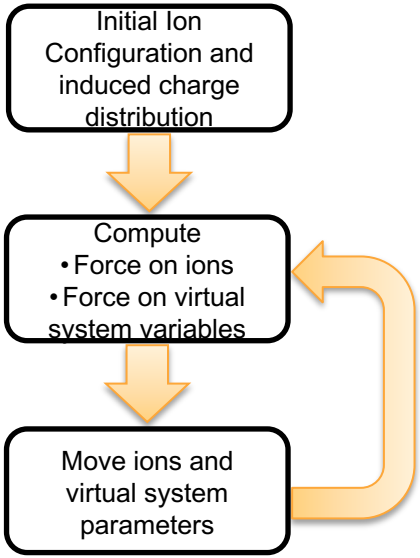
Abrua et al. Physics Today 61, 43 (2008)

- Nanoparticles are polarized in most solvents
- Simulating the dynamics of ions near polarizable nanoparticles is challenging: Need to solve Poisson equation at every timestep

Traditional approach



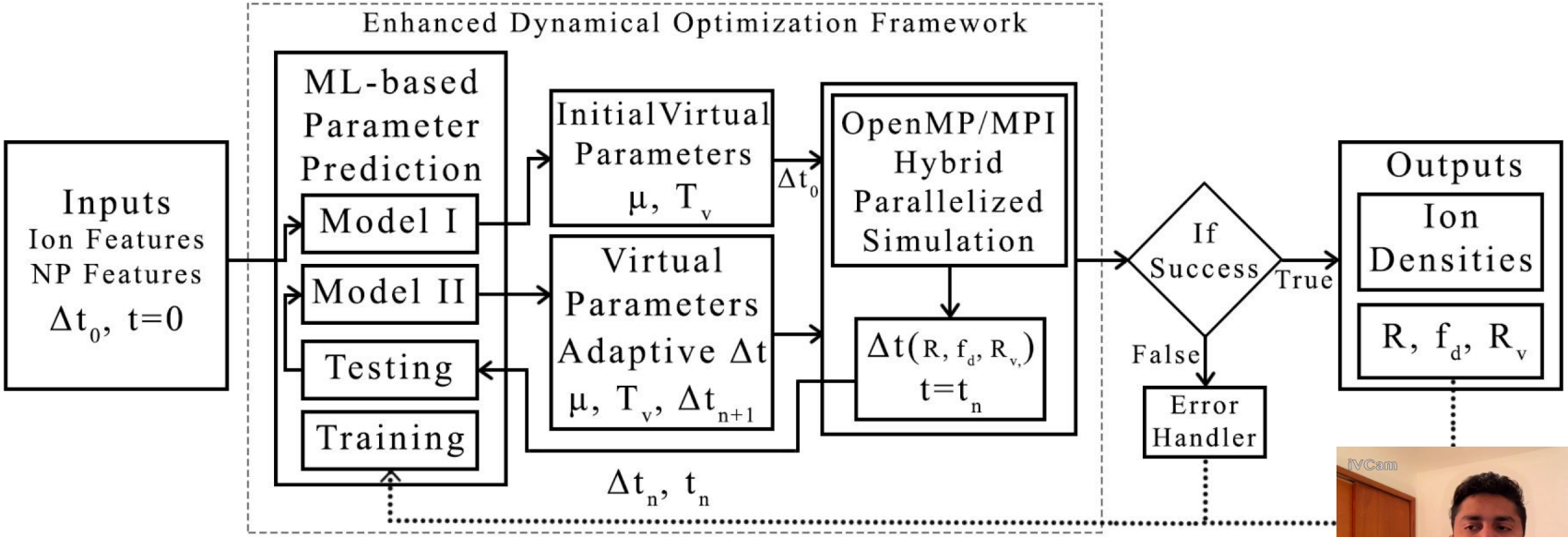
Dynamical optimization framework



The electrostatic problem is solv
fly and this framework is imple
using Car-Parrinello molecular d
(CPMD)

ML-based selection and auto-tuning of virtual parameters in CPMD

- Previously, tedious process of trial and error is involved to find the virtual parameters in CPMD
- We apply ML to select and auto-tune the virtual parameters in CPMD method



