Classical Charged Systems: Breaking symmetries, Building structure

Strongly Coupled Coulomb Systems
July 28, 2025

Lorin Swint Matthews
Center for Astrophysics, Space Physics, and Engineering Research (CASPER)
Baylor University, Waco, TX

Baylor University

Classic Coulomb Interaction

$$\vec{F} = -\nabla\Phi$$

$$\Phi = \frac{1}{4\pi\epsilon_0}\frac{q}{r}$$

Same charged particles, different interaction

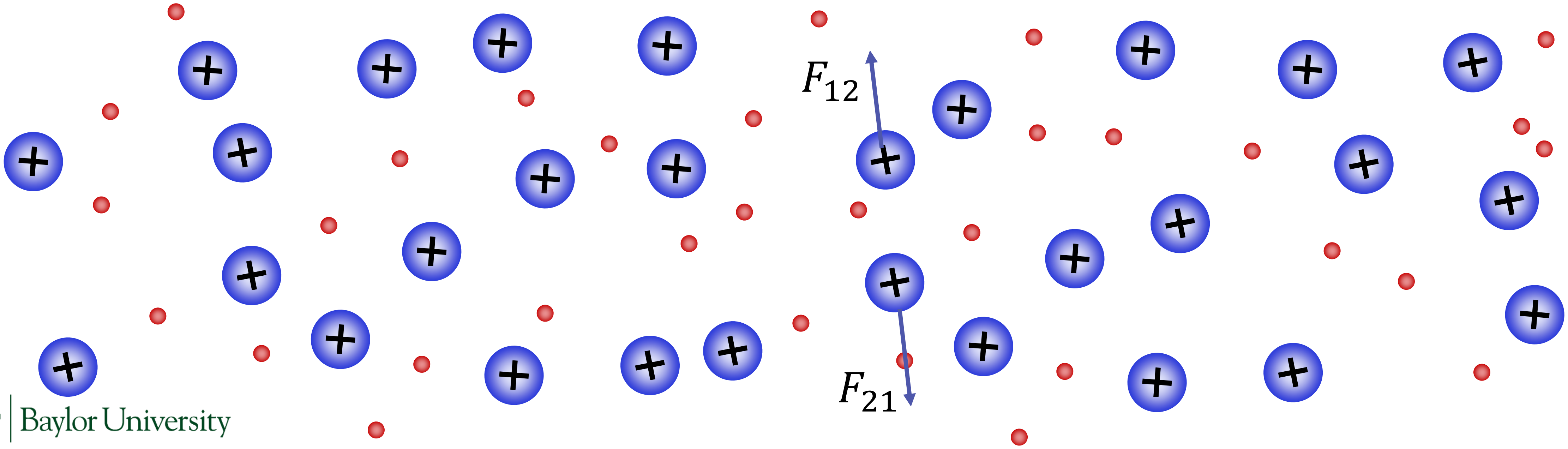
Same charged particles, different interaction

$$\vec{F} = -\nabla\Phi$$

$$\Phi = \frac{1}{4\pi\epsilon_0}\frac{q}{r}\exp\left(-\frac{r}{\lambda}\right)$$

Classical Charged Systems

- Want to examine behavior in a system of many interacting particles
- Key is to understand how all the other particles in the system affect the interaction between two particles



Areas of interest

- Particle diffusion / transport
  - Waves
  - Shocks
  - Instabilities
- Heat diffusion
  - Energy loss in plasmas
  - Thermalization
- Viscosity

Svante Arrhenius

- 1903 Nobel Prize: salts disassociate into paired charged particles (ions) when dissolved
- Since the electrolyte solution is charge neutral and the ions are uniformly distributed, the **average force** acting on each particle is **null**
- But electrostatic interactions ***are*** important to describe strong electrolytes

Image from Wikipedia, public domain

Tamashiro, Levin, & Barbosa, Physica A, 268, 24-49 (1999)

Debye – Hückel Theory 1923

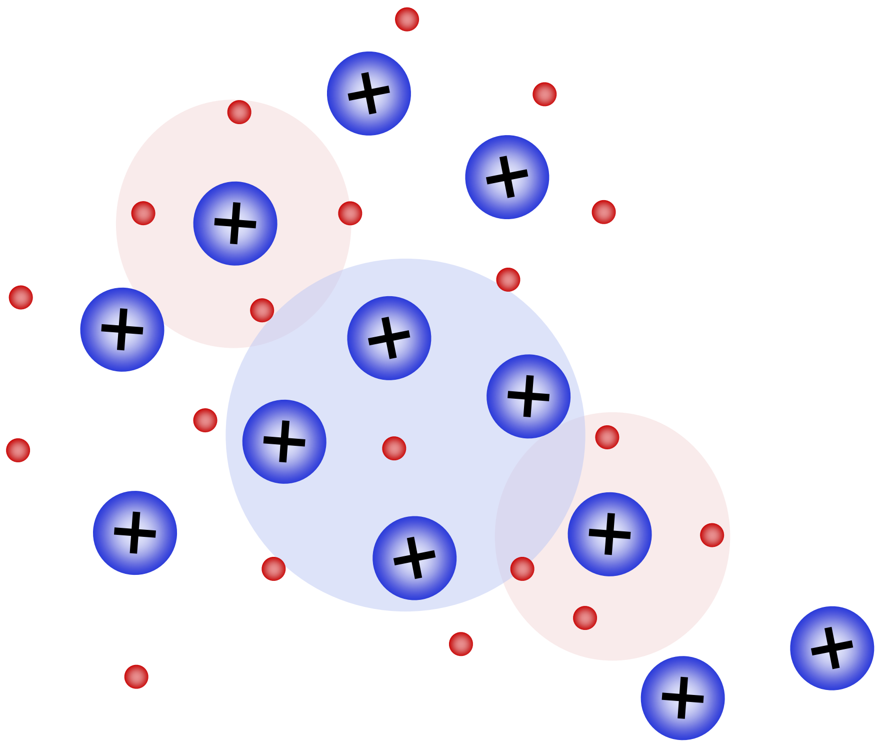
- Explain departures from ideality in electrolytic solutions and plasmas
- Each ion is closely surrounded by ions of opposite charge

$$\Phi = \frac{1}{4\pi\epsilon}\frac{q}{r}\exp\left(-\frac{r}{\lambda}\right)$$

ϵ dielectric constant of media

$$\Phi = \frac{1}{4\pi\epsilon}\frac{q}{r}\frac{\exp\left(\frac{a_0}{\lambda}\right)}{1+\frac{a_0}{\lambda}}\exp\left(-\frac{r}{\lambda}\right)$$

a_0 distance of closest approach between ions



Images from Wikipedia, public domain

Peter Debye

Erich Hückel

Strongly Coupled Coulomb Systems

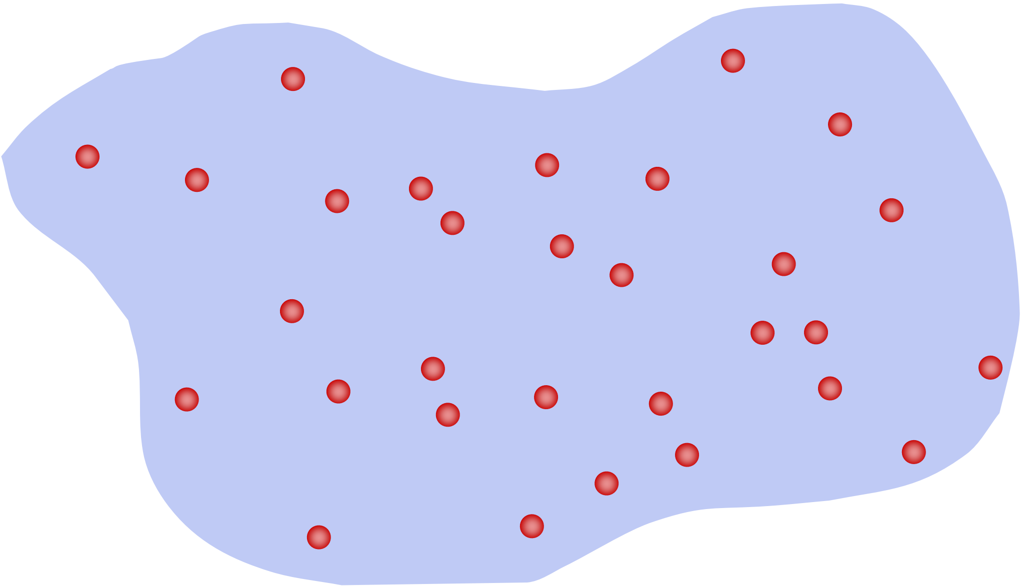
- Describe system behavior when the potential energy is greater than or equal to the thermal energy

$$\Gamma = \frac{q^2}{4\pi\epsilon_0 a_{ws} k_B T} > 1$$

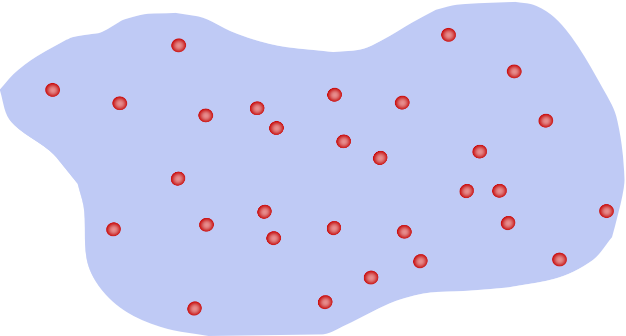
- Strongly coupled systems: potential varies from Debye-Hückel

Simplest System: One Component Plasma (OCP)

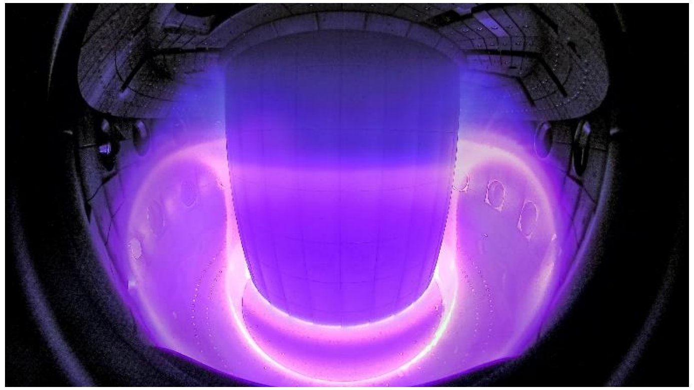
- Model system for strongly coupled atomic plasmas
- N identical particles
- Neutralizing background



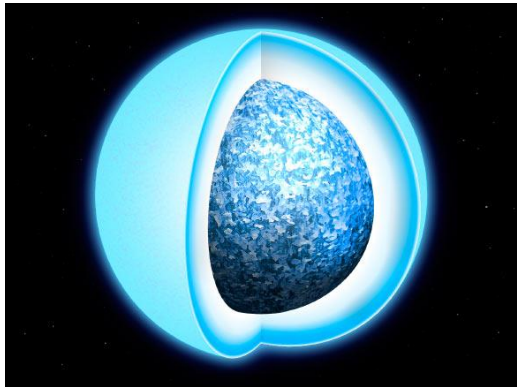
Simplest System:
One Component Plasma (OCP)



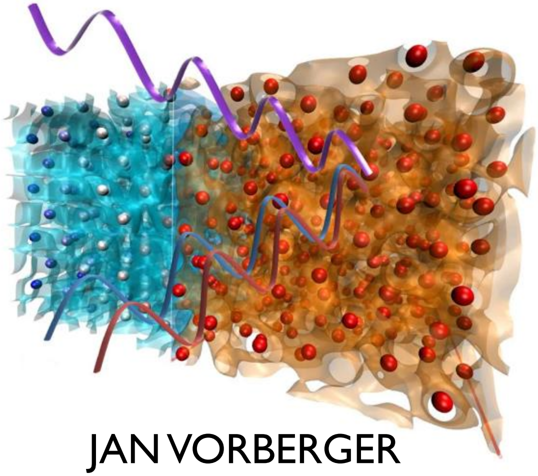
- Equation of state
- Collective modes
- Transport properties
- Viscosity
- Energy deposition



