Workshop 1: Computational Challenges in Hot Dense Plasmas,
IPAM, UCLA, March 29th 2012

Multiscale Simulation of Streaming Plasmas

Patrick Ludwig[1], Hanno Kählert[1],
Michael Bonitz[1], James Dufty[2]

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[2] University of Florida, USA

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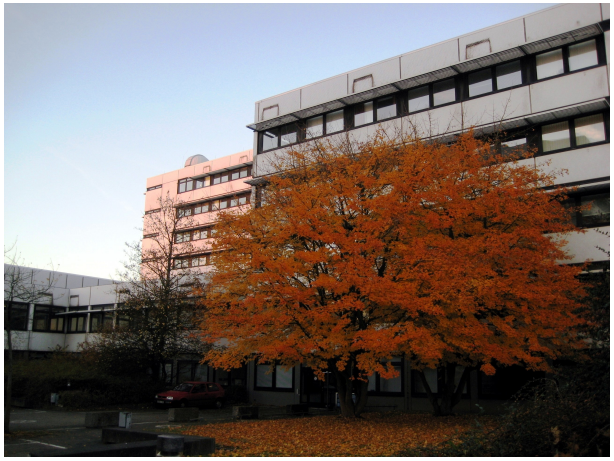
Chair Statistical Physics, CAU Kiel



Christian-Albrechts-Universität zu Kiel
Institut für Theoretische Physik und Astrophysik
Lehrstuhl Statistische Physik
Leibnizstraße 15, 24098 Kiel, Germany

Back from left: L. Filinov*, Lasse Rosenthal, Tim Schoof, Patrick Ludwig, Torben Ott, Hanno Kählert, David Hochstuhl (+ family), H. Kersten**, W. Kraeft**, J. Dufty**, F. Geisler*, Mrs. Kraeft*

Front: Sebastian Bauch, Henning Baumgartner, Karsten Balzer, Hauke Thomsen, Alexej Filinov, Christian Henning, Michael Bonitz

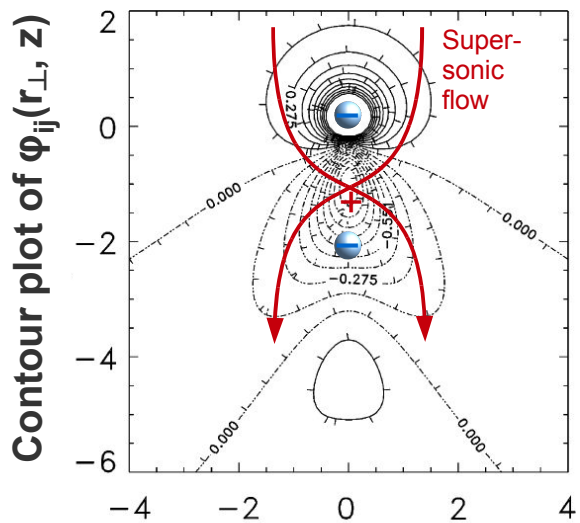
** Collaborators
* Guests

TR 24 complex plasmas

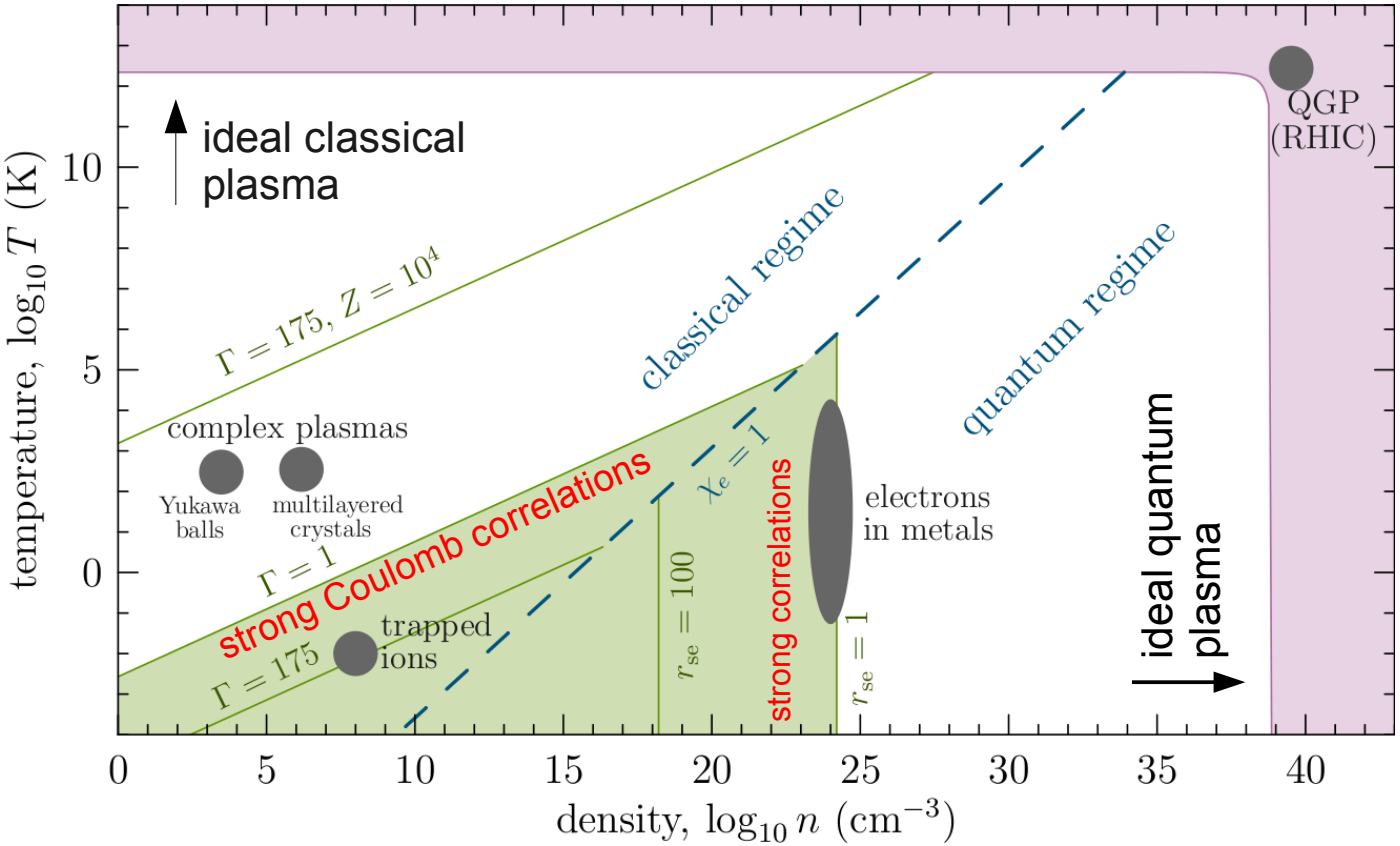
Multiscale Concept. Dynamical Screening Approach

Goal: First principle description of (strongly) correlated classical and quantum, multi-component plasmas in non-equilibrium situations.

Ansatz: Statistical description of the lighter plasma constituents by means of *Linear Response Theory*. Coulomb correlations of the heavy species are *fully included* in the Langevin Dynamics simulations.

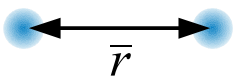


Strong Correlations in Nature and Laboratory



Coulomb interaction

$$U_{ab}(r) = e_a e_b / (\epsilon r)$$



Degeneracy parameter

$$\chi \equiv n \Lambda^{dim} \sim (\Lambda / \bar{r})^{dim}$$

$$(\Lambda = h / \sqrt{2 \pi m k_B T})$$

$$\Gamma \equiv \frac{Q^2}{\bar{r} k_B T}$$

Classical systems ($\chi < 1$)

$$r_s \equiv \frac{\bar{r}}{a_B} \sim Q^2 m \bar{r}$$

Quantum systems ($\chi \geq 1$)

$\Gamma, r_s \gg 1$: ***strongly correlated behavior***

$\longrightarrow$ ***Coulomb (Wigner) crystallization***

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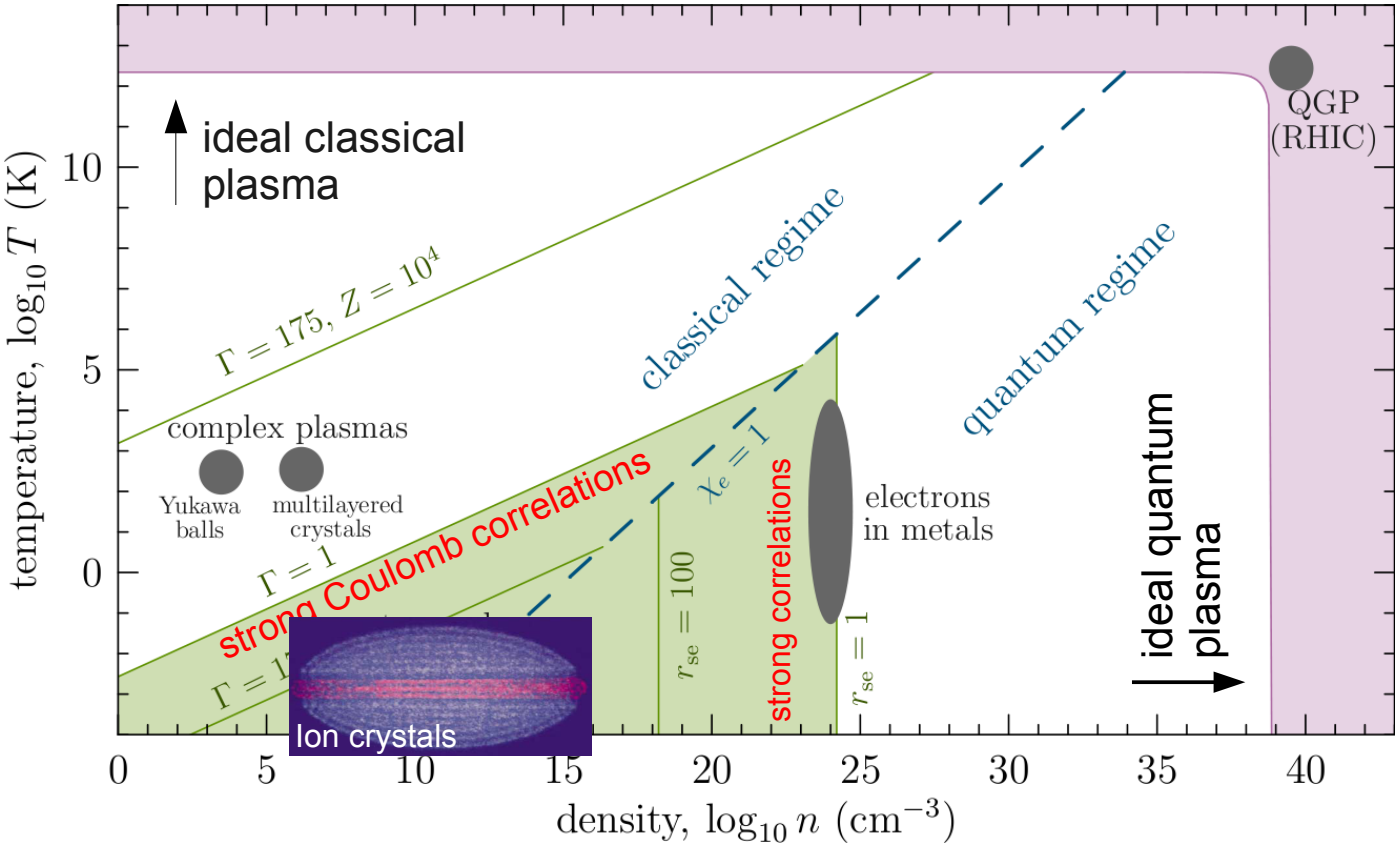

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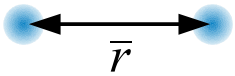

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a) low temperatures

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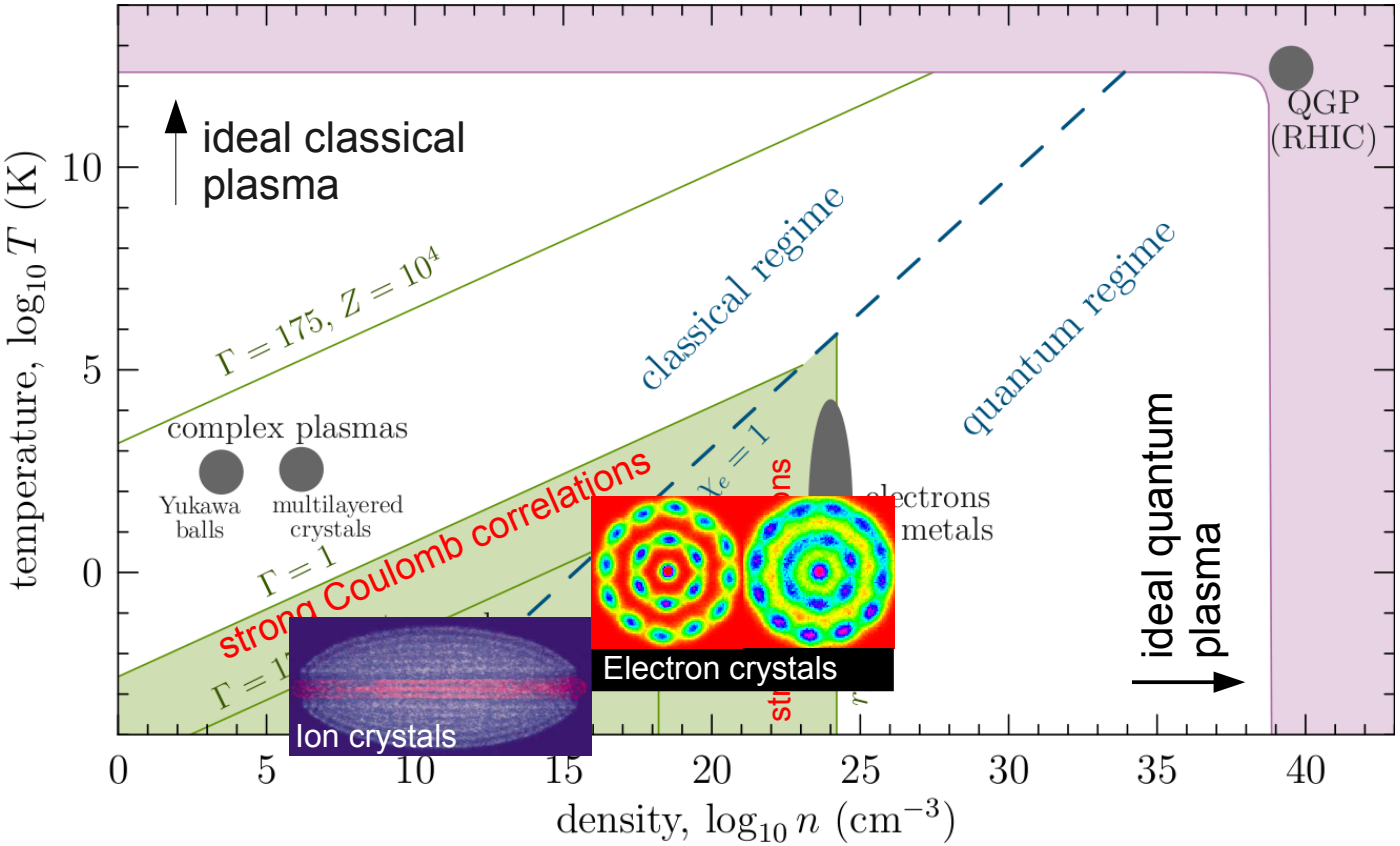