Nanosphere Electrostatics Lab

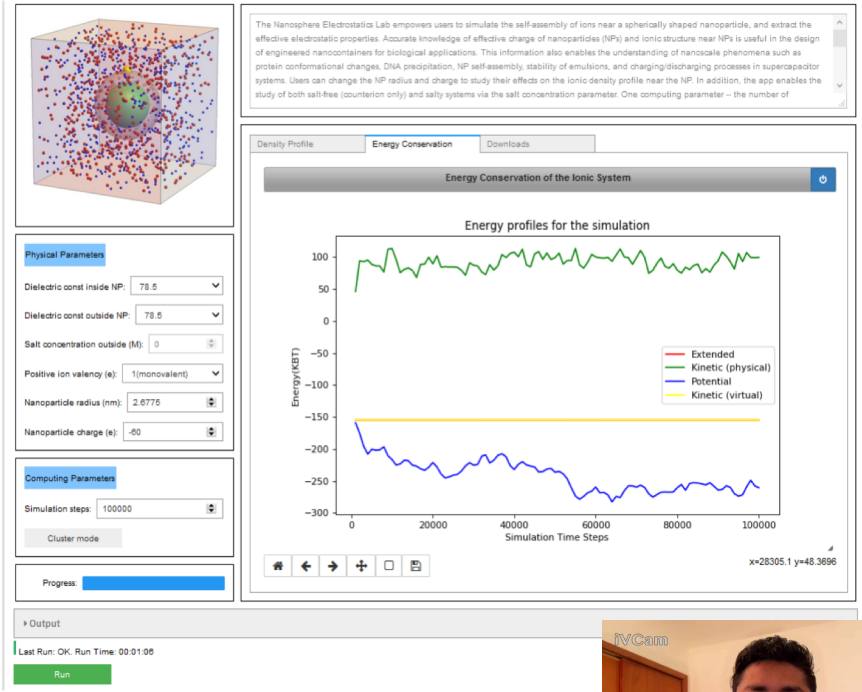
- Frontend: Jupyter
- Backend: C++
- OpenMP/MPI Hybrid parallelized
- Open source on github

Input parameters

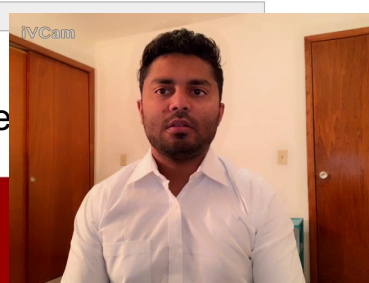
1. Dielectric const inside NP: (2, 78.5)
2. Dielectric const outside NP: (78.5)
3. Salt concentration outside (M): (0)
4. Positive ion valency (e): (1, 2, 3)
5. Nanoparticle radius (nm): (2.6775)
6. Nanoparticle charge (e): (-60)

Outputs

1. Positive/Negative density profiles
2. Energy conservation
3. Movie file of the simulation



https://nanohub.org/tools/nse



Demo of Nanosphere Electrostatics Lab

nanoHUB.org - Members: Vie | npelectrostatics | npelectrostatics

https://nanohub.org/members/184552

Home › Members › JCS Kadupitiya › Dashboard

JCS Kadupitiya

Public Profile :: Your profile is currently public.

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All Projects | New Project

Nano Confinement
By me | manager

MY SESSIONS

Workspace

LAST ACCESSED:
October 02, 2019 @ 12:04am

Open | Terminate

Jupyter Notebook with anaconda 5.1

Ions in Nanoconfinement

Nanosphere Electrostatics Lab

Nanosphere Electrostatics Lab (12:22 am)

Storage (manage)

66% of 10GB

MY TOOLS

Recent | Favorites | All Tools

electro

Dualfoil.py: Porous Electrochemistry for Rechargeable Batteries

Electrochemical Simulation

ElectroMat

Electron Magnetic Resonance (EMR) in Nanoparticles

Electrostatic Properties Simulatic
Material Devices

Illinois Solid State Electronic Dev

RESOURCES

- Learning Modules

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Conclusion

- The Nanosphere Electrostatics Lab empowers users to simulate the self-assembly of ions near a spherically shaped nanoparticle and extract the effective electrostatic properties.
- In addition, the app enables the study of both salt-free (counterion only) and salty systems via the salt concentration parameter.
- The app was enhanced using a Hybrid MPI/OpenMP parallelization method as well as a machine learning approach designed to automate the evolution of the polarized charges.
- The app is being tested experimentally by measuring zeta potentials of NPs of different radius and bare charge under various ionic conditions; numerical validation has been performed via LAMMPS.

Acknowledgements

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Thank you!