GURDIN WÜTHRICH, SPC/EPFL



MARK GARLICK / UNIVERSITY OF WARWICK



JAN VORBERGER

Early Applications of OCP

- Correlation function

$$g(r) = n(r)/n$$

- Potential energy

$$U = \Sigma_{i<j}^{N} \phi(r_i, r_j)$$

- Average U

$$\frac{\langle U \rangle}{\mathrm{NkT}} = \frac{2\pi n}{kT} \int_0^\infty \phi(r) g(r) r^2 dr$$

- Pressure

$$\frac{PV}{NkT} = 1 - \frac{2n}{3kT} \int_0^\infty r^3 g(r) \frac{d\phi(r)}{dr} dr$$

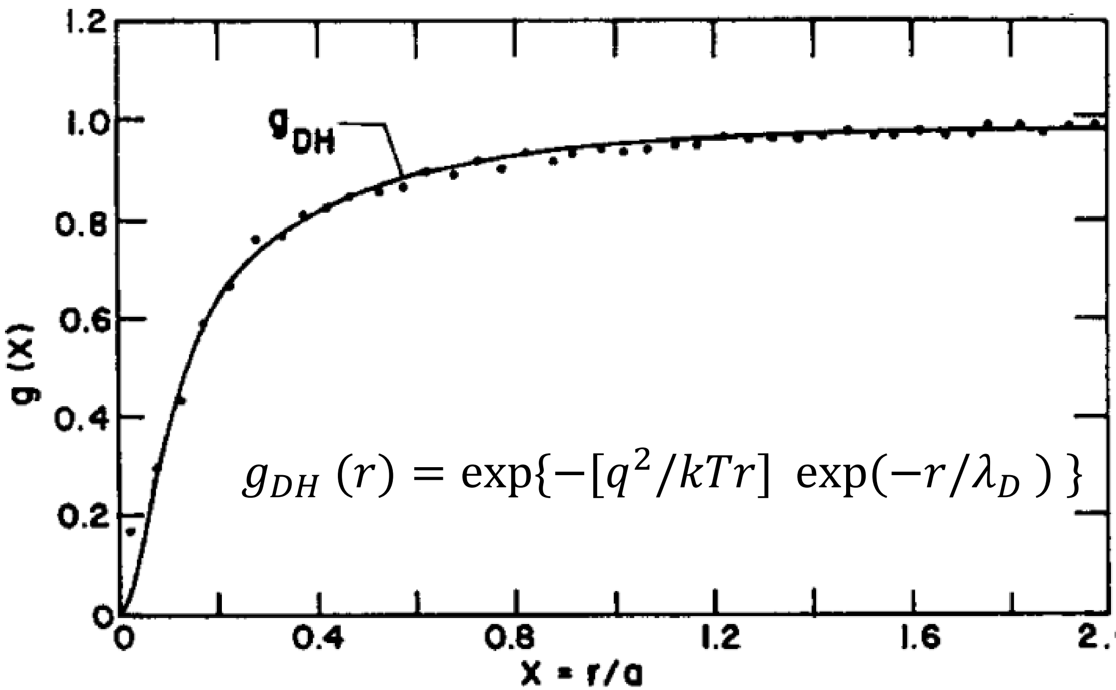


FIG. 6. Comparison of the MC and DH radial distribution functions $g(x)$ at $\Gamma=0.1$ for $N=108$. ●, Monte Carlo.

Brush, Sahlin, Teller, J Chemical Physics 45, 2102-2118 (1966)

Early Applications of OCP

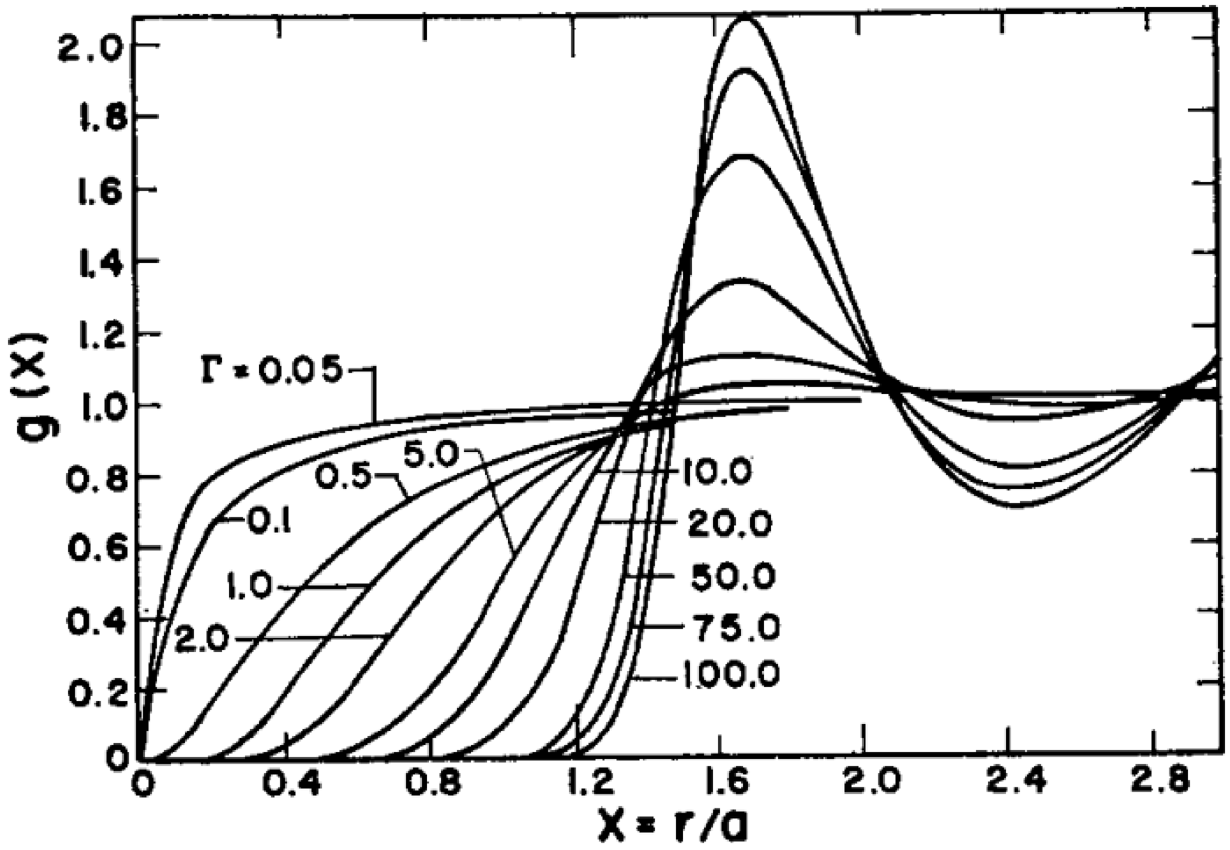


FIG. 5. Radial distribution functions $g(x)$ for $0.05 \leq \Gamma \leq 100.0$.

Brush, Sahlin, Teller, J Chemical Physics 45, 2102-2118 (1966)

Predicted phase transition for $\Gamma = 168$

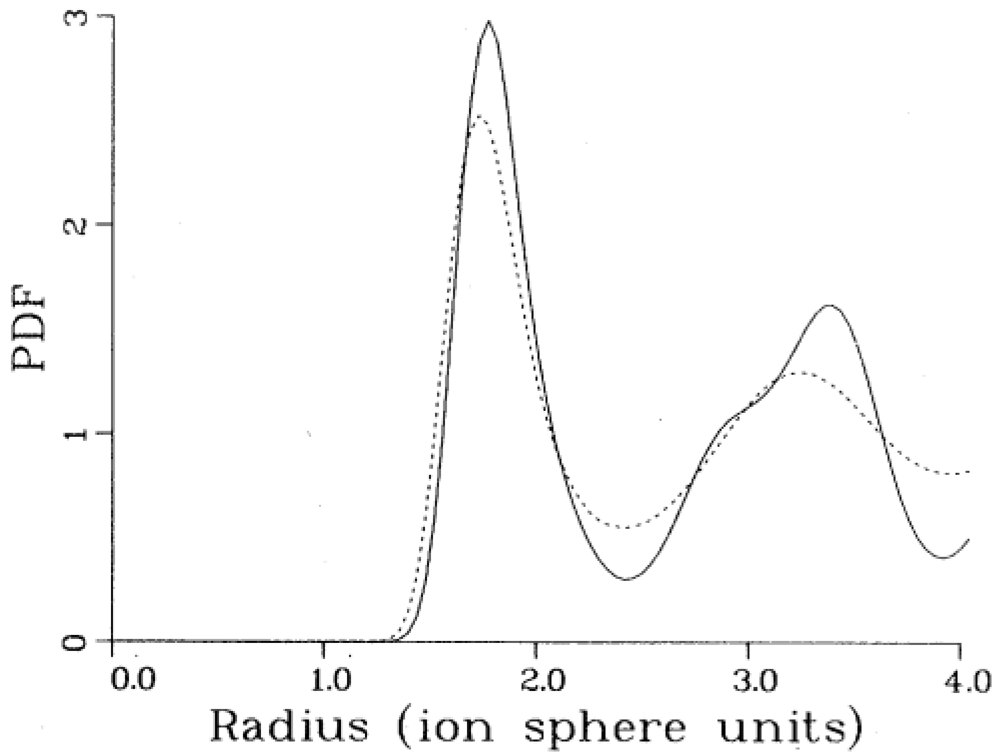


FIG. 1. Pair distribution functions for the liquid (dashed curve) and the solid (solid curve) for $\Gamma = 180$.

Slattery, Doolen, DeWitt Phys Rev A 21(6), 2087 (1980)

Current applications of OCP

- Modifications of Debye-Hückel interaction potential
- Molecular gases
- Anisotropies in density, velocity, temperature

Bremsstrahlung Radiation in the Strongly Coupled Limit

- Binary collisions modeled via the "potential of mean force"

$$\overline{\boldsymbol{F}}_i^n(\vec{r}) = \boldsymbol{F}_i^{ext} + \sum_{\substack{j=1 \\ j\neq i}}^{n} \boldsymbol{F}_{ij}^C + \int \boldsymbol{F}_{i,n+1}^C \frac{\rho^{(n+1)}(\boldsymbol{r}^{n+1})}{\rho^n(\boldsymbol{r}^n)} d\boldsymbol{r}_{n+1}$$

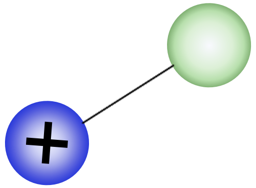
Baalrud and Daligault, Phys. Plasmas 26, 082106 (2019)

- Potential of mean force:

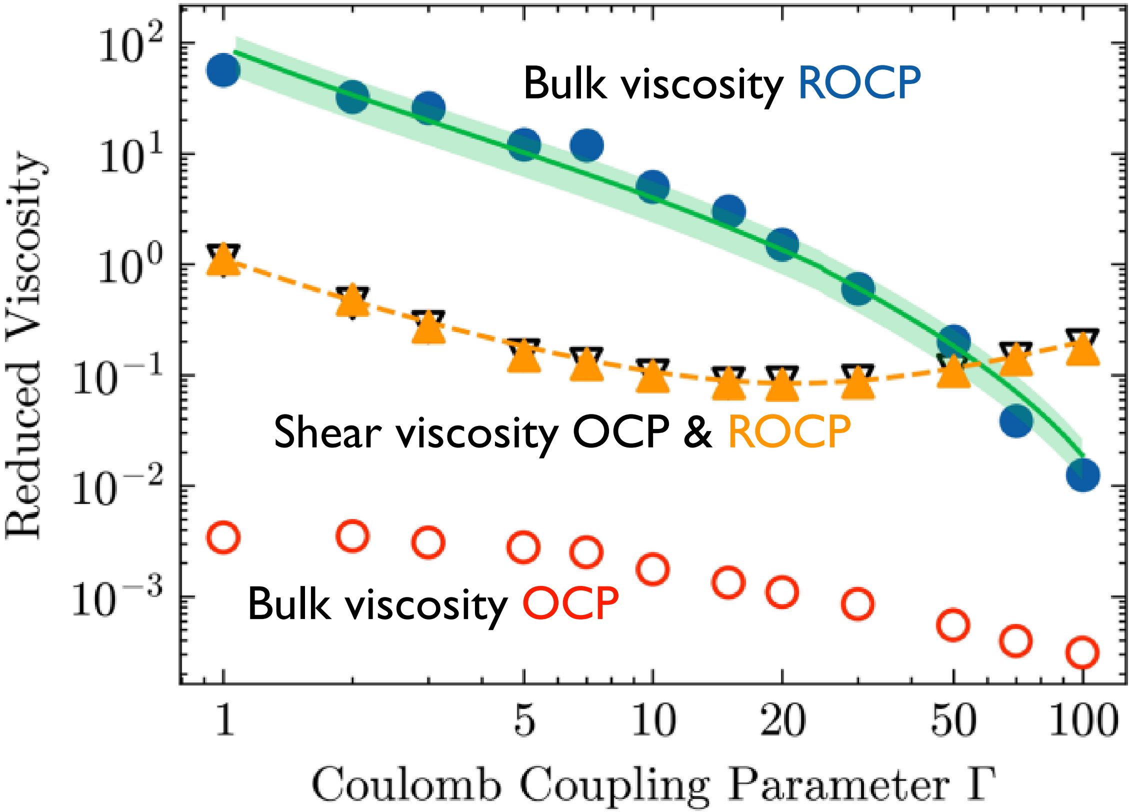
$$w^n(\boldsymbol{r}^n) = -k_b T ln\left[\frac{\rho^{(n)}(\boldsymbol{r}^n)}{\rho^n}\right]$$

Scott Baalrud, Monday 10:10 am

Effect of molecular ions



- Rigid rotor OCP (ROCP): neutral atom bonded to an ion
- Bulk viscosity of OCP is small compared to shear viscosity
- For a rigid rotor one component plasma (ROCP), the bulk viscosity can exceed shear viscosity by several orders of magnitude
- Include bulk viscosity in fluid simulations of turbulence, shock waves, instabilities



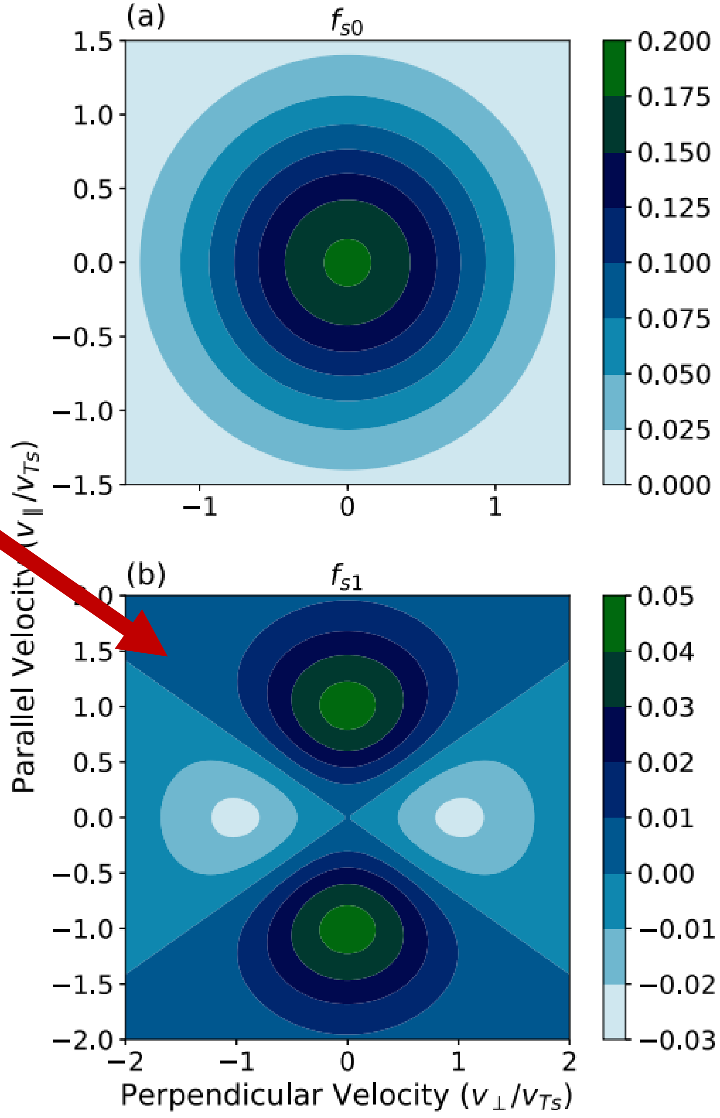
Levan, Acciarri, and Baalrud, Phys Rev E 110, 015208 (2024)

Jarett Levan, Monday 9:30 am

Magnetization

Jose, Welch, Tharp, and Baalrud, Phys Rev E 111, 035201 (2025)

- Differences in relaxation times in parallel and perpendicular directions
- Introduces anisotropies in temperature and velocity distributions
- Affects screening factors and collisions rates → fusion processes

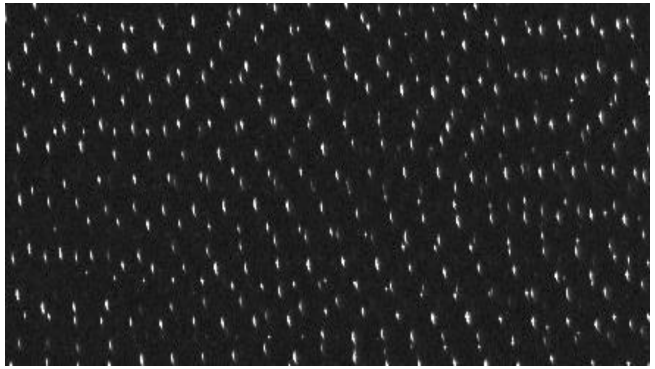


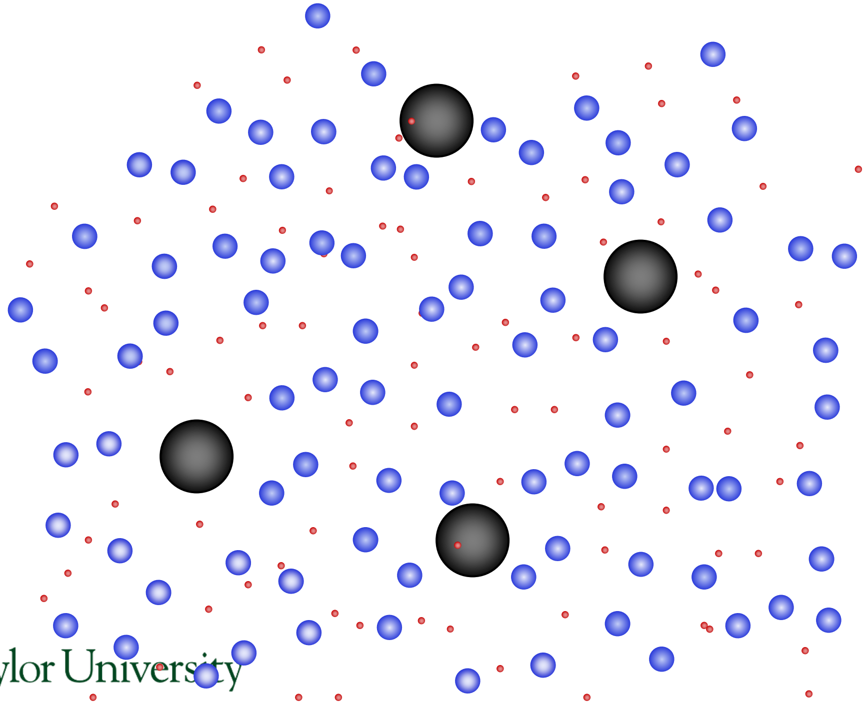
Louis Jose, Monday, 9:50 am

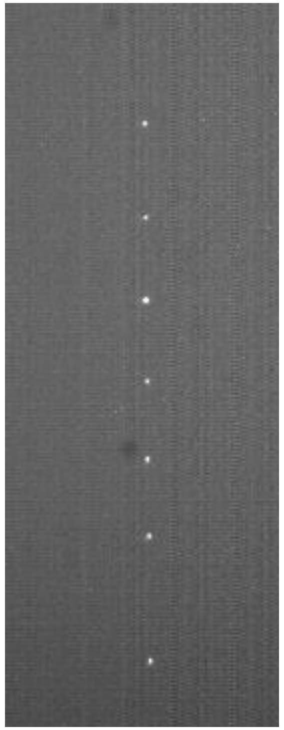
www.baylor.edu/CASPER

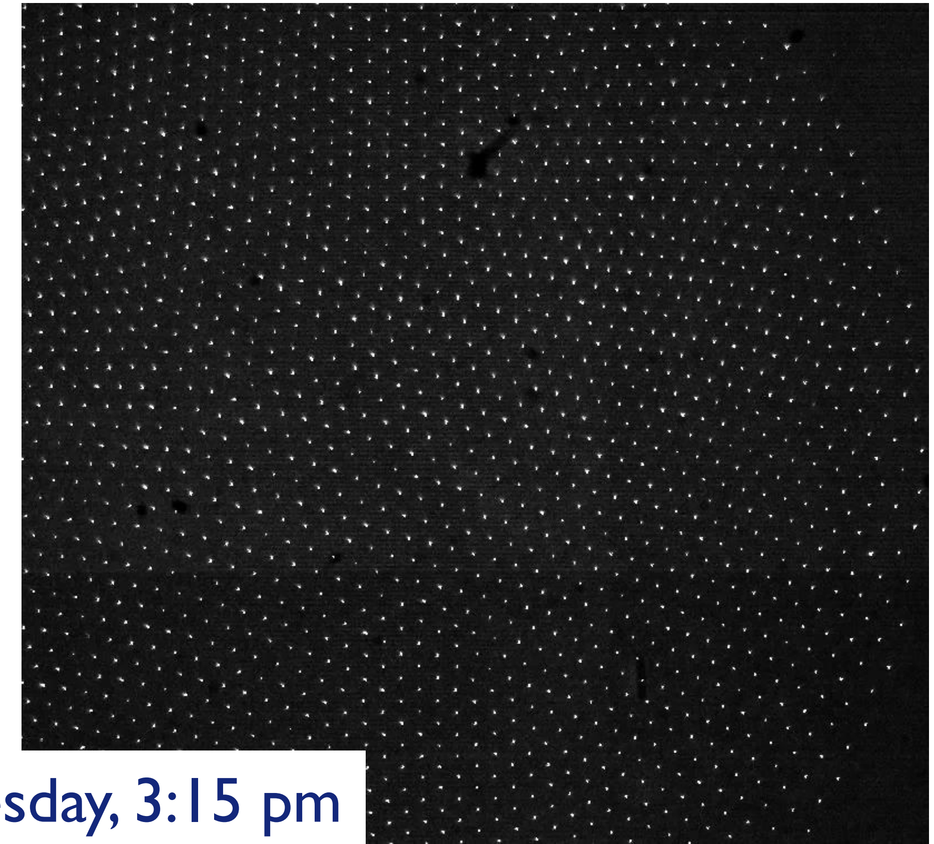
Dusty Plasmas

- Useful analog for atomic systems
- Dust is easily imaged
- Dynamics tracked at molecular level
- Self organization and stability