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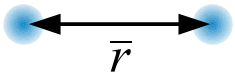

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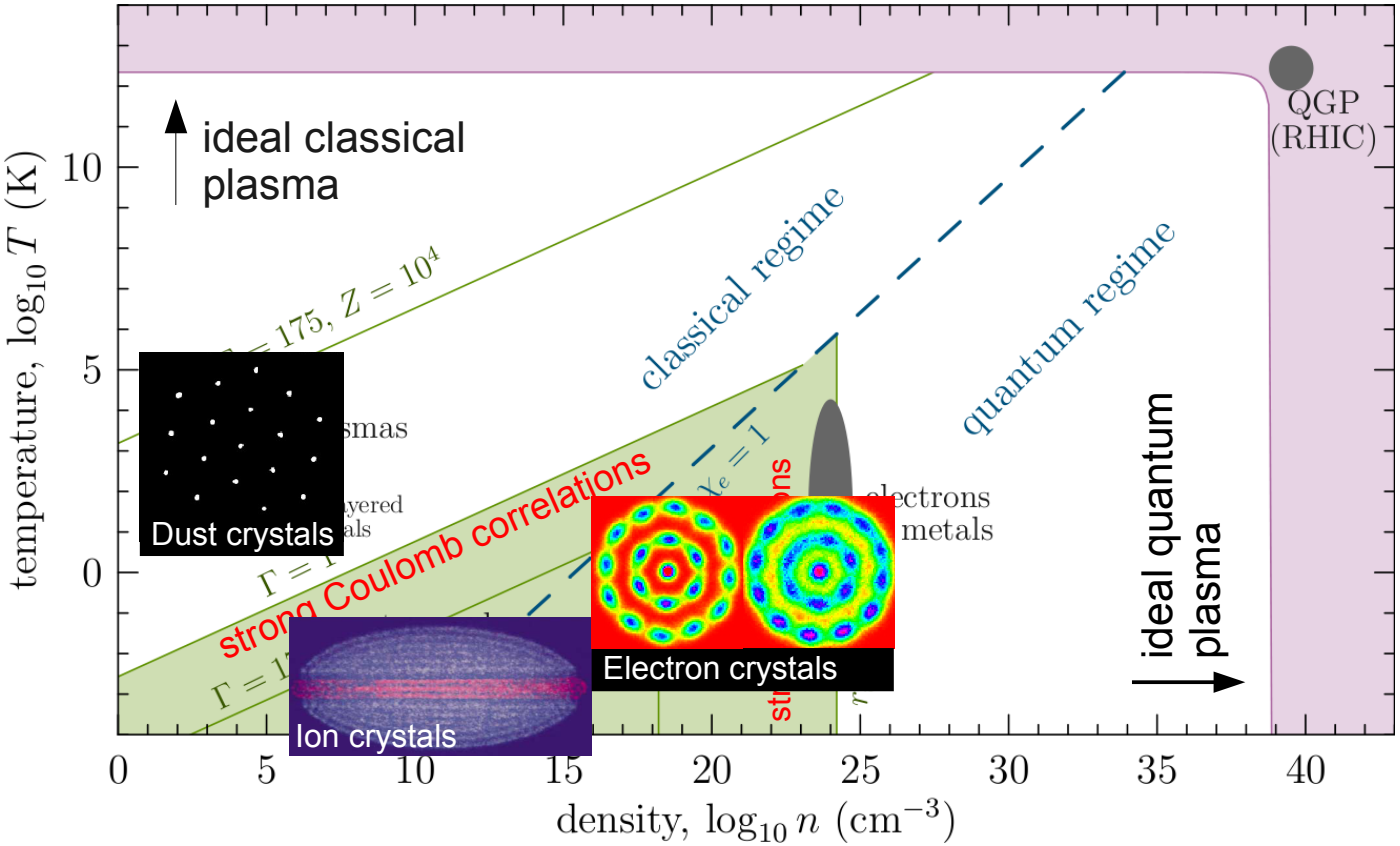

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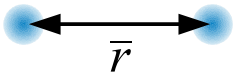

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c) charge increase

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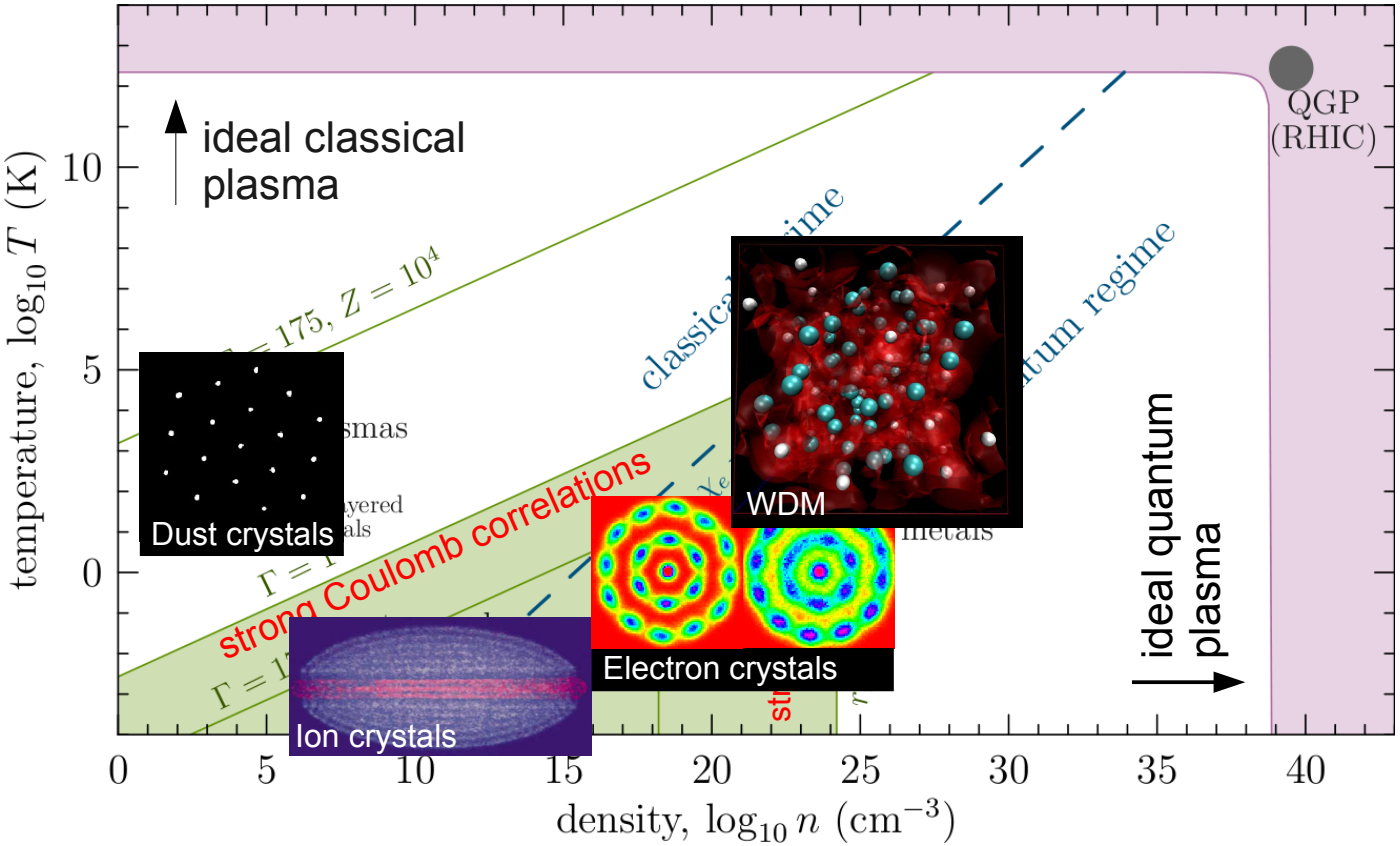

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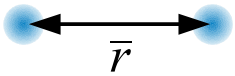

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WDM (Warm Dense Matter)

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Quantum systems ($\chi \geq 1$)

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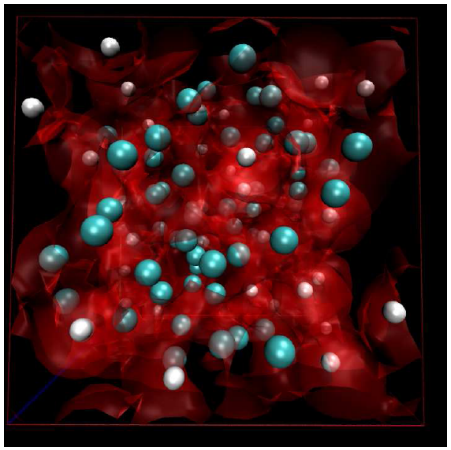
First Principle Description of Dense Quantum Plasmas



Ion-Electron Plasma
Fig.: D. Gericke et al.

Warm Dense Matter:

- light species: degenerate electrons, weakly coupled

- heavy species: classical ions, (possibly) strongly coupled

- weak e-i coupling

- non-equilibrium situations: streaming electrons and/or ions, particle beams etc. (not included in standard QMC, DFT simulations)

Goal: description of the correlated dynamcis of a multi-component plasma with full time-resolution

Problem: very different r, t – scales!
selfconsistent simulation impossible

ion-to-electron mass ratio ≥ 2000

ion-to-electron plasma frequency ratio ≥ 45

→ Multiscale approach required

First Principle Description of Dense Quantum Plasmas

Multiscale concepts: *Semiclassical Hybrid Simulations*

(i) DFT - MD (J. Clerouin, M. Desjarlais, J. Kress, W. Lorenzen, etc.)

(ii) KTMD (F.Graziani *et al.*, *High Energy Density Physics* **8**, 105 (2012))

(iii) **<u>Dynamical Screening Approach</u>**

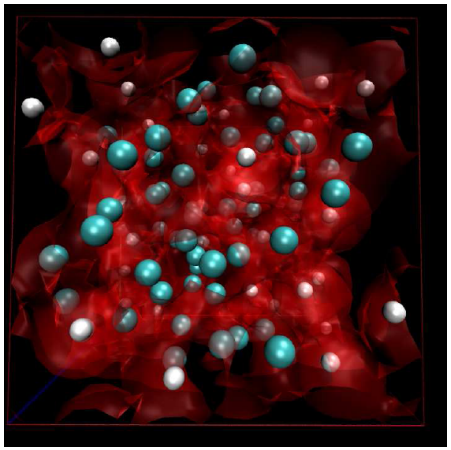
→ MD + (Dynamic) Dielectric Function: MCP → OCP

- classical (complex) plasmas:
  M. Lampe, G. Joyce, et al., Phys. Plas. **7**, 3851 (2000)

  Test against nonlinear simulations:
  *Hutchinson, Phys. Plasmas **18**, 032111 (2011)*
  Ludwig, Miloch et al., 2010-2012

- extension to quantum plasmas (WDM):
  P. Ludwig, M. Bonitz, H. Kählert, and J.W. Dufty,
  J. Phys. Conf. Series **220**, 012003 (2010)

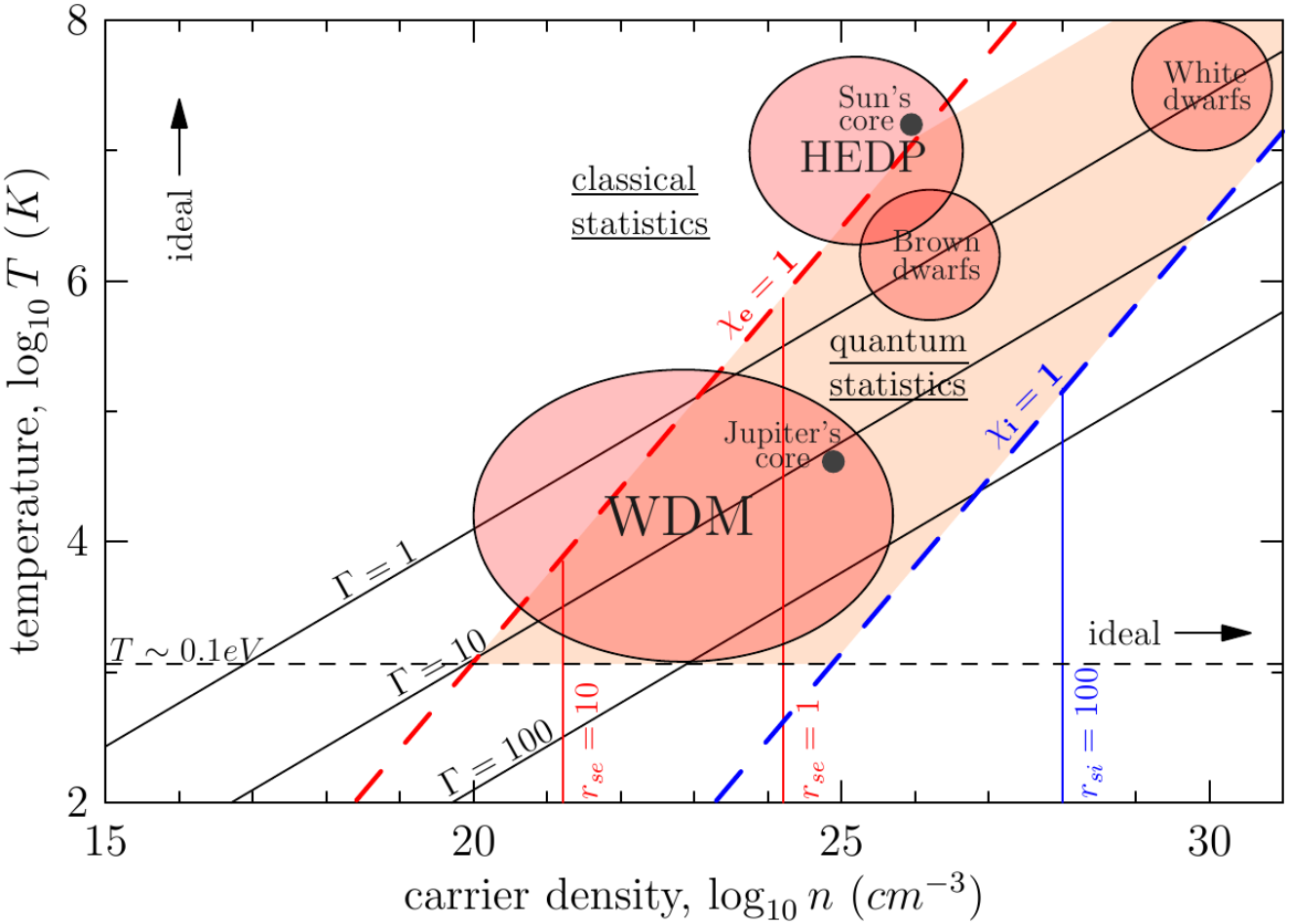
→ full nonequilibrium dynamics of ions including streaming effects (MD)
→ ion pair interaction dynamically screened by quantum electrons



Ion-Electron Plasma
Fig.: D. Gericke et al.

Strongly coupled quantum plasmas

Strongly coupled ions + weakly coupled quantum electrons

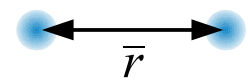


Astrophysics: planet interiors, white dwarf and neutron stars

Laboratory plasmas: laser/FEL produced plasmas
WDM (Warm Dense Matter), **HEDP** (High-Energy Density Plasmas)

Coulomb interaction

$$U_{ab}(r) = e_a e_b / (\epsilon r)$$



Degeneracy parameter

$$\chi \equiv n \Lambda^{dim} \propto (\Lambda / \bar{r})^{dim}$$

$$(\Lambda = h / \sqrt{2 \pi m k_B T})$$

Coupling parameter

classical systems ($\chi < 1$):

$$\Gamma = \langle U \rangle / k_B T \propto q^2 / (\epsilon \bar{r} k_B T)$$

quantum systems ($\chi \geq 1$):

$$r_s \equiv \bar{r} / a_B \propto \langle U \rangle / E_F$$

(a_B - Bohr radius)

(E_F - Fermi energy)

Dynamical Screening Model
for a (partially) ionized quantum plasma

Equation of motion of N-ion density operator (BBGKY-hierarchy [1])

$$i\hbar\frac{\partial \widehat{F}_i(1,..,N_i)}{\partial t} - \left[\widehat{H}_i(1,..,N_i), \widehat{F}_i(1,..,N_i)\right] = \sum_{b=e,n}\sum_{k=1}^{N_i} n_b Tr_{2_b}\left[\widehat{V}_{ib}(k,2_b), \widehat{F}_{ib}(1,..,N_i;2_b)\right]$$

*operator of binary interactions between an ion and **particle of type b***

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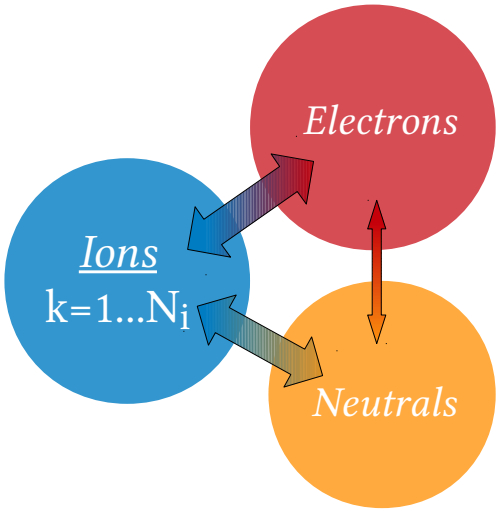

$$\widehat{H}_i(1,..,N_i) = \sum_{k=1}^{N_i}\hat{h}_i(k) + \frac{1}{2}\sum_{k\neq\ell}^{N_i} V_{ii}(|\mathbf{r}_k - \mathbf{r}_\ell|),$$

$$\hat{h}_i(k) = \frac{1}{2m_k}\left(\frac{\hbar}{i}\nabla_k - \frac{e_i}{c}\mathbf{A}(\mathbf{r}_k,t)\right)^2 + e\phi(\mathbf{r}_k,t)$$

$$n_i^{N_i}\cdot\widehat{F}_i(1,..,N_i,t) \rightarrow \Psi^\dagger(\mathbf{r}_1,t)\ldots\Psi^\dagger(\mathbf{r}_{N_i},t)\Psi(\mathbf{r}'_{N_i},t)\ldots\Psi(\mathbf{r}'_1,t)$$

$$\left[\Psi(\mathbf{r},t),\Psi^\dagger(\mathbf{r}',t)\right]_\mp = \delta(\mathbf{r}-\mathbf{r}'), \quad (\mathrm{B/F})$$

$$n_i^{N_i}\cdot \mathrm{Tr}_{1\ldots N_i}\langle\widehat{F}_i\rangle = N_i^{N_i}$$

[1] M. Bonitz, *Quantum Kinetic Theory*, Teubner, Stuttgart, Leipzig (1998)

[2] P. Ludwig, M. Bonitz, H. Kählert, and J.W. Dufty, J. Phys. Conf. Series 220, 012003 (2010)

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*operator of binary interactions between an ion and **particle of type b***

*joint density operator for N_i ions and one **particle of type b***

***Approximations**:*

1. classical limit for ions → Newton's equations

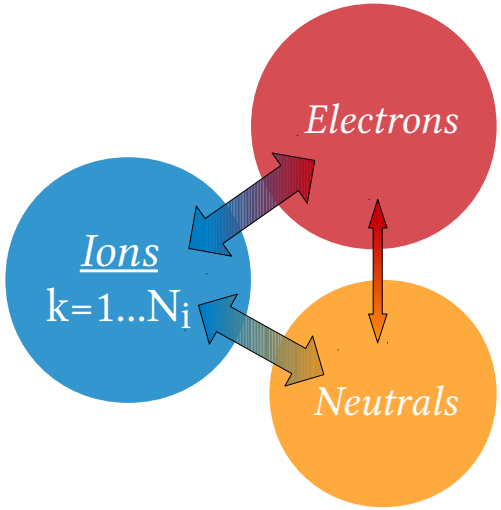
2. weak electron-ion correlations: mean field approximation $\widehat{F}_{ie}(1,..,N_i;2_e) \simeq \widehat{F}_i(1,..,N_i)\widehat{F}_e(2_e)$

   → *electrons create a Hartree potential for ion 'k':* $\widehat{W}_{ie}(k) \equiv n_e Tr_{2_e}\widehat{V}_{ie}(k,2_e)\widehat{F}_e(2_e)$

   → *electron contribution becomes:* $n_e Tr_{2_e}\left[\widehat{V}_{ie}(k,2_e), \widehat{F}_{ib}(1,..,N_i;2_e)\right] \simeq \left[\widehat{W}_{ie}(k), \widehat{F}_i(1,..,N_i)\right]$

   → *effective single particle Hamiltonian for each ion:* $\widehat{\widehat{h}}_i(k) = \widehat{h}_i(k) + \widehat{W}_{ie}(k)$

3. Langevin-Fokker-Planck approximation for ion-neutral interaction



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Semiclassical equations

$$\frac{d\mathbf{p}_k}{dt} = -\frac{d}{d\mathbf{r}}\left(V_i^{\text{eff}}(\mathbf{r},t) + e_i\phi^{ext}(\mathbf{r},t)\right)\Big|_{\mathbf{r}=\mathbf{r}_k} + \mathbf{F}^{i,n}(\mathbf{r}_k,\mathbf{p}_k,t), \qquad k = 1,\ldots,N_i$$

friction force + Langevin white noice term

$$V_k^{\text{eff}}(\mathbf{r}_k,t) = e_k\sum_{l=1}^{N_i}\phi_l^{\text{tot}}(\mathbf{r},t), \qquad \tilde{\phi}_l^{\text{tot}}(\mathbf{k},\omega;\mathbf{R},t) = \frac{\tilde{\phi}_l(\mathbf{k})}{\epsilon(\mathbf{k},\omega;\mathbf{R},t)}$$

total effective ion-ion interaction energy (screened by electrons)

total electrost. potential produced by ion 'l'

Ion potential dynamically screened by electrons

P. Ludwig, M. Bonitz, H. Kählert, and J.W. Dufty, J. Phys. Conf. Series 220, 012003 (2010)

Dynamical Screening Model: electron dynamics

1. First equation of BBGKY-hierarchy

$$i\hbar\frac{\partial \widehat{F}_e(1)}{\partial t} - \left[\widehat{H}_e(1), \widehat{F}_e(1)\right] = \sum_{b=e,i,n} n_b Tr_{2_b}\left[\widehat{V}_{ib}(k, 2_b), \widehat{F}_{eb}(1; 2_b)\right]$$

$$\widehat{H}_e(1) = \left[\frac{1}{2m_e}\left(\frac{\hbar}{i}\nabla_1 + \frac{e_0}{c}\mathbf{A}(\mathbf{r}_1, t)\right)^2 - e_0\phi(\mathbf{r}_1, t)\right]$$

2. Perturbation ansatz with respect to e-i coupling: $\widehat{F}_e = \widehat{F}_e^0 + \widehat{F}_e^1$

$$i\hbar\frac{\partial \widehat{F}_e^0(1)}{\partial t} - \left[\widehat{\overline{H}}_e^0(1), \widehat{F}_e^0(1)\right] = \widehat{I}_e^0(1),$$

$$i\hbar\frac{\partial \widehat{F}_e^1(1)}{\partial t} - \left[\widehat{\overline{H}}_e^0(1), \widehat{F}_e^1(1)\right] - \left[\widehat{W}_e^1(1) + \widehat{W}_i(1), \widehat{F}_e^0(1)\right] = \widehat{I}_e^{RTA,1}(1).$$

3. Compute $\widehat{F}_e^1$ in linear response → quantum dielectric function with collisions (Mermin)

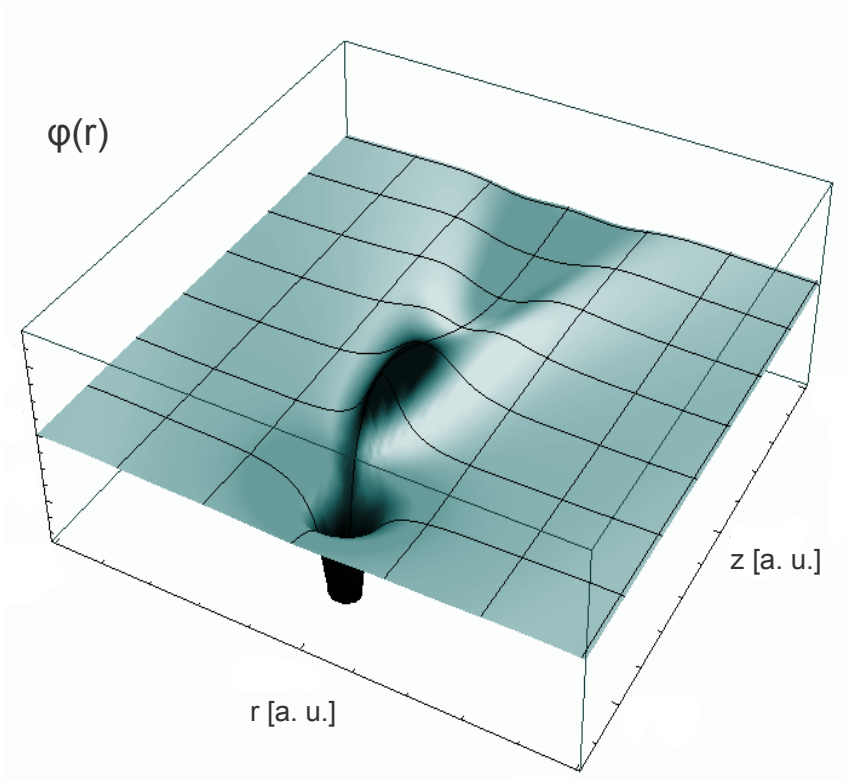
Ion potential, dynamically screened by degenerate electrons

$$\phi(\mathbf{r},t;\mathbf{v}_a) = e_a \int \frac{d^3k}{2\pi^2} \frac{e^{i\mathbf{k}(\mathbf{r}-[\mathbf{r}_{0a}+\mathbf{v}_a t])}}{\sum_{ij} k_i k_j \epsilon_{k,ij}(\mathbf{k}\mathbf{v}_a)}$$

dynamic dielectric function

- Equilibrium: isotropic Yukawa potential
- Nonequilibrium (streaming electrons): anisotropic potential, wake effects
- Space and time-dependent screening

→ used in Newton's equations
→ dramatic effect in ion dynamics

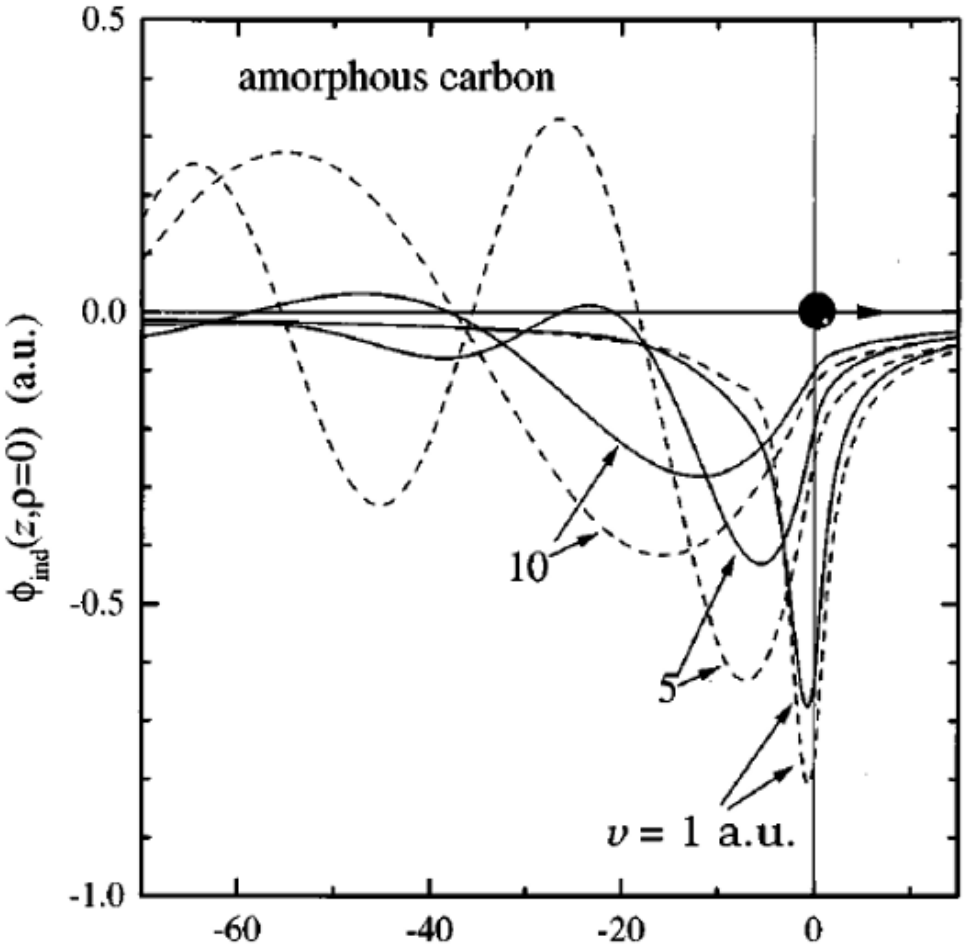


total potential of a single ion moving relative to the electrons with constant velocity $\mathbf{v}_a$

The quality of the solutions depends fully on the **quantum dielectric function**

- D. Mermin, Phys. Rev. B **1**, 2362 (1970)
- I. Abril, R. Garcia-Molina, C.D. Denton, J. Perez-Perez, and N.R. Arista, Phys. Rev. A **58**, 357 (1998)
- A. Selchow, G. Röpke, A. Wierling, Contrib. Plasma Phys. **42**, 43 (2002)
- M. D. Barriga-Carrasco, Phys. Plasmas **15**, 033103 (2008)

Wake effects in streaming quantum plasmas: stopping power of ions



Potential of a single proton (at z = 0)
Moving with v=const along the z-axis
in amorphous carbon
(for three values of v shown in the figure).