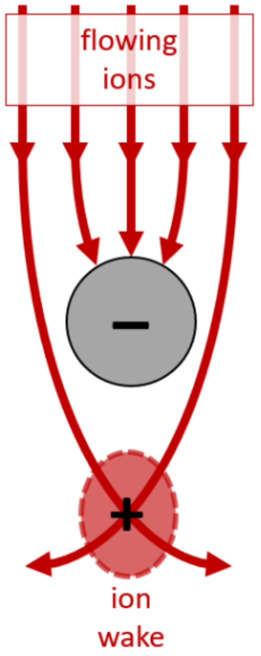


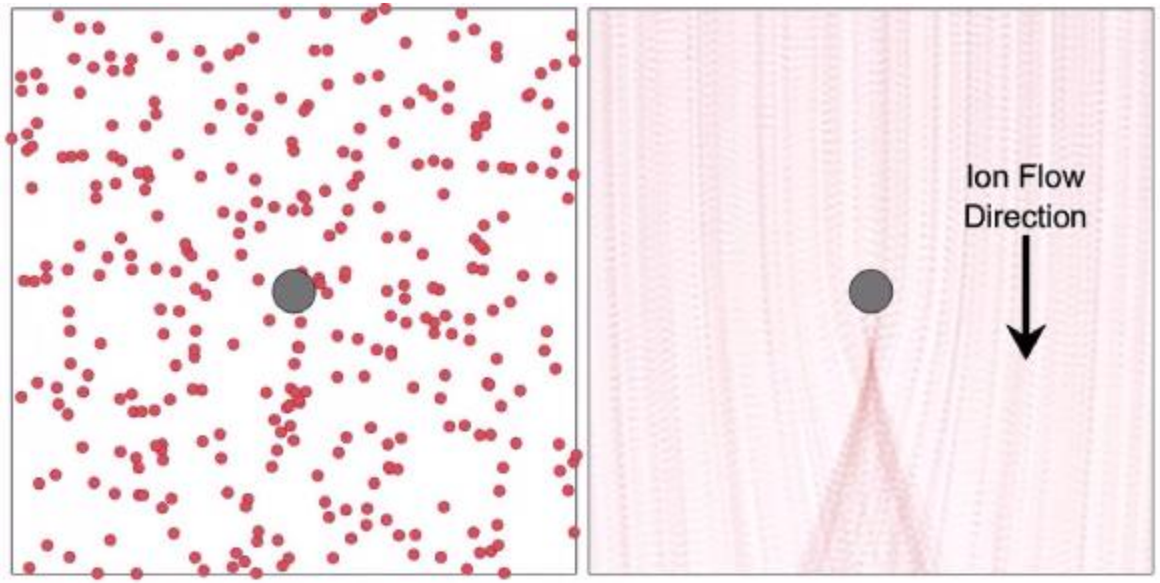


Peter Hartmann, Tuesday, 3:15 pm

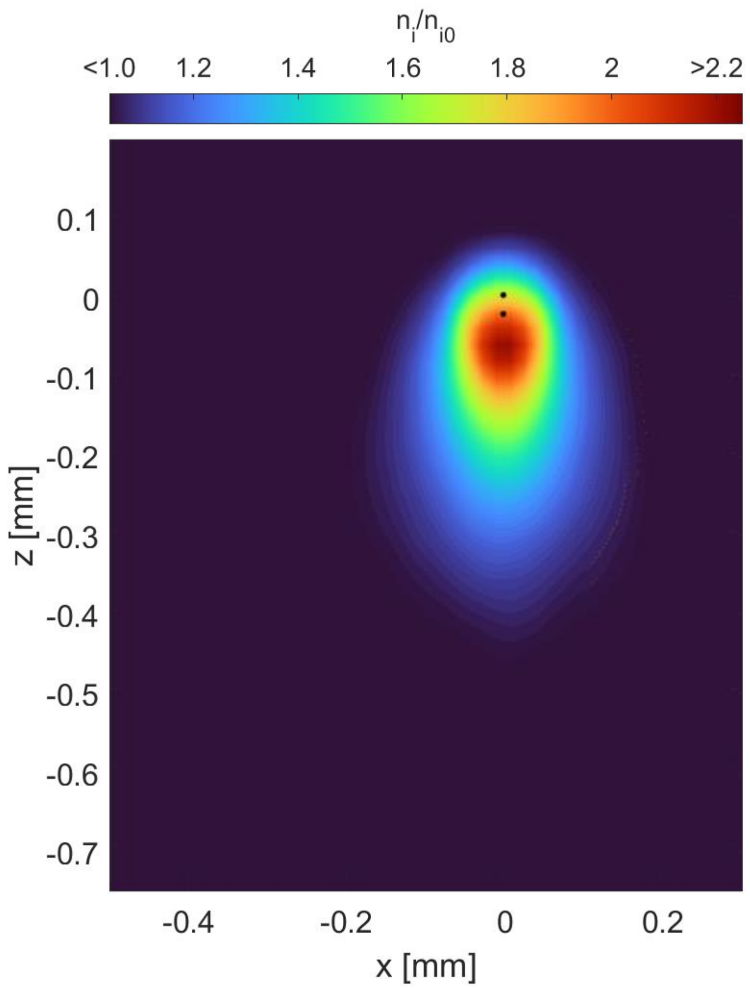
Ion Wakes

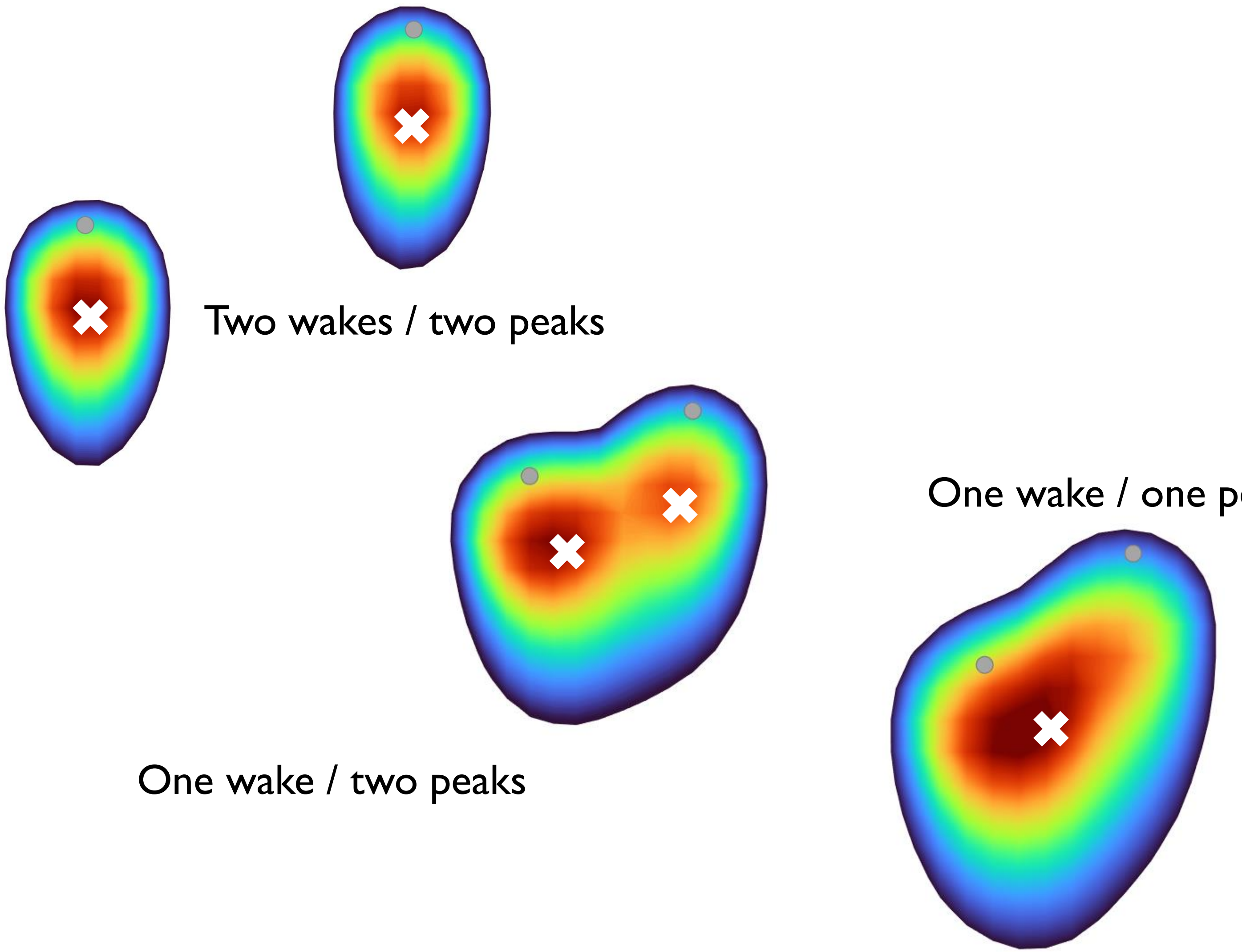
- Accumulation of positive charge density
  - depends on:
    - dust grain charge
    - ion flow speed
    - presence of additional dust grains