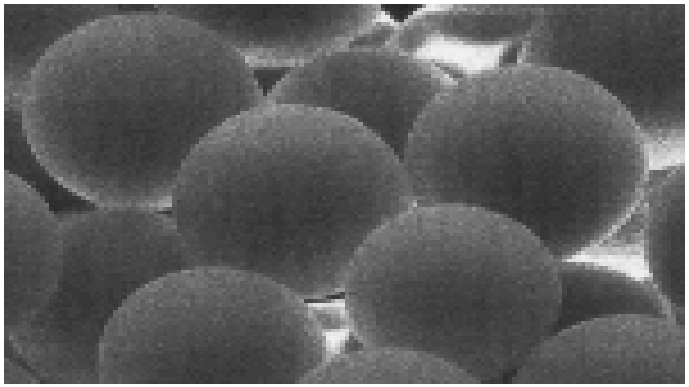
Dotted line: Lindhard dielectric function

Full line: Mermin DF (collisions included)

Fig.: I. Abril, R. Garcia-Molina, C. D. Denton, J. Perez-Perez, and N.R. Arista, Phys. Rev. A **58**, 357 (1998)

So far, the quantum DF has not been used to compute a screened pair potential and to study the N -particle dynamics of strongly correlated ions.

Classical analog: ***Complex (Dusty) Plasmas***

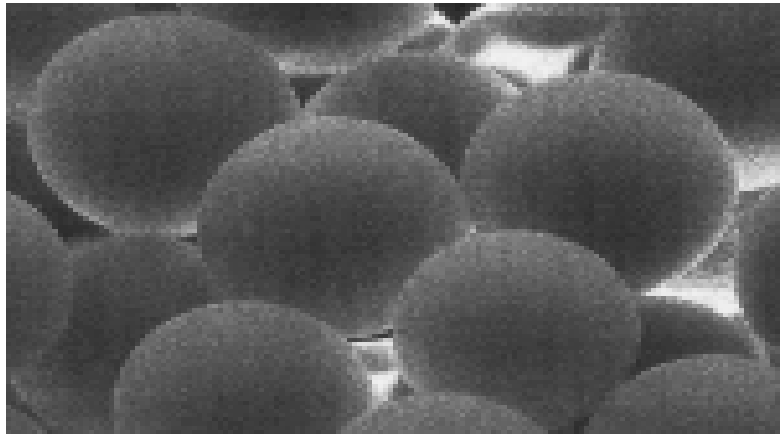


- light species: ions, neutrals, electrons (weakly coupled)

- heavy species: dust grains (strongly coupled)

→ **Problem:** very different r, t – scales!

Complex – Dusty – Plasmas in laboratory



dust particles:

- polymer micro-spheres (melamine), monodisperse
- diameter of a few µm ($d \approx 10\mu m$)
- highly charged ($Q \approx 10{,}000e$)
- strongly coupled at room temperature ($T \approx 300K$)
- low density ($n \approx 1...50mm^{-3}$)
- weak to moderate neutral gas friction (gas pressure $p_d \approx 10Pa$)

→ observable with the naked eyes and standard CCD-camera
→ low charge-to-mass-ratio → slow system dynamics
(dust plasma frequency: $f \approx (1...10)Hz$)

Complex – Dusty – Plasmas in laboratory

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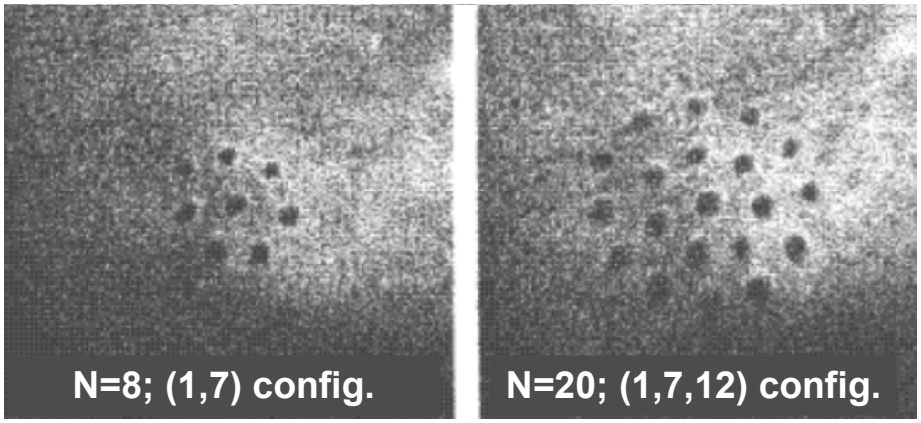
- low density ($n \approx 1...50mm^{-3}$)
- weak to moderate neutral gas friction (gas pressure $p_d \approx 10Pa$)

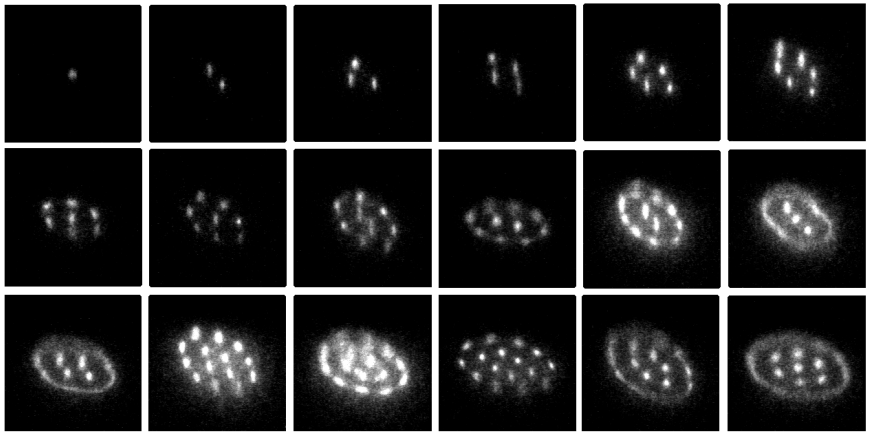
→ observable with the naked eyes and standard CCD-camera
→ low charge-to-mass-ratio → slow system dynamics
(dust plasma frequency: $f \approx (1...10)Hz$)

→ ideal test system for many-particle correlation effects
(due to the universal character of Coulomb correlations)

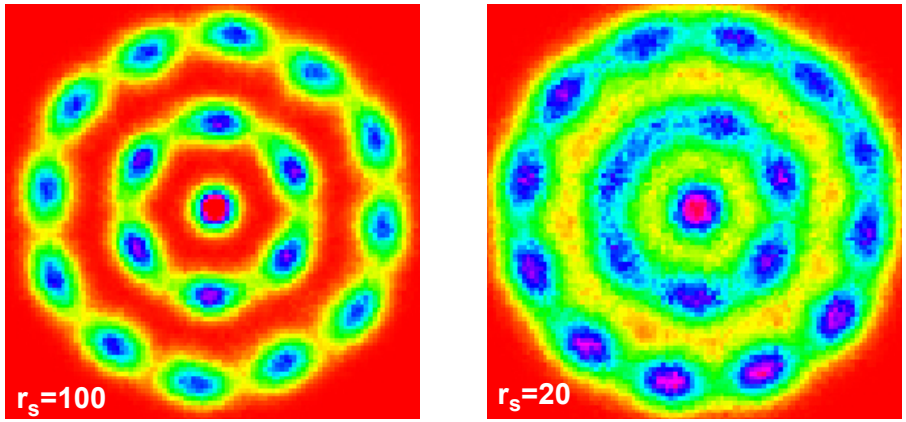
Strongly Coupled Coulomb Systems in Traps
('2D Artifical Atoms')



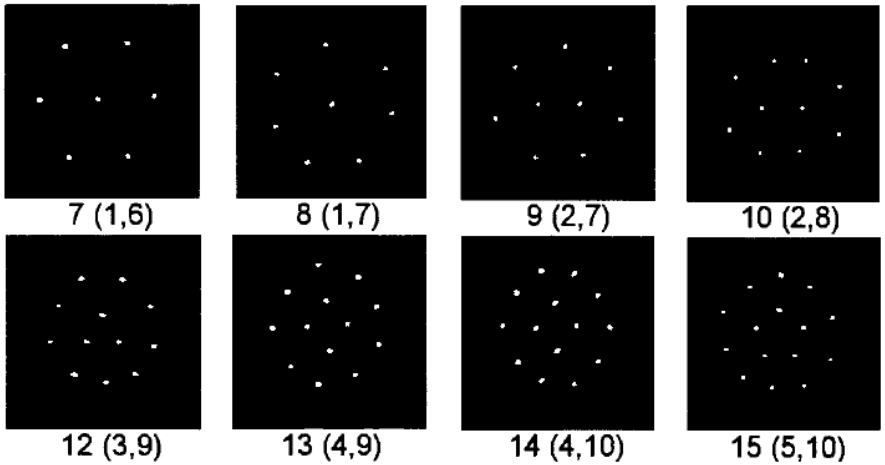
2D Electron Dimples on the Surface of Liquid ^{4}He
(Leiderer *et al.*, Surface Science **113**, 405 (1982))



2D Ca^+ Ion Crystals in a Paul Trap
(Werth *et al.*, University Mainz, Germany (2000))

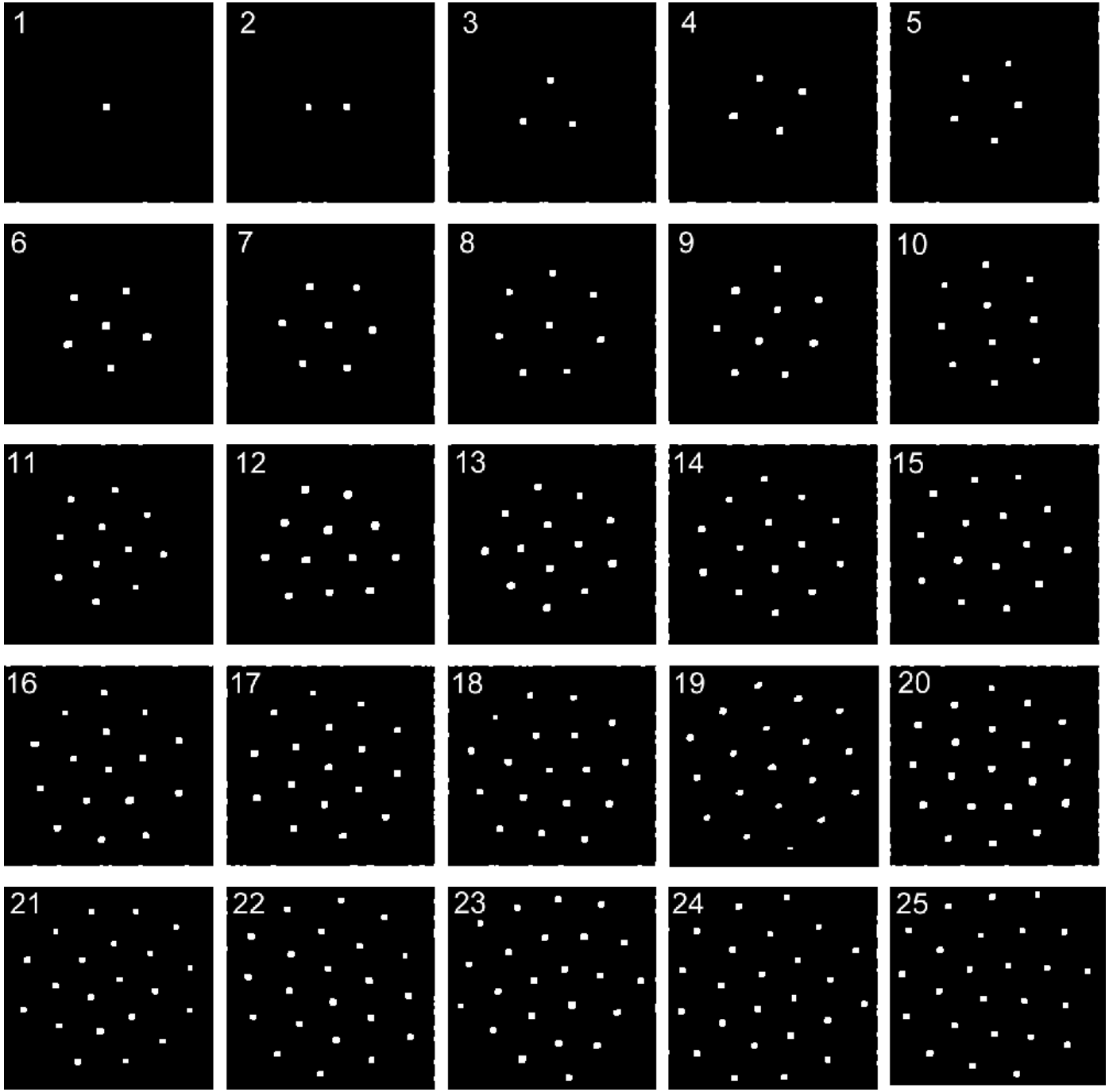


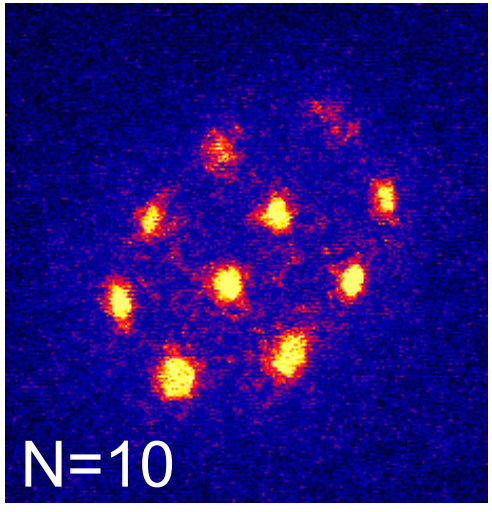
2D Electron 'Wigner' Crystals in Quantum Dots
(A. Filinov, M. Bonitz, Yu.E. Lozovik, PRL (2001))



2D Finite Dust Crystals in a rf Plasma Trap
(Lin I *et al.*, Taiwan (1999))

„Mendeleyev table“ for 2D Coulomb Clusters

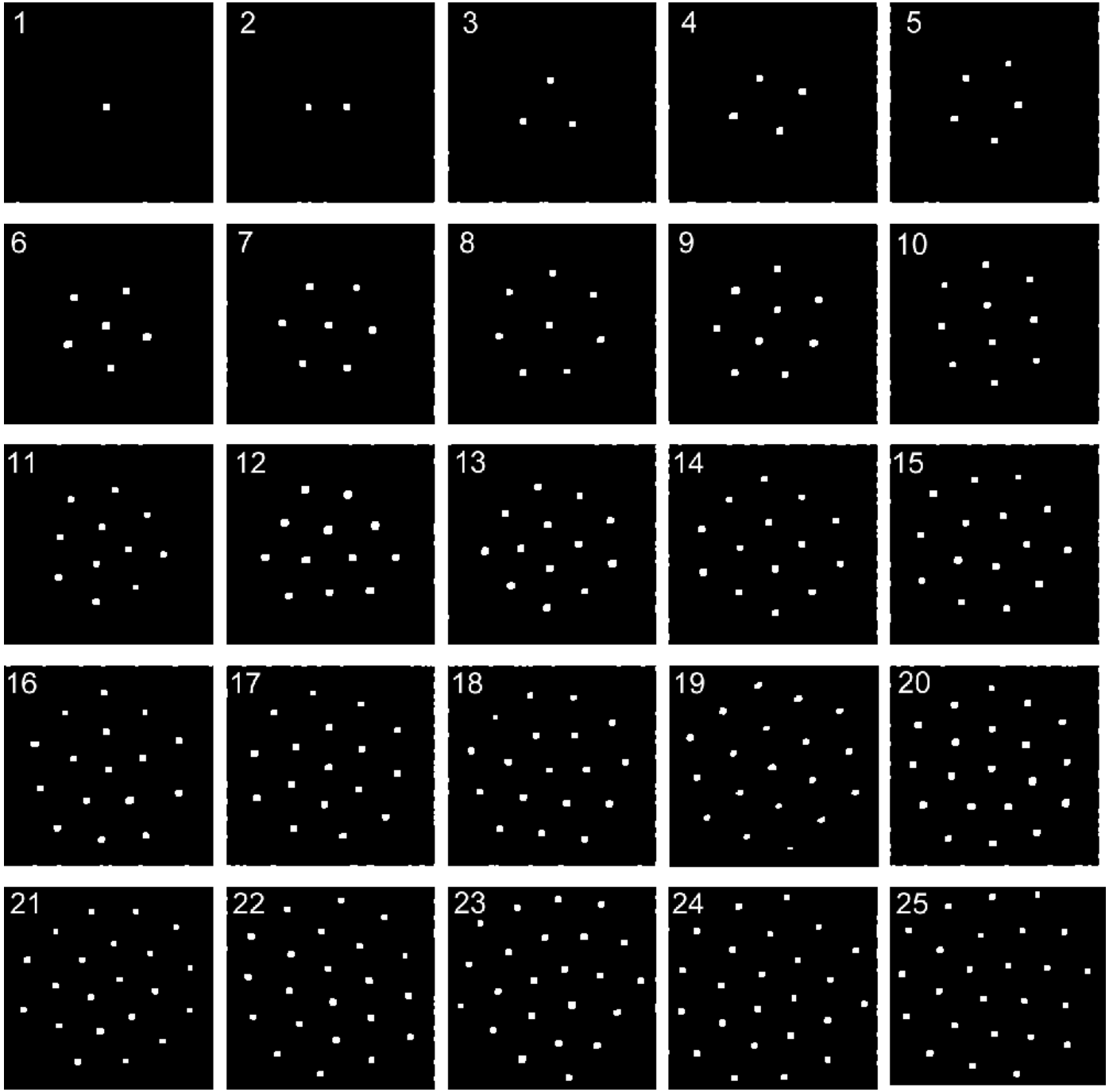


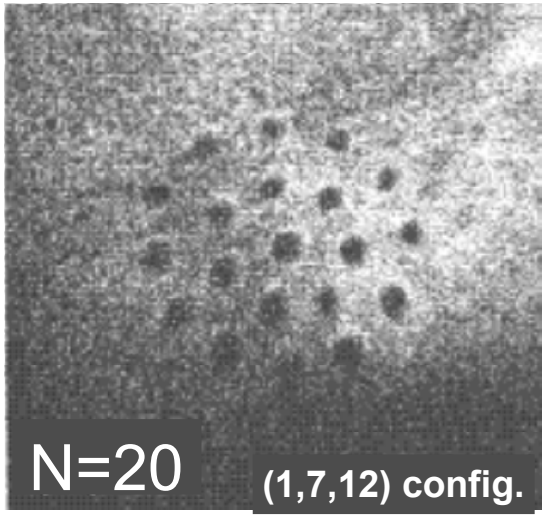


Ca^+ ion crystals
in a Paul trap
G. Werth, Uni Mainz

Dusty Plasma,
Melzer et al.

„Mendeleyev table“ for 2D Coulomb Clusters

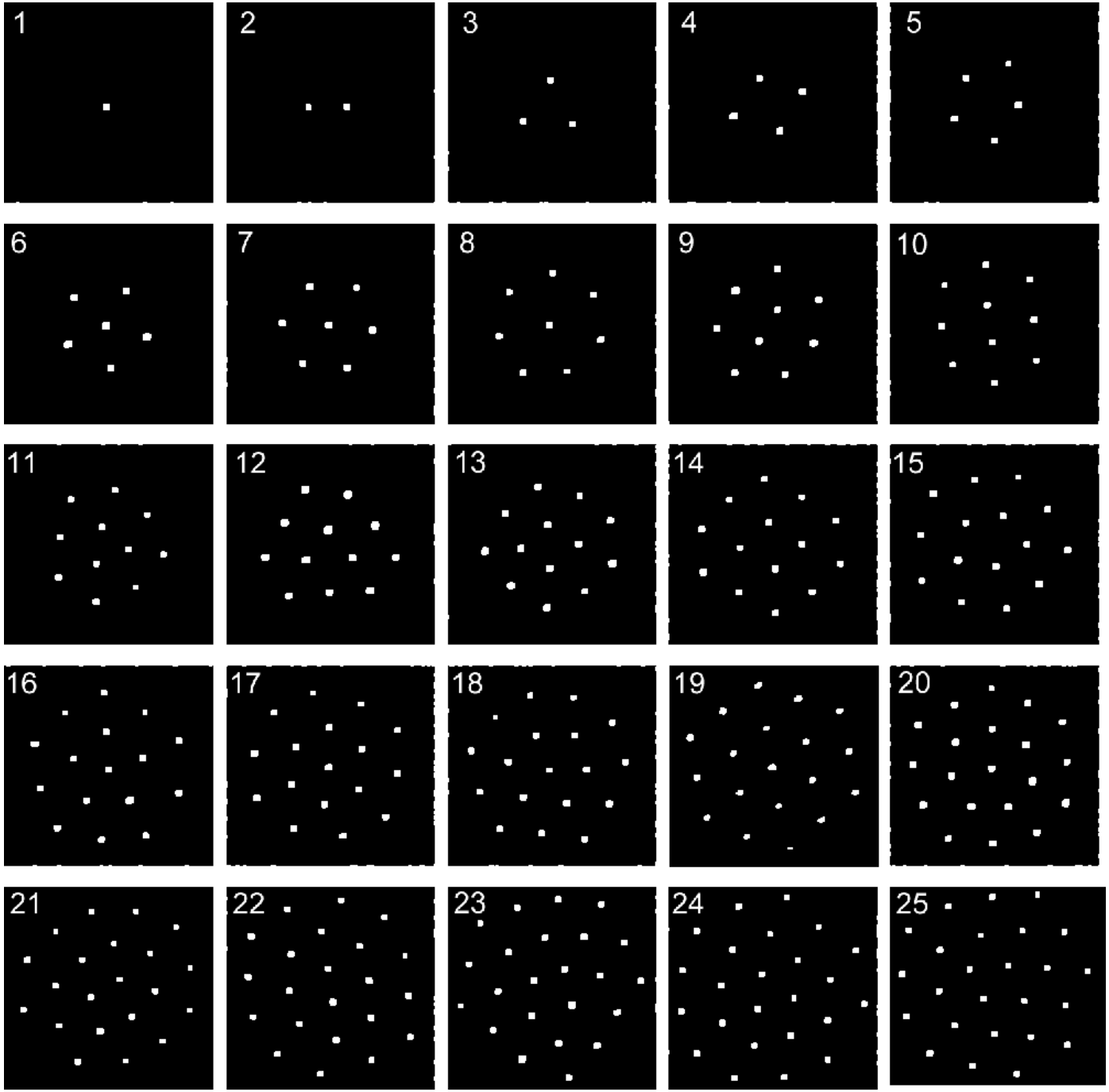


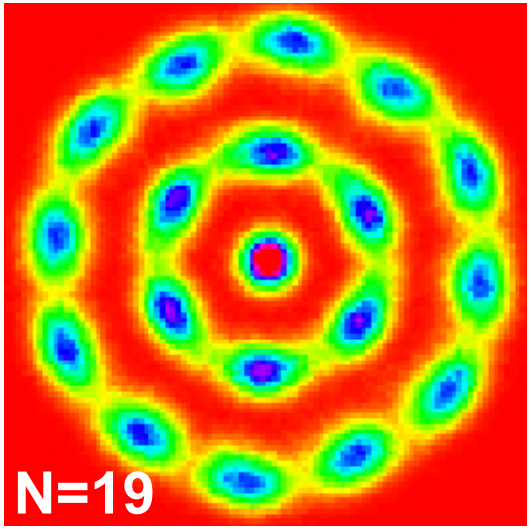


Electrons on a liquid helium surface, P. Leiderer (1982)

Dusty Plasma, Melzer et al.

„Mendeleyev table“ for 2D Coulomb Clusters

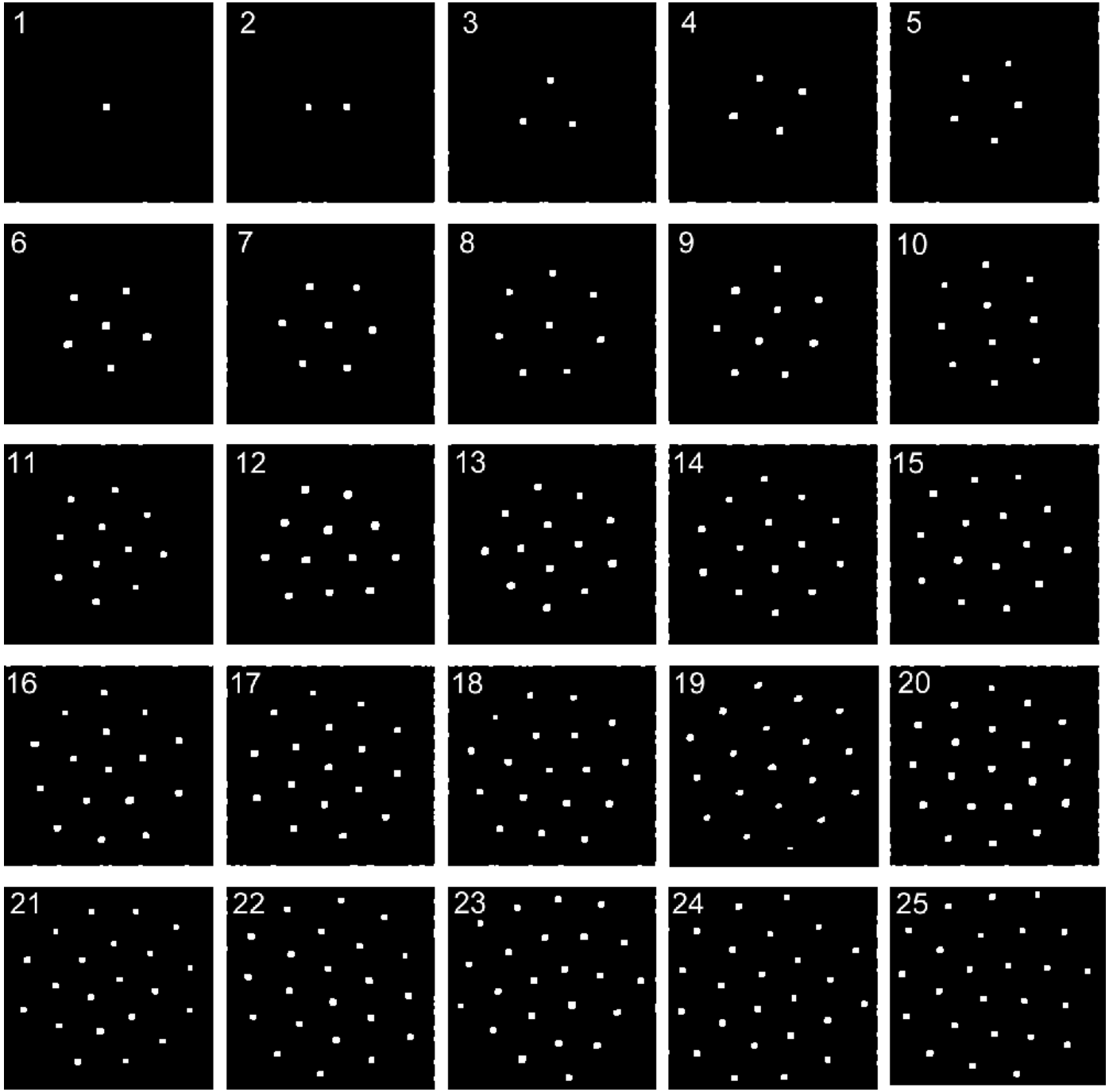


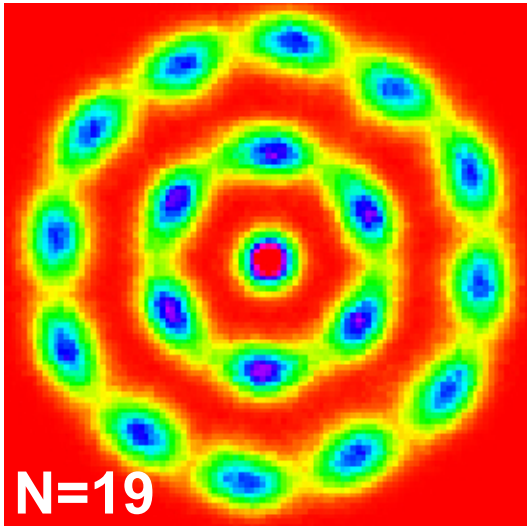


Wigner Crystal of Electrons
in a Quantum Dot
A. Filinov et al., 2001

Dusty Plasma,
Melzer et al.

„Mendeleyev table“ for 2D Coulomb Clusters





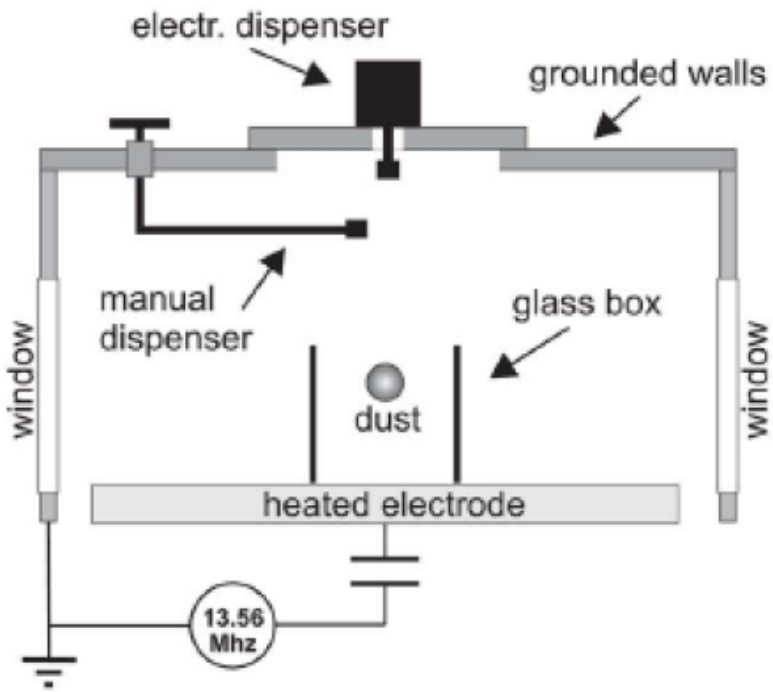
Wigner Crystal of Electrons
in a Quantum Dot
A. Filinov et al., 2001

→ Complex (dusty) plasmas – a laboratory for strong correlations

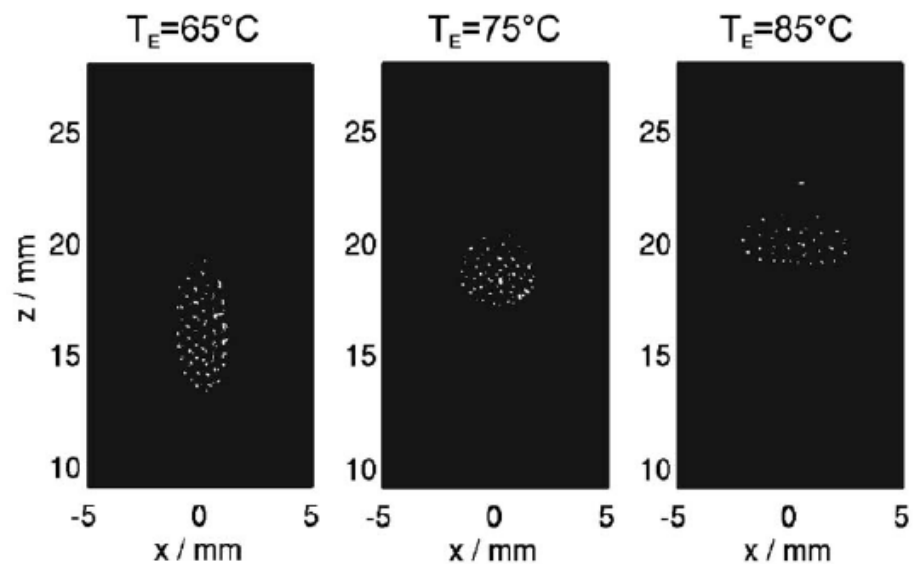
Dusty Plasma,
Melzer et al.