Interacting wakes





Dust and Wake Potential: 2 Dust Grains

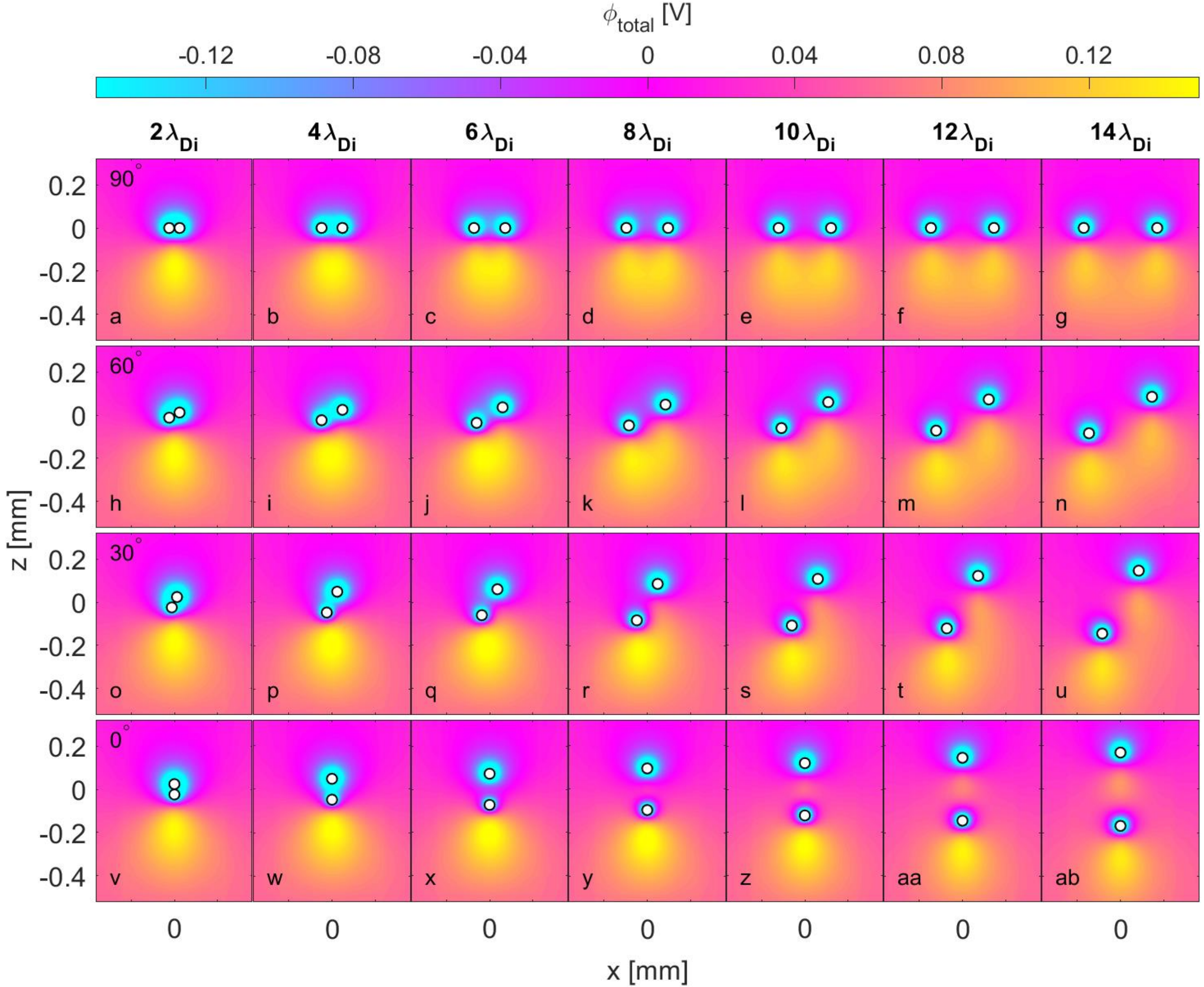
Physics of Plasmas

AIP Publishing

Vol. 31, Iss. 7, Jul. 2024

Interacting dust grains in complex plasmas: Ion wake formation and the electric potential

K. Vermillion, R. Banka, A. Mendoza, B. Wyatt, L. Matthews, and T. Hyde

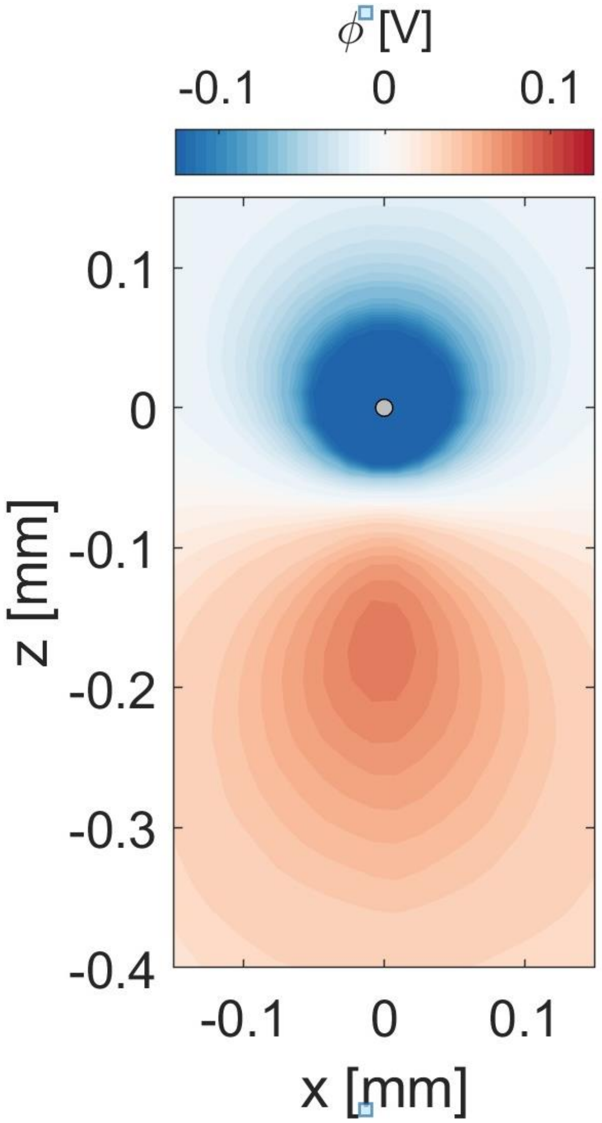


Electric Potential of Dust + Wake

- $\phi = \phi_{dust} + \phi_{wake}$

ϕ_{dust}

- $\phi_{dust}(r,\theta) = \frac{Q_d}{4\pi\epsilon_0 r}\exp\left[\frac{-r}{\lambda}\right]$

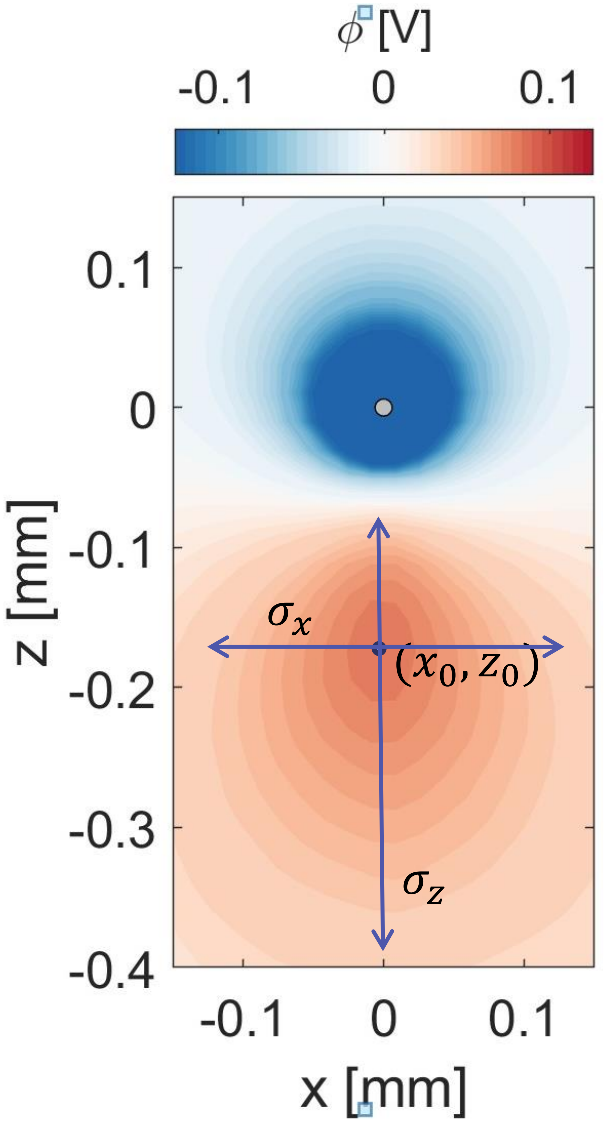


Electric Potential of Dust + Wake

- $\phi = \phi_{dust} + \phi_{wake}$

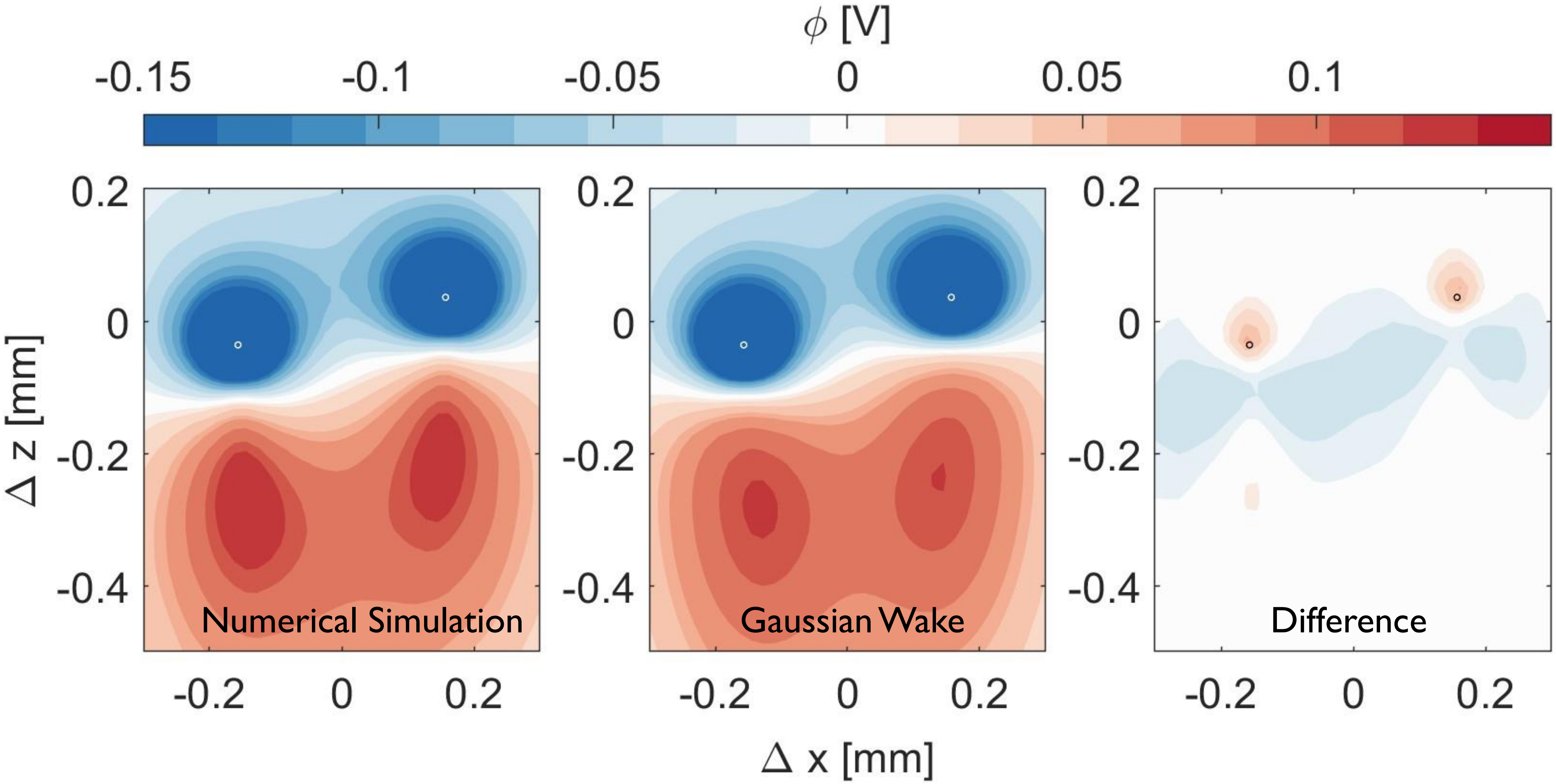
ϕ_{wake}

- $\phi_{wake} = \frac{\alpha Q_d}{4\pi\epsilon_0 \lambda_{De} M^2} \exp[\beta(x,z)]$
- $\beta(x,z) = -a(x - x_0)^2 - 2b(x - x_0)(z - z_0) - c(z - z_0)^2$
- $a = \frac{\cos^2\theta}{2\sigma_x^2} + \frac{\sin^2\theta}{2\sigma_z^2}$
- $b = -\frac{\sin 2\theta}{4\sigma_x^2} + \frac{\sin 2\theta}{2\sigma_z^2}$
- $c = \frac{\sin^2\theta}{2\sigma_x^2} + \frac{\cos^2\theta}{2\sigma_z^2}$

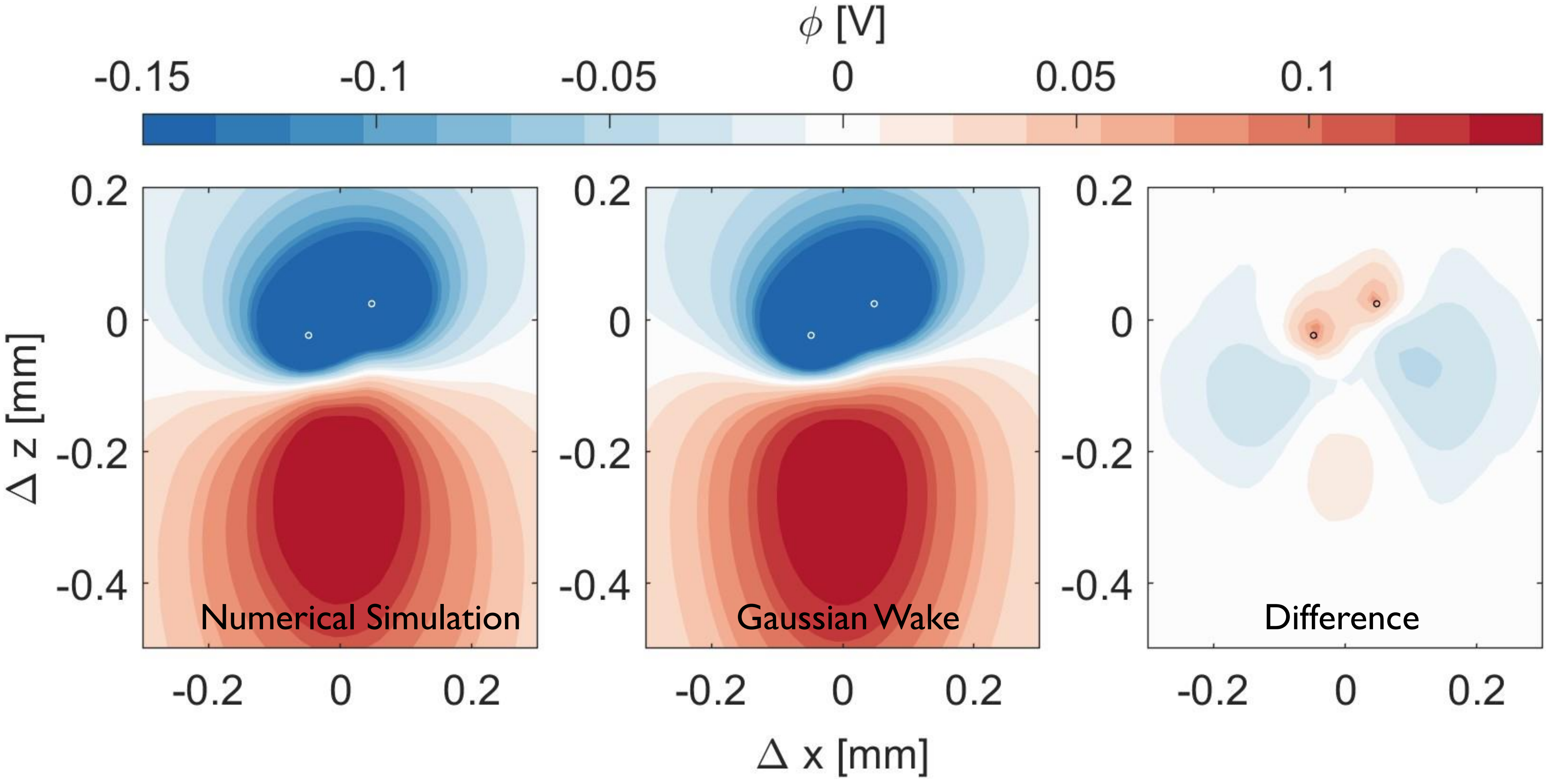


Diana Jimenez, Thursday poster

Comparison of Results



Comparison of Results



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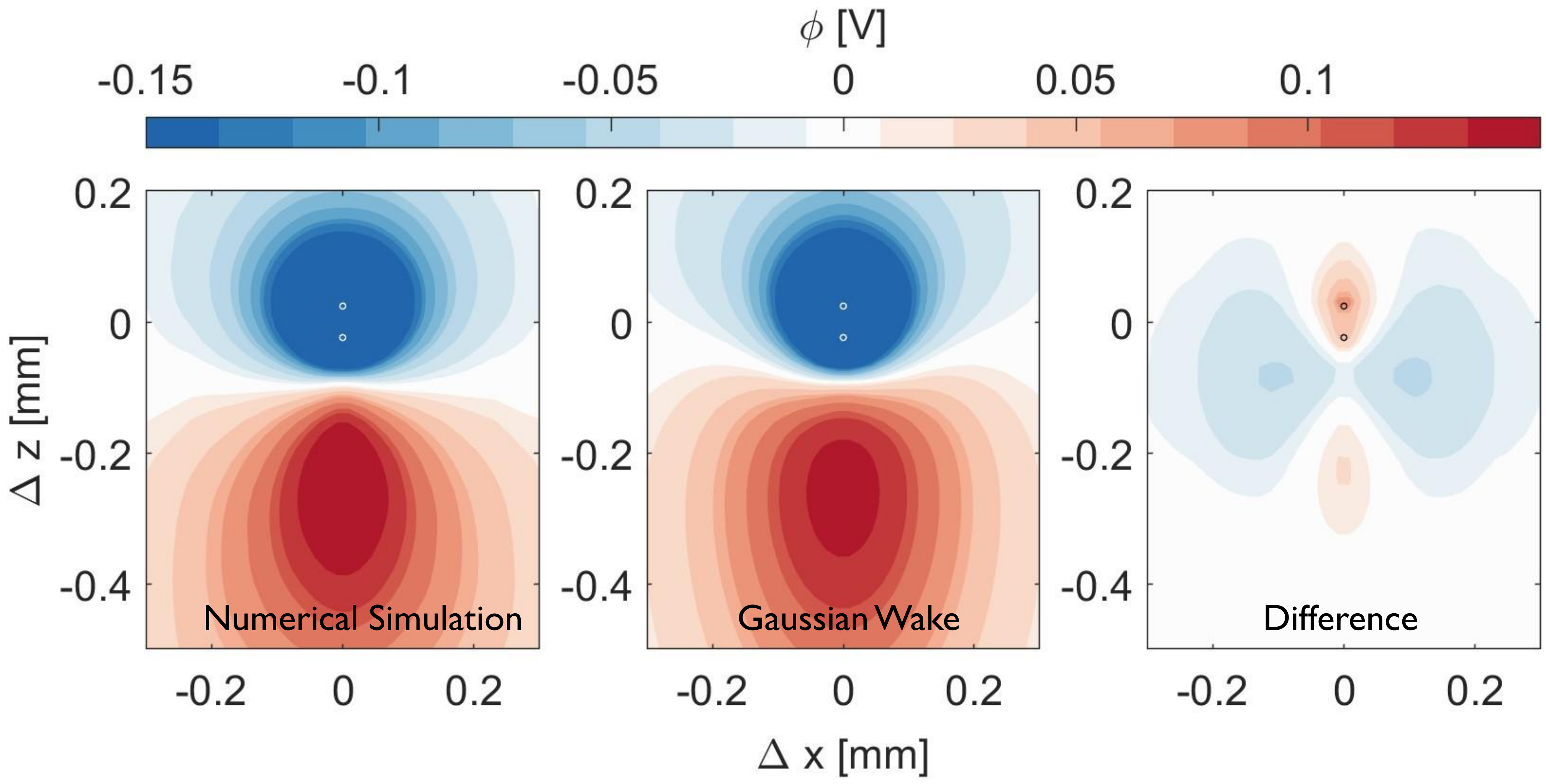
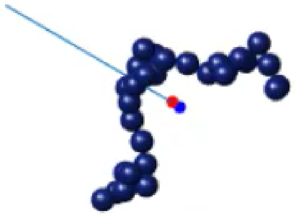
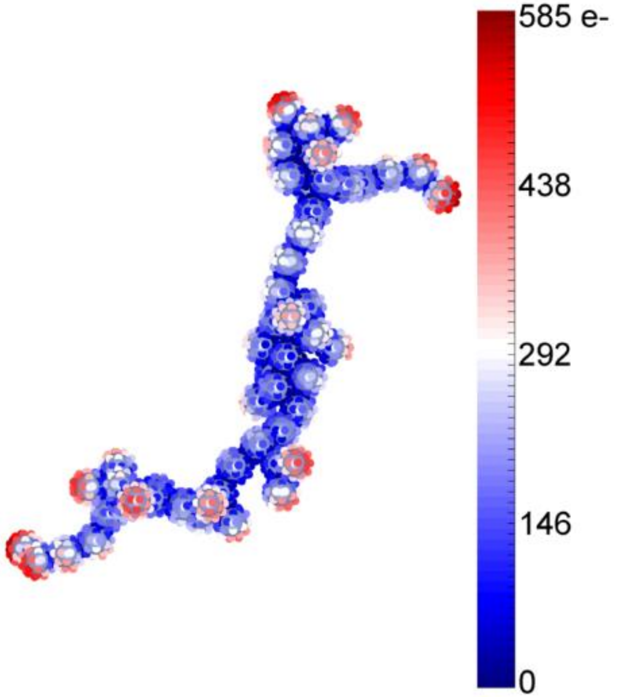


"Natural" Dusty plasmas

- Aggregate, irregular grains
- Charge dipole
- Modified wakes
- Altered transport





Benny Saenz, Thursday poster

Back to Chemistry: Colloidal Particles in Electrolyte Solutions

- Stability of colloidal particles in solution depends on surface charge
- which in turn depends on pH and salt concentration.
- Complex systems require computational approach

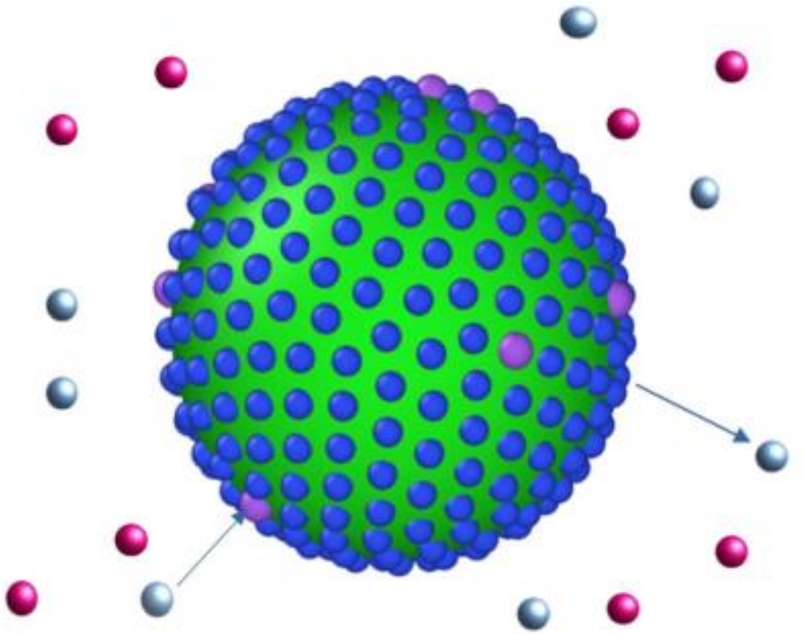


Fig. 2 A colloidal particle inside the simulation cell. The blue sites are protonated. The gray spheres are the hydronium ions. The arrows indicate protonation/deprotonation moves.