Laboratory dusty plasmas
„Yukawa balls“: spherical crystals

RF discharge chamber



3D Plasma Crystals



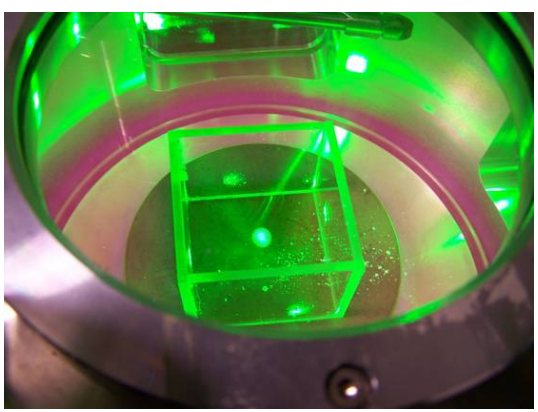


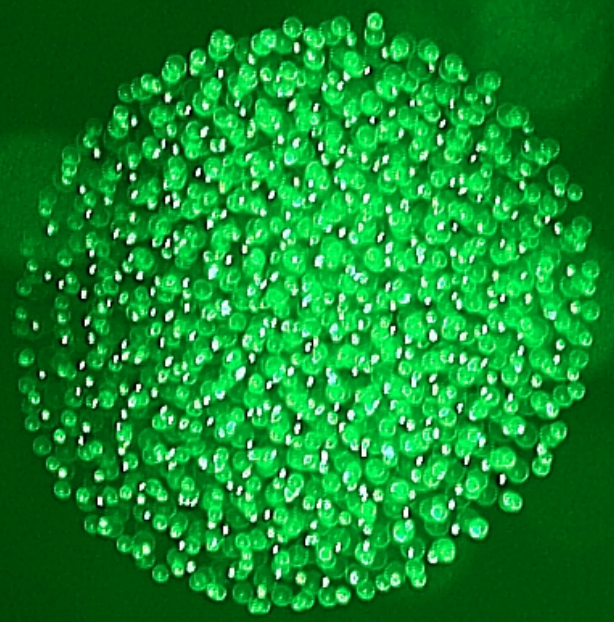
Foto: S. Käding, U Greifswald

Experiments
- dust negatively charged (≈10,000e_0)
- gravity compensated by thermophoretic force and electric fields
- glass box avoids formation of void region inside the dust cloud
- confinement (almost) isotropic [1)]
- dust particles surrounded by electrons, ions and neutrals

1) O. Arp et al., Phys. Plasmas **12**, 122102 (2005)

3D Spherical Dust Crystals

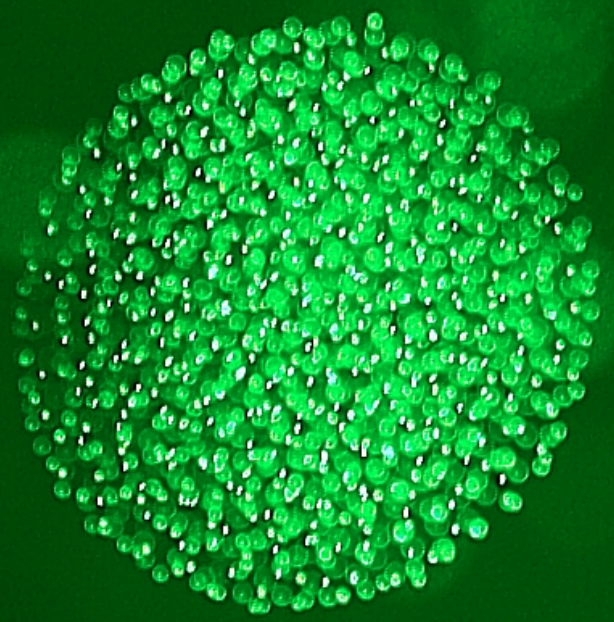
strongly coupled Coulomb clusters in traps

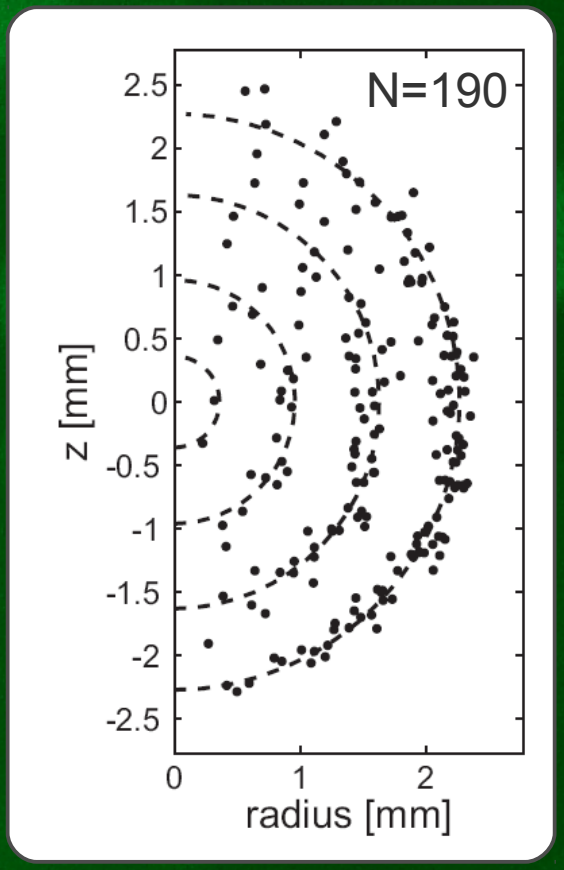


- Dusty plasma crystal consisting of several tens to thousands dust particles (white dots) [Arp, Block, Piel & Melzer, Phys. Rev. Lett. **93**, 165004 (2004)]
- Room temperature, coupling parameter $\Gamma \approx 1000$

3D Spherical Dust Crystals

strongly coupled Coulomb clusters in traps

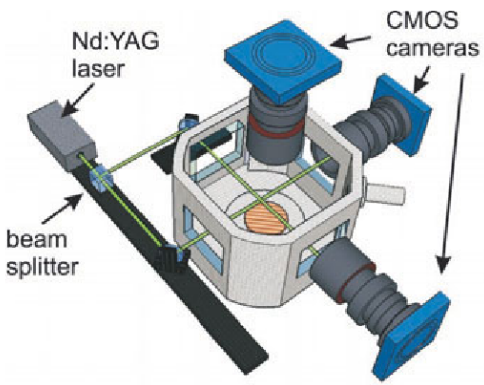


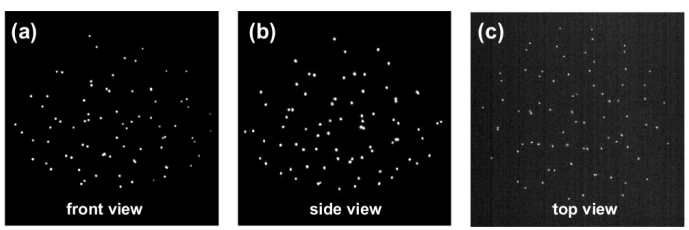


- Particles arranged on concentric spherical shells
- Multi-component plasma: electrons, ions, neutral (e.g. argon) atoms, and dust grains
- Subsystem of grains (OCP) well described by isotropic Yukawa potential $(Ze)^2\exp(-\kappa\cdot r)/r$
- isotropic 3D parabolic confinement [Arp et al., Phys. Plas. **12**, 122102 (2005)]

Particle Tracking in 3D Dusty Plasmas

Stereoscopy



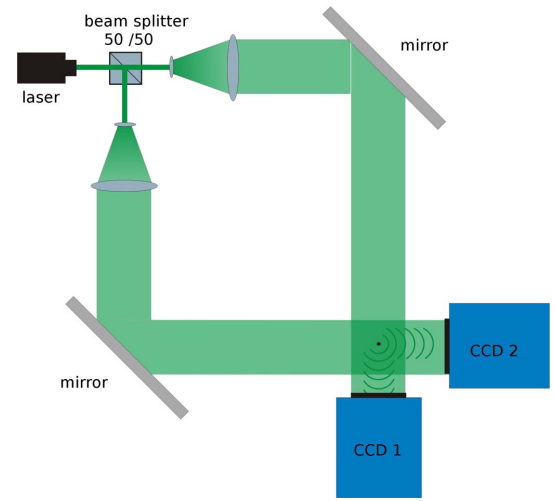


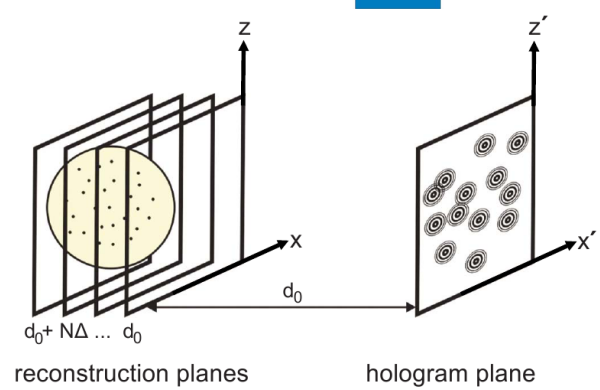
<u>Top:</u> Scheme of the stereoscopic setup with 3 orthogonal cameras and the expanded laser beam for illumination.
<u>Bottom:</u> Single snap shots of a Yukawa ball with about 60 particles from each camera

Restricted to small clouds (shadowing effects)

A. Melzer, S. Käding, D. Block, A. Piel, "Stereoscopy in dusty plasmas", Photonik International Nr. 2/2008, 56

Digital Holography





<u>Top:</u> Schematic setup of the stereoscopic digital holography system. The system consists of two identical digital inline holographic setups, with perpendicular orientation of their optical axis.

Stereoscopic holography is suitable for high resolution measurements of 3D dust clouds

M. Kroll, L. Mühlfeld, D. Block, "Stereoscopic Digital Holography", IEEE Transactions on Plasma Science **38**, No. 4, 897 (2010)

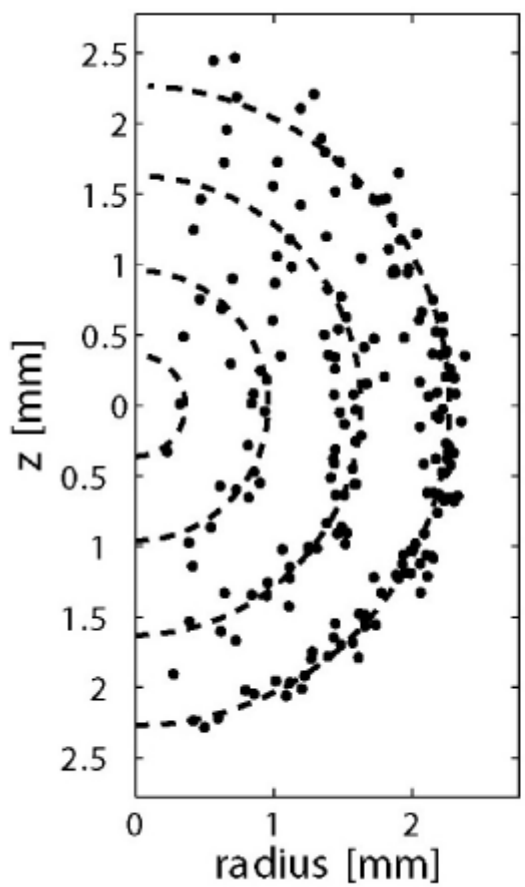
Experiment vs. Simulation

N=190

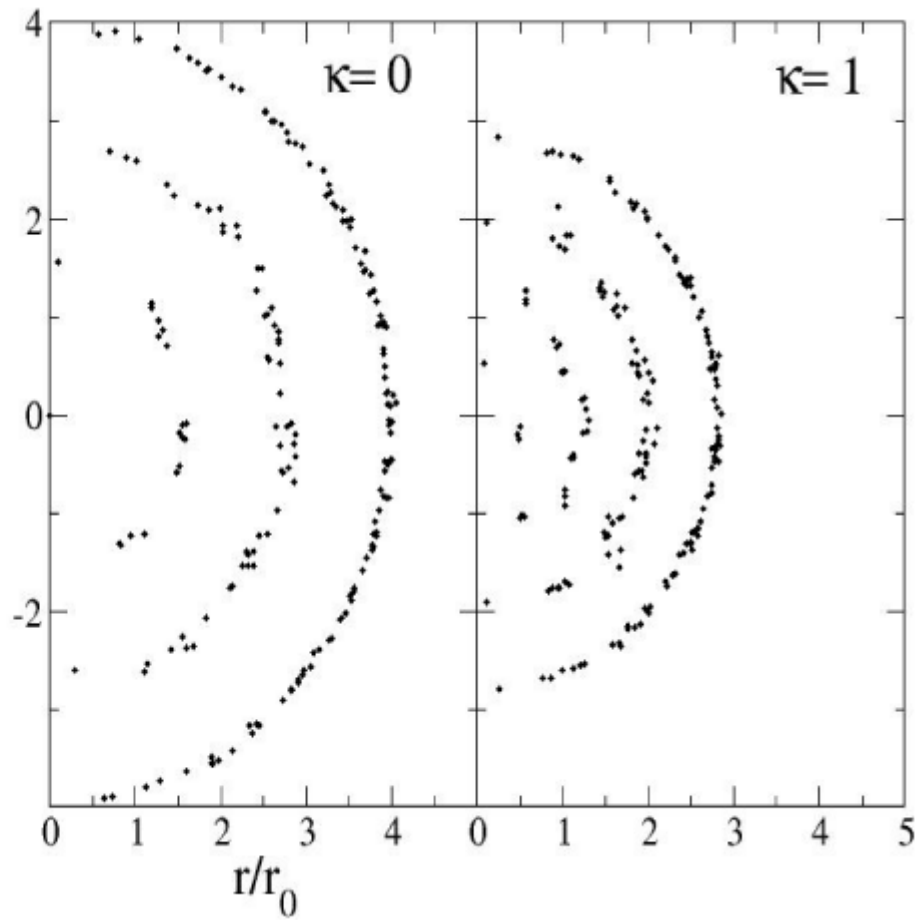
Molecular dyamics with
Coulomb and Yukawa-potential
(→ particle correlations exact)

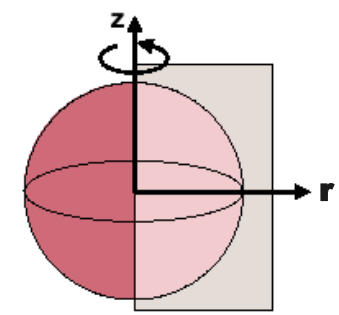
$$V(r) = \frac{Q^2 e^{-\kappa r}}{4\pi\epsilon_0 r}$$

Experiment



Simulation





z-r-projection

*Bonitz et al, PRL **96**, 075001 (2006)*

(**2, 21, 60, 107**) (1, 18, 56, 115) (4, 24, 60, 102)

→ shell configuration from MD for κ=0.6: (2, 21, 60, 107) !!

Experiment vs. Simulation (cont.)

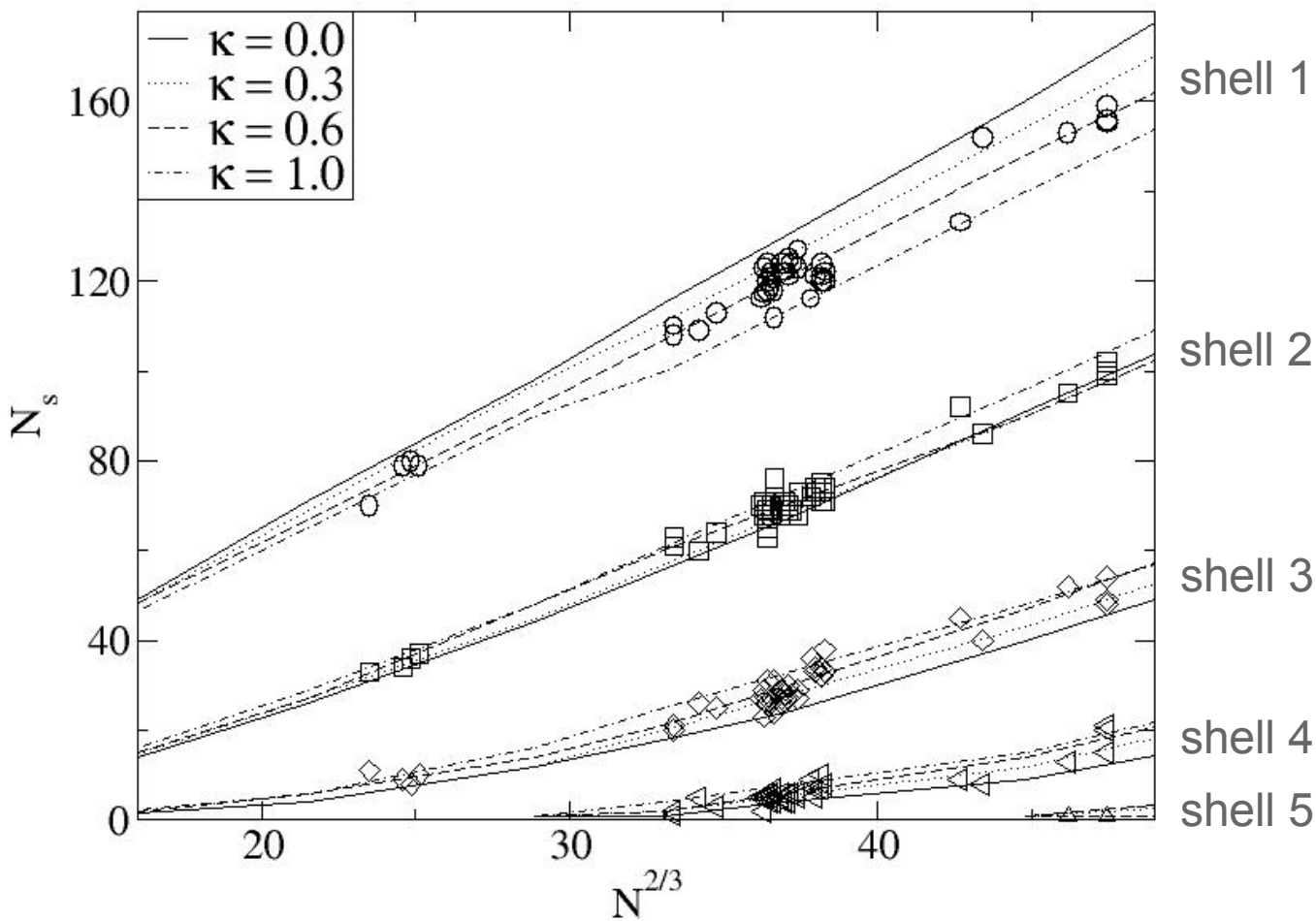
Experiment (symbols):
43 clusters,
N=100...500

Molecular dyamics with
Coulomb and
Yukawa potential

$$V(r) = \frac{Q^2 e^{-\kappa r}}{4\pi\epsilon_0 r}$$

$$\kappa = \frac{1}{\lambda_D} \qquad \lambda_D^2 = \sum_a \frac{k_B T_a}{e^2 n_a}$$

Shell populations



Systematic screening dependence!
→ Non-invasive diagnostics for
plasma parameter in experiment:

outer (1th) shell: $\kappa = 0.62 \pm 0.23$
2nd shell: $\kappa = 0.58 \pm 0.43$

Experiment vs. Simulation (cont.)

Experiment (symbols):
43 clusters,
N=100...500

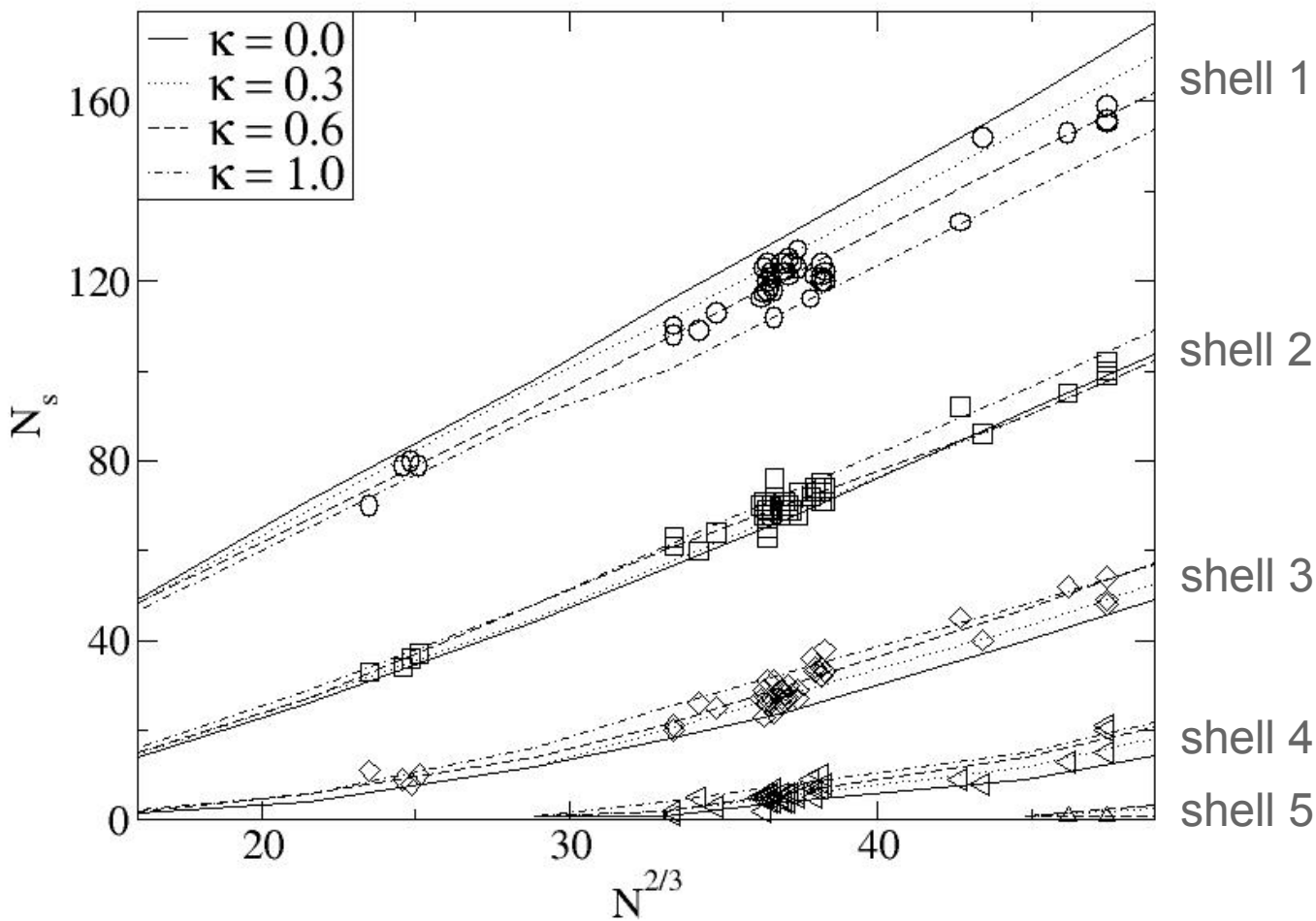
Molecular dyamics with
Coulomb and
Yukawa potential

$$V(r) = \frac{Q^2 e^{-\kappa r}}{4\pi\epsilon_0 r}$$

$$\kappa = \frac{1}{\lambda_D} \qquad \lambda_D^2 = \sum_a \frac{k_B T_a}{e^2 n_a}$$

→ *excellent agreement with dusty plasma experiments (Phys. Rev. Lett. 2006)*

Shell populations



Systematic screening dependence!
→ Non-invasive diagnostics for plasma parameter in experiment:

outer (1th) shell: $\kappa = 0.62 \pm 0.23$
2nd shell: $\kappa = 0.58 \pm 0.43$

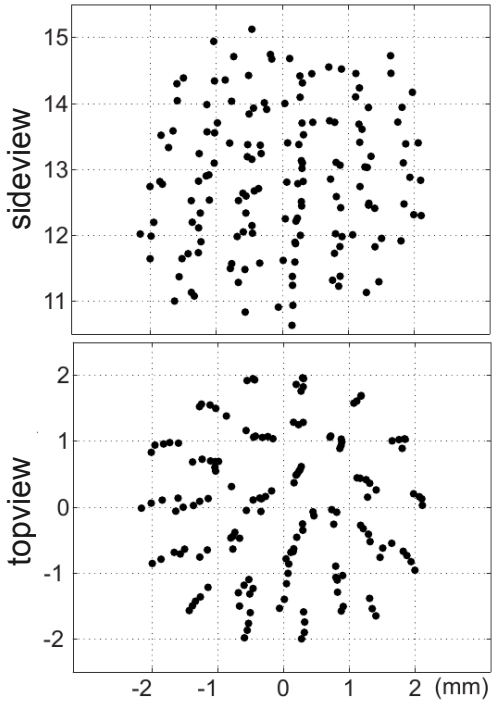
Attraction of identical particles

- wake effects

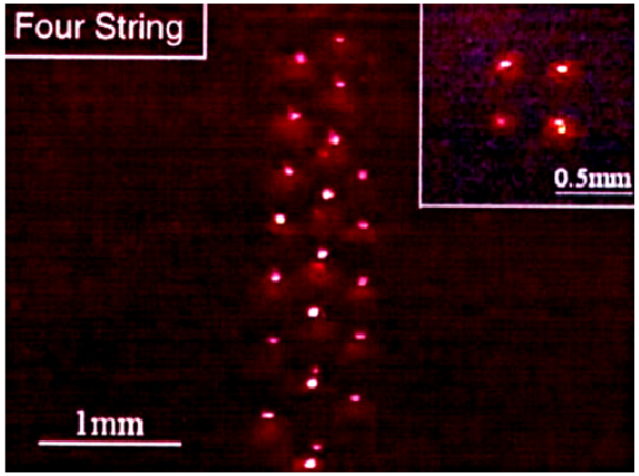
Experiments with fast streaming ions

String Formation in Vertically Elongated 3D Confined Dusty Plasmas

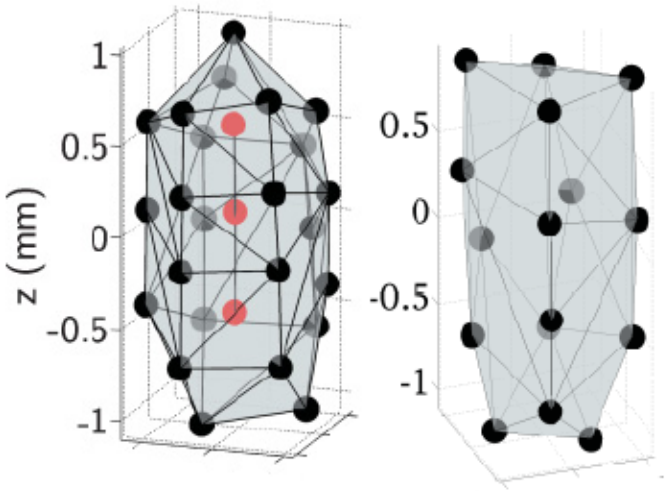
Representative examples for various plasma parameters



M. Kroll, J. Schablinski, D. Block, and A. Piel, Phys. Plas. **17**, 013702 (2010)



N. Sato et al. (2001)



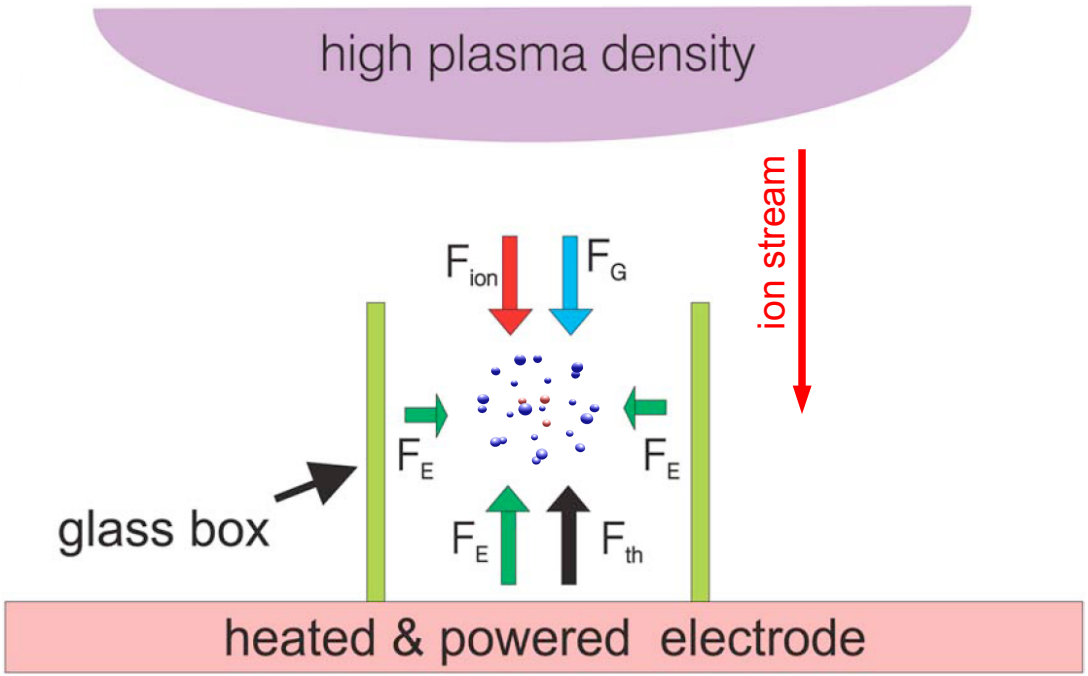
C. Killer, A. Schella, T. Miksch, and A. Melzer, PRB **84**, 054104 (2011)

VIDEO

Vertical alignment not explainable with repulsive Yukawa potential!