Bakhshandeh & Levin, Phys. Chem. Chem. Phys., 2023, 25, 32800–32806

Back to Chemistry: Colloidal Particles in Electrolyte Solutions

- Potential of colloidal particle

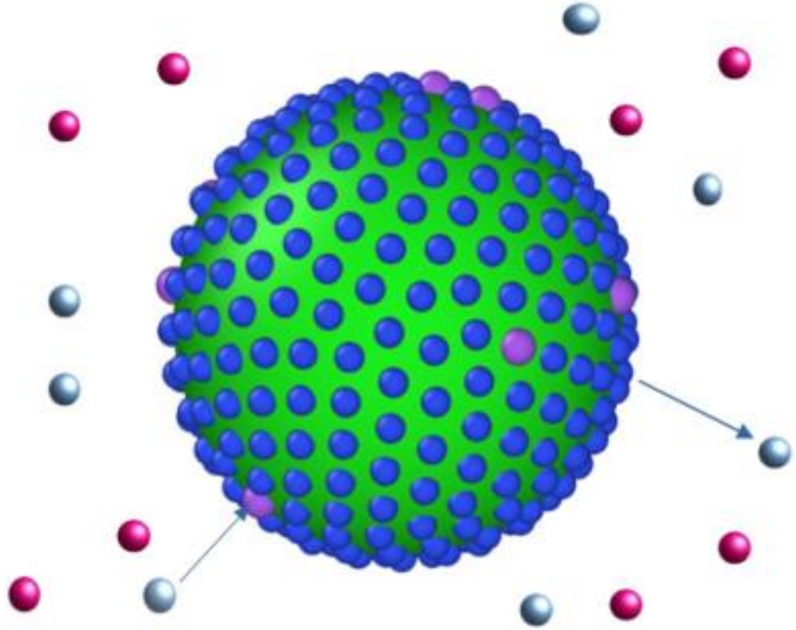
$$\varphi(\boldsymbol{r}) = \sum_{k=0}^{\infty} \sum_{j=1}^{N} \frac{4\pi q^j}{\epsilon_w V|\boldsymbol{k}|^2} \exp\left[-\frac{|\boldsymbol{k}|^2}{4\kappa_e^2} + i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}^j)\right]$$

$$+ \sum_{j=1}^{N} \sum_{\boldsymbol{n}} q^j \frac{\operatorname{erfc}(\kappa_e|\boldsymbol{r}-\boldsymbol{r}^j-L\boldsymbol{n}|)}{\epsilon_w|\boldsymbol{r}-\boldsymbol{r}^j-L\boldsymbol{n}|}$$

$$+ \frac{1}{V}\sum_{k=0}^{\infty} \tilde{\varphi}_b(\boldsymbol{k}) \exp[i\boldsymbol{k}\cdot\boldsymbol{r}],$$

Long + Short range interactions

Neutralizing background



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Bakhshandeh & Levin, Phys. Chem. Chem. Phys., 2023, 25, 32800–32806

Distribution of positive and negative ions near colloidal particle

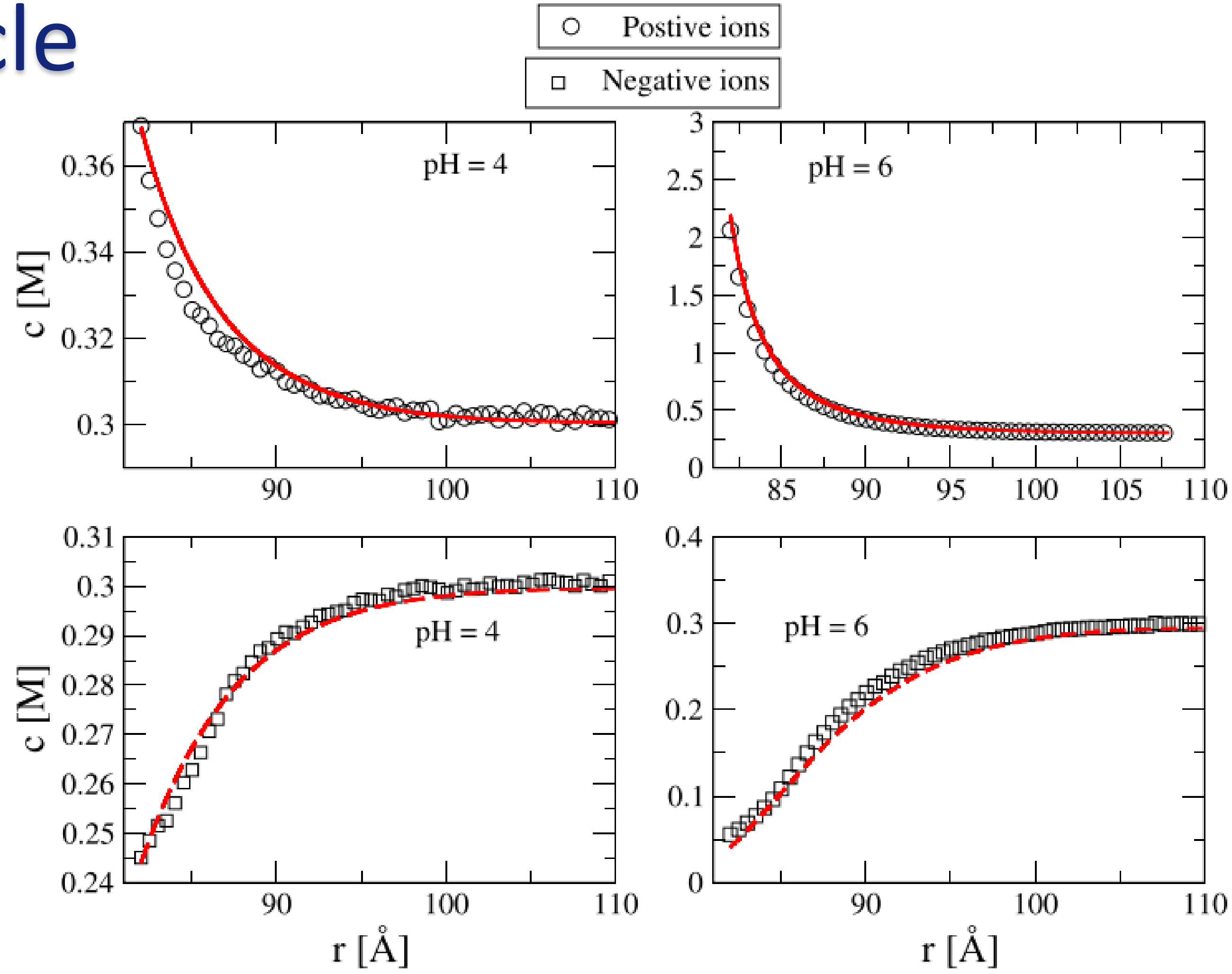


Figure 5. Comparison of ionic density profile for pH 4 and 6 of a colloidal particle with 600 active sites with $K_a = 1/K = 3.95 \times 10^{-6}$ M and radius 80 Å, the concentration of 1:1 salt is 300 mM. Symbols are simulation results and solid curve is the theory.

Bakhshandeh, Frydel, & Levin, Langmuir 2022, 38, 13963−13971

Computational Model

- Each colloidal particle is modeled inside a Wigner-Seitz (WS) cell
- Infinite replication of WS cells to determine long-range electrostatic interaction
- Adding a proton (changes the pH) adds an infinite number of charges – thus the need for the neutralizing background.
- Inserted proton experiences a jump in potential energy (Bethe potential) which changes the pH calculation.

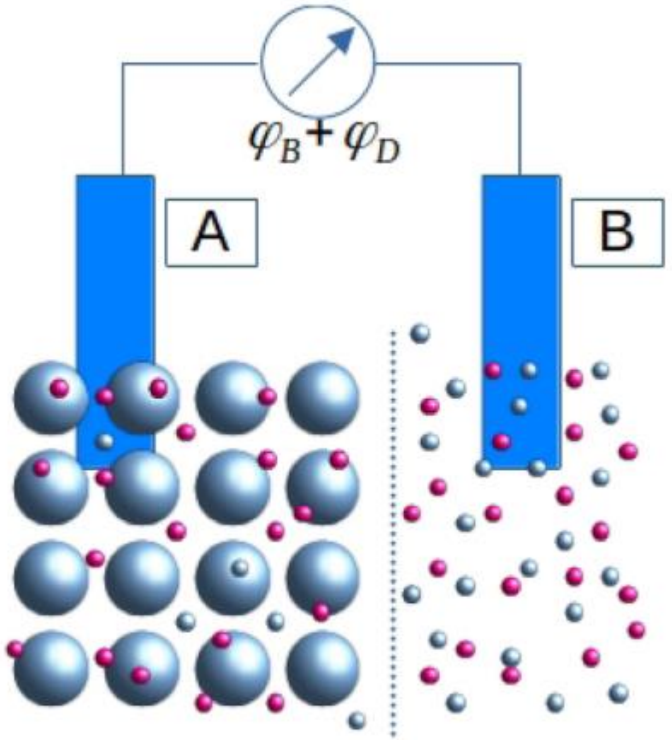
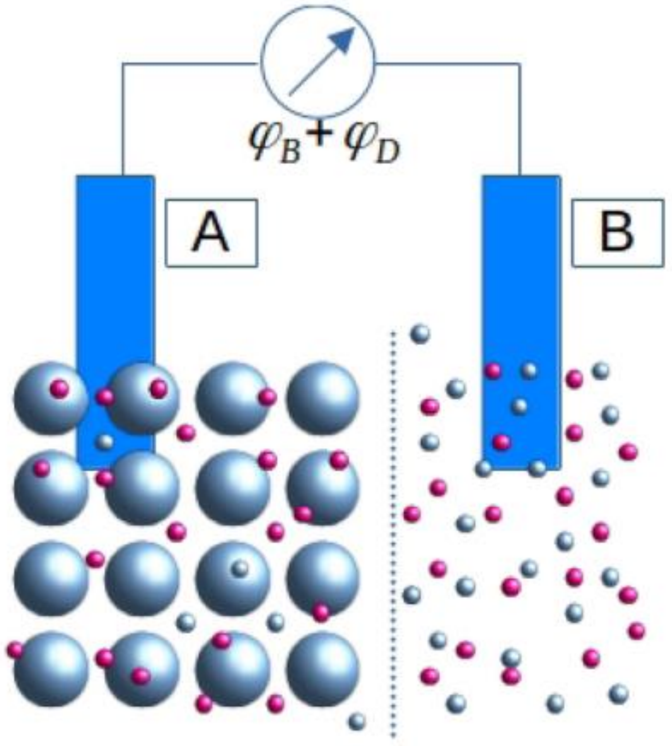


FIG. 2. Periodically replicated system separated from the reservoir by a semi-permeable membrane: the electrostatic potential difference between the two is $\phi_B + \varphi_D$.

Levin & Bakhshandeh, J. Chem. Phys. 159, 111101 (2023)

Computational Model

- Bethe potential - average of the local electrostatic potential inside the periodically replicated crystal
- Donnan potential is the potential drop between the system and the reservoir



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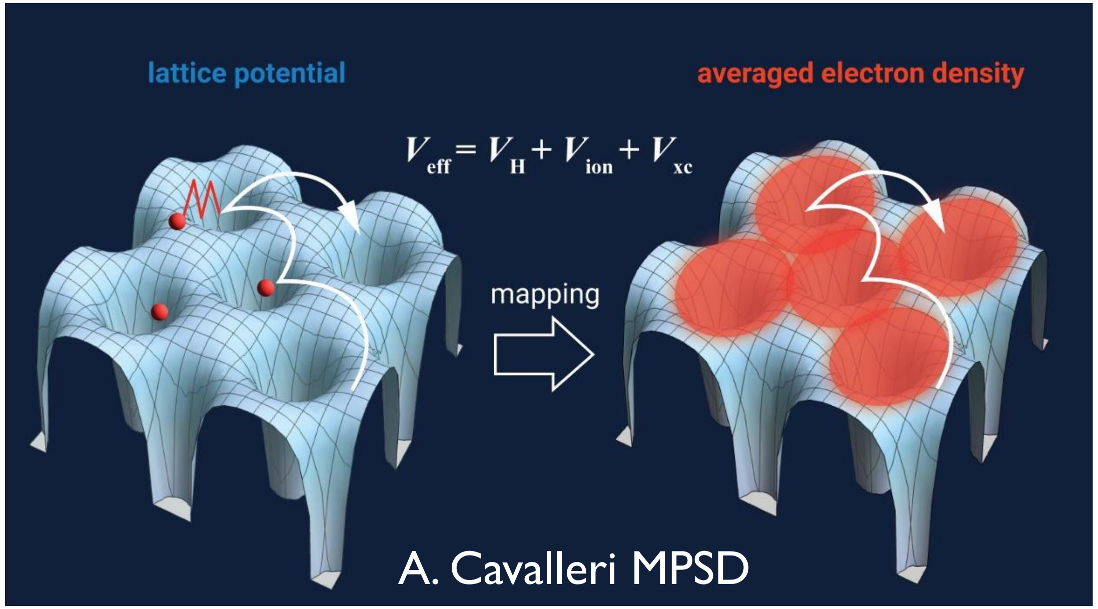
Levin & Bakhshandeh, J. Chem. Phys. 159, 111101 (2023)

Even Higher Densities – Quantum Effects

- Track motion of ions *and*
- Quantum dynamic response of electrons
- Density Functional Theory
- Many body effects
- Temperature dependence



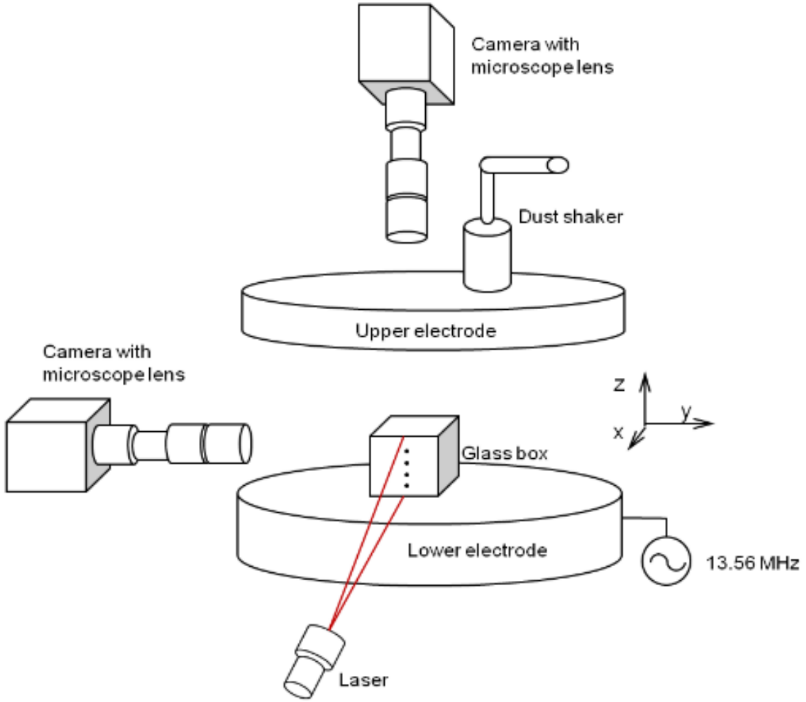
Conclusions

- Challenges remain for classic charged systems!
- Anisotropic shielding
- Anisotropies in distributions
- Multi-components
- Chemistry

THANK YOU

L. Matthews acknowledges support from the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under award number DE-SC0024681, National Science Foundation under award number 2308743, and NVIDIA Corporate Applied Research Program.

Dust Structures



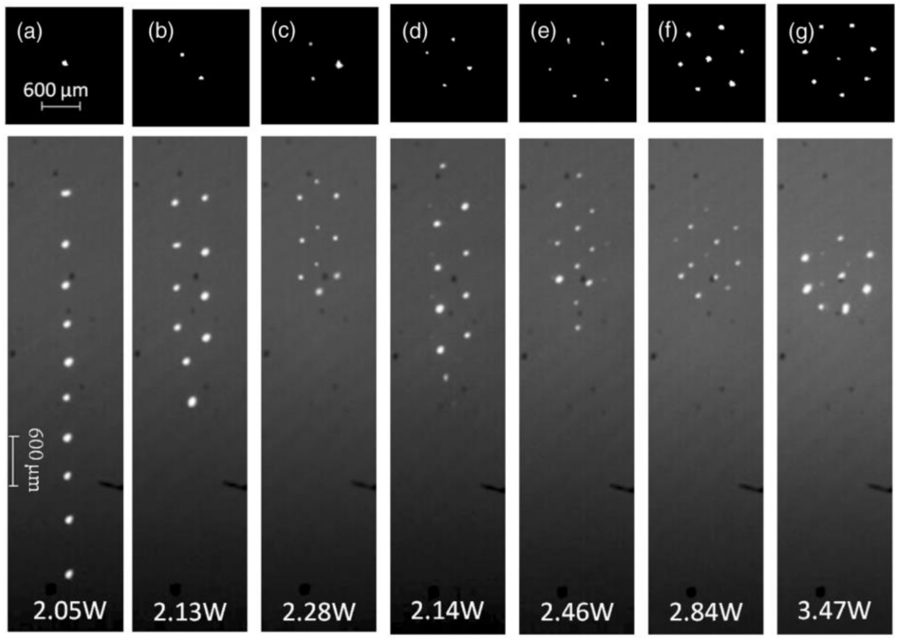
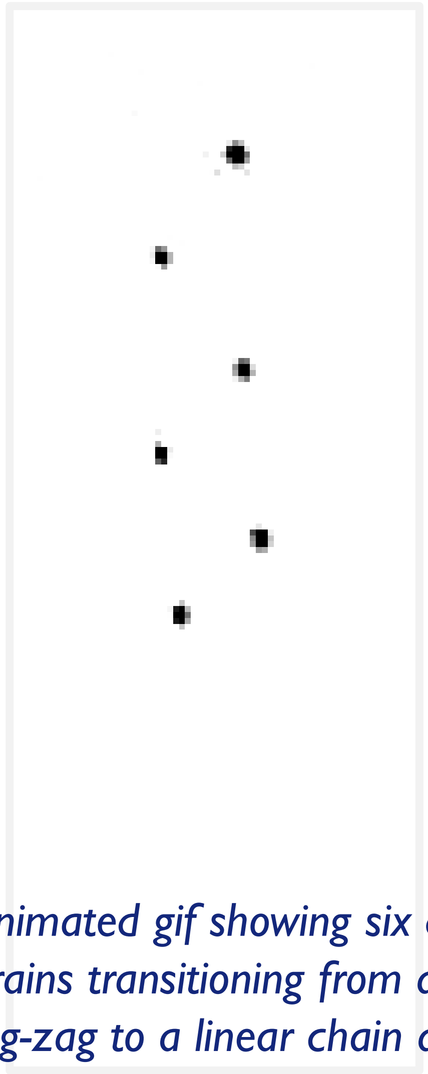


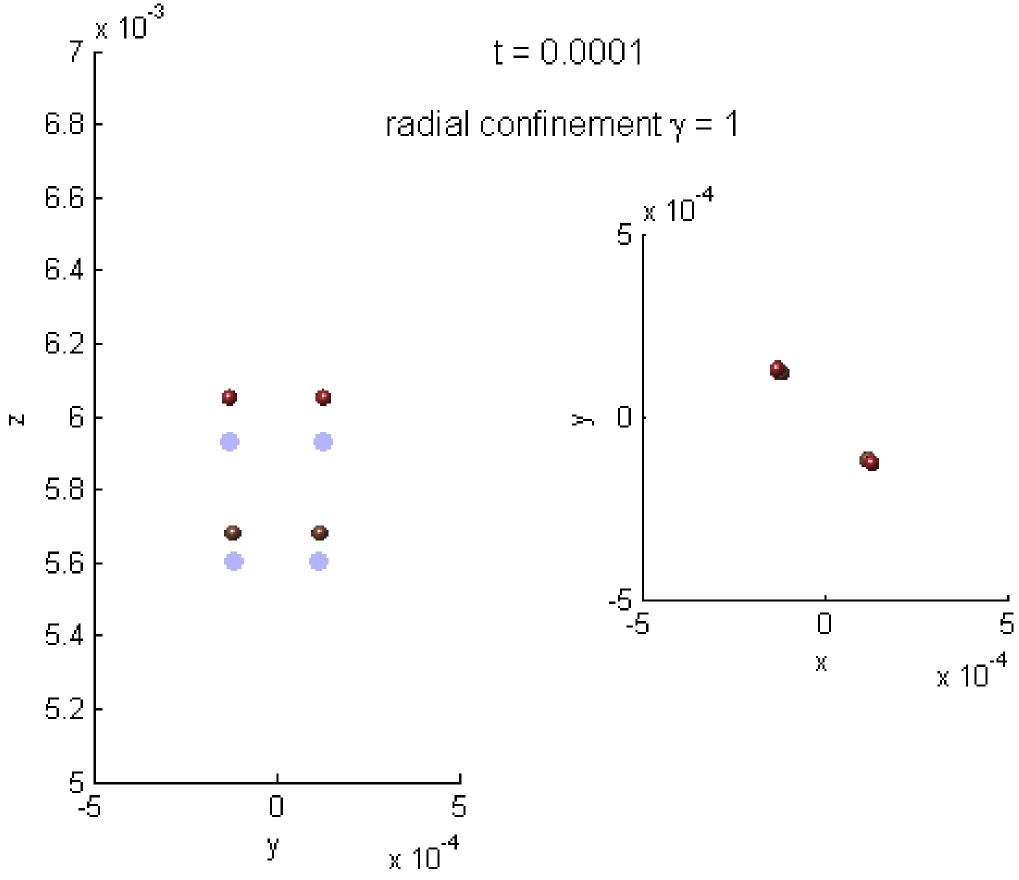
Figure 3 from T. Hyde, J. Kong, L. Matthews (2013) “Helical structures in vertically aligned dust particle chains in a complex plasma” doi: 10.1103/PhysRevE.87.053106



Animated gif showing six dust grains transitioning from a zig-zag to a linear chain and back.

Goal: One-Component Model for Charged Dust Interactions

Colored spheres: dust
Gray cloud: point ion-wake



Animated gif of a simulation of four dust grains with point-wakes transitioning from a double chain to a single linear chain as the radial confinement is increased. The point wake charges and positions are adjusted as dust grains align in the ion flow direction.

Challenges

- Large difference in time scales, distance scales
- diagnostics

- Interaction of particles and their surroundings determine stability and structure
- Easy to imagine for a building – solid objects which are physically touching. Truss – the components of the truss act the same whether the truss is in air or in water, if it is raining (and hopefully) if the wind is blowing.
- What about when the interaction force is Coulombic – particles are not touching? What about when the strength of this interaction depends on conditions in the surrounding medium?
- This has effects on static structures as well as fluid flow

Current topics in dusty plasmas

- Model systems for condensed matter phenomena
  - Phase transitions, lattice formation, density waves
- Dust contamination control in plasma processes
  - Extreme UV lithography, ultra-clean industrial processes
- Magnetic fusion research
- Ionospheric and space dusty plasmas: heliosphere, space-debris, lunar dust, planetary debris disks
- Atmospheric pressure plasmas with aerosols
  - Synthesis of nanoparticles, nitrogen fixation, deactivation of pathogens

- Chaotic dynamics governs the thermalization of the world (existence of heat) – Linda Reichl

Main features of dusty plasmas

- Charged dust
  - OML theory works great, until it doesn't
  - Theory doesn't take into account plasma screening
  - Electron emission, electron screening
- Plasma screening
  - Effect on charging
    - Anisotropic screening in ion flows
- Ion drag force

Conclusions

- New model of ion wake
- Takes into account variations due to the spatial configuration of dust
- Eliminates the singularity in the point-wake model of the ion wake.