Effect of fast streaming ions

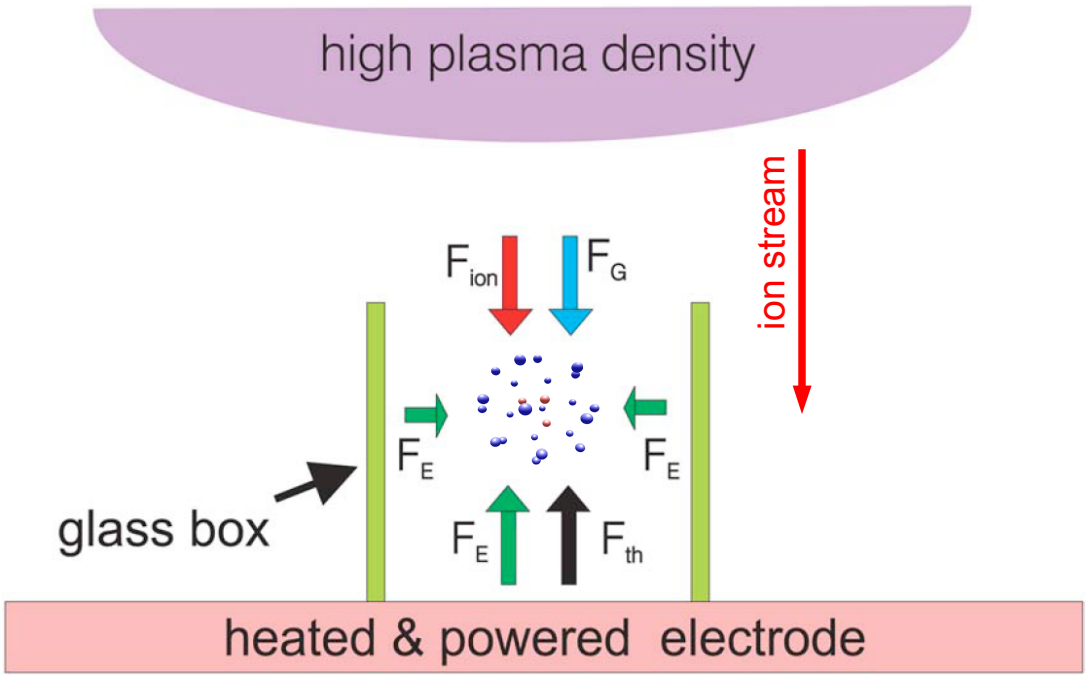
Scheme of the experimental setup



Close to electrode: strong field, fast ions
→ supersonic motion, Mach cone

Effect of fast streaming ions

Scheme of the experimental setup

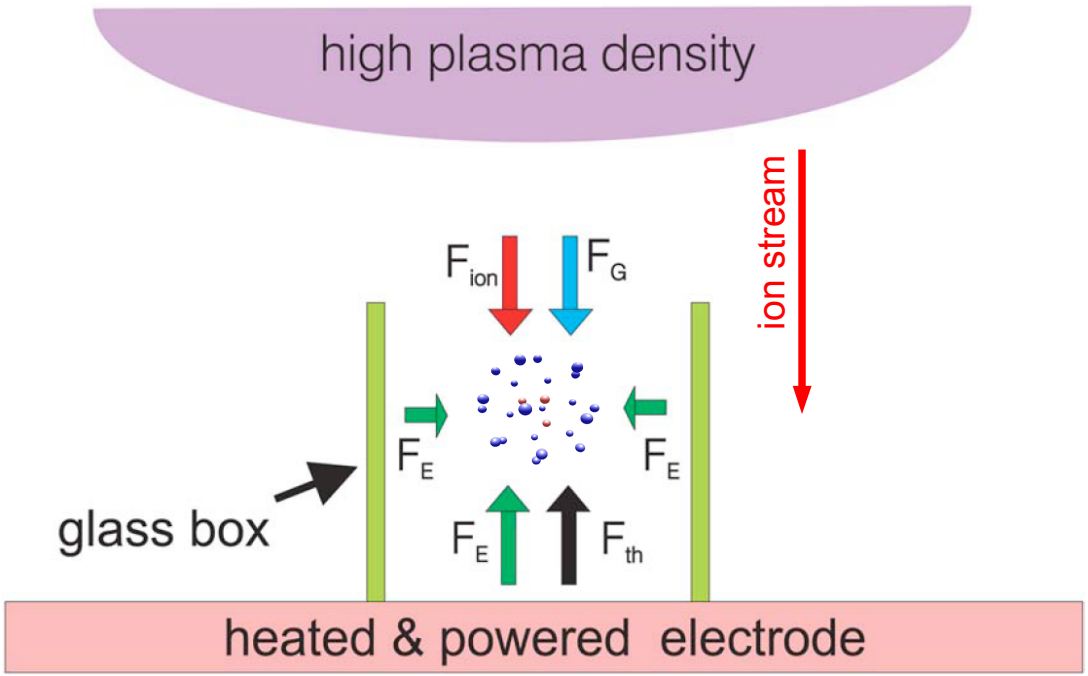


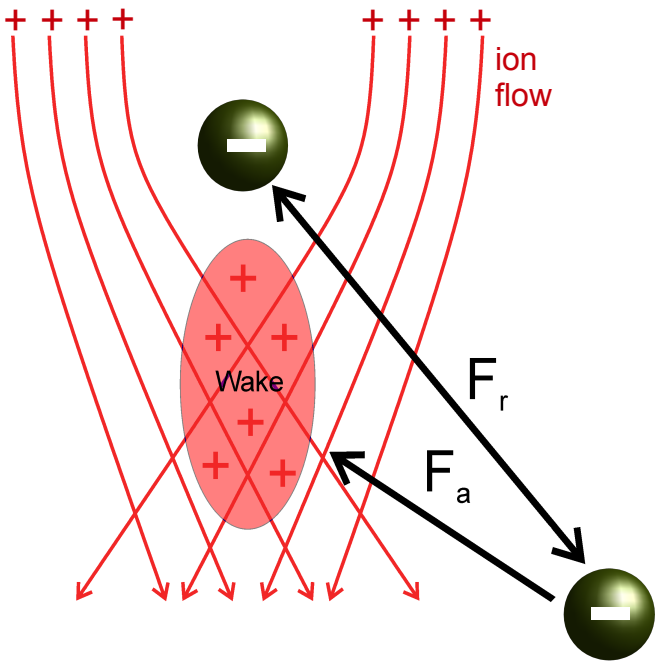
Close to electrode: strong field, fast ions
→ supersonic motion, Mach cone

Non-static problem!

Effect of fast streaming ions

Scheme of the experimental setup





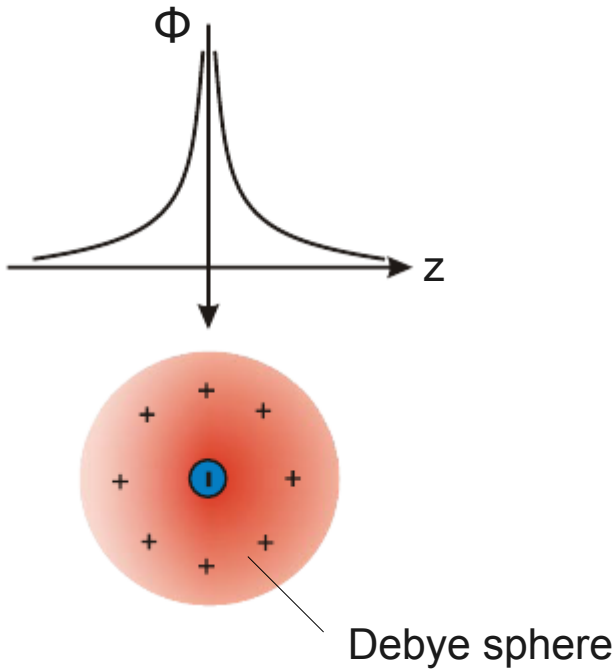
Close to electrode: strong field, fast ions
→ supersonic motion, Mach cone

Non-static problem!

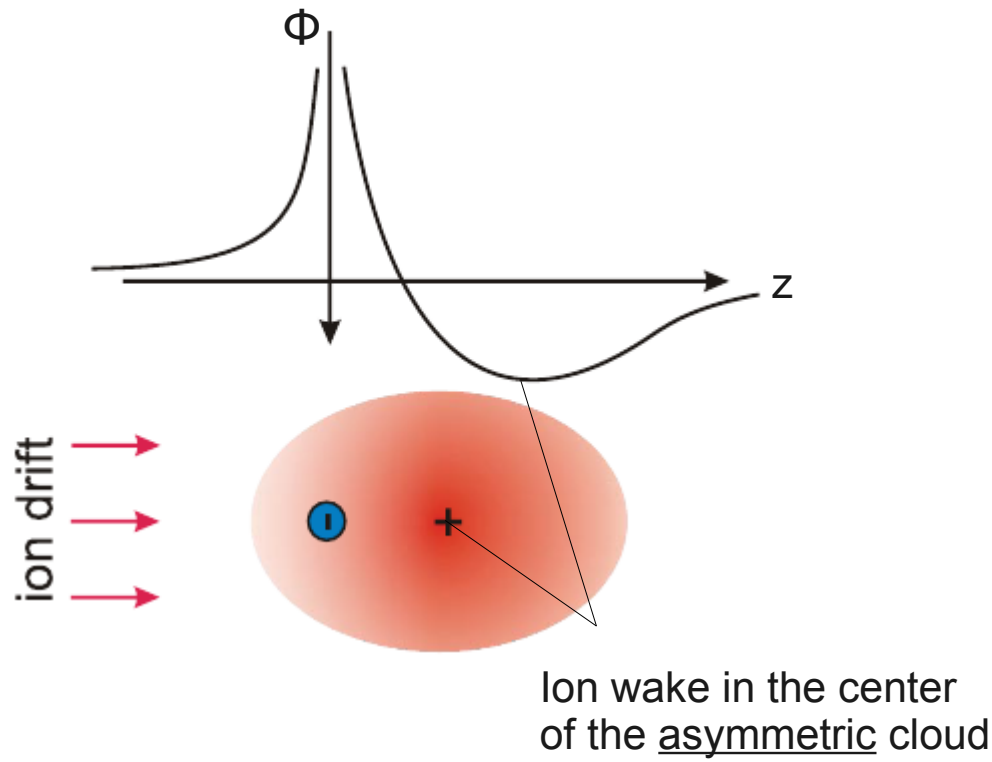
Streaming plasma (non-eq.)
→ wake-field behind charged grain
→ anisotropic potential
→ non-reciprocal grain interaction
→ vertical grain alignment

Grain Potential in a Complex Plasma

No drift:



Electric field-induced ion drift



Isotropic Yukawa (Debye) Potential:

$$\frac{(Ze)^2 e^{-\kappa \cdot |r_i - r_j|}}{|r_i - r_j|}$$

$$\kappa = \frac{1}{\lambda_D} \qquad \lambda_D^2 = \sum_a \frac{k_B T_a}{e^2 n_a}$$

POTENTIAL?

Fig.: Ivlev *et al*, PRL **100**, 095003 (2008)

Dynamically screened potential

$$\Phi_i(\mathbf{r},t) = \int \frac{d^3k}{2\pi^2} \frac{q}{k^2} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}_i t)}}{\epsilon^{\mathrm{l}}(\mathbf{k},\mathbf{k}\cdot\mathbf{v}_i)}$$

Each dust grains is 'dressed' by the e-i plasma (mediated by the dielectric function)

Fourier transform of bare Coulomb potential

Dynamically screened potential

$$\Phi_i(\mathbf{r},t) = \int \frac{d^3k}{2\pi^2}\frac{q}{k^2}\frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}_i t)}}{\epsilon^l(\mathbf{k},\mathbf{k}\cdot\mathbf{v}_i)}$$

Each dust grains is 'dressed' by the e-i plasma (mediated by the dielectric function)

Dielectric function for a (shifted) Maxwellian plasma with BGK-type collisions included

$$\epsilon^l(\mathbf{k},\omega) = 1 + \frac{1}{k^2\lambda_{De}^2} + \frac{1}{k^2\lambda_{Di}^2}\left[\frac{1+\zeta_i Z(\zeta_i)}{1+\frac{i\nu_{in}}{\sqrt{2}kv_{T_i}}Z(\zeta_i)}\right]$$

$\omega \rightarrow \mathbf{k}\cdot\mathbf{v}_i$

electrons: statical screening ($u_e \ll V_{Te}$)
ions: dynamical screening ($T_i < T_e$) (collisionless)

$$\lambda_{D_\alpha}^2 = \frac{v_{T_\alpha}^2}{\omega_p^2} = \frac{\varepsilon_0 k_B T_\alpha}{n_\alpha q_\alpha^2}$$

static screening → Yukawa potential

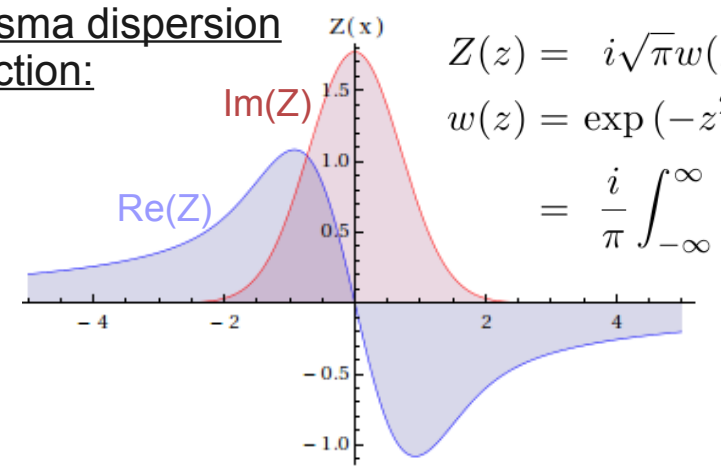
dynamical screening → wake effects

Ion-neutral scattering → collisional damping

$$\zeta_i = \frac{\mathbf{k}(\mathbf{v}_d - \mathbf{u}_i) + i\nu_{in}}{\sqrt{2}kv_{T_i}}$$ — ion neutral collison frequency

thermal velocity $v_{T_\alpha} = \sqrt{\frac{k_B T_\alpha}{m_\alpha}}$

Plasma dispersion function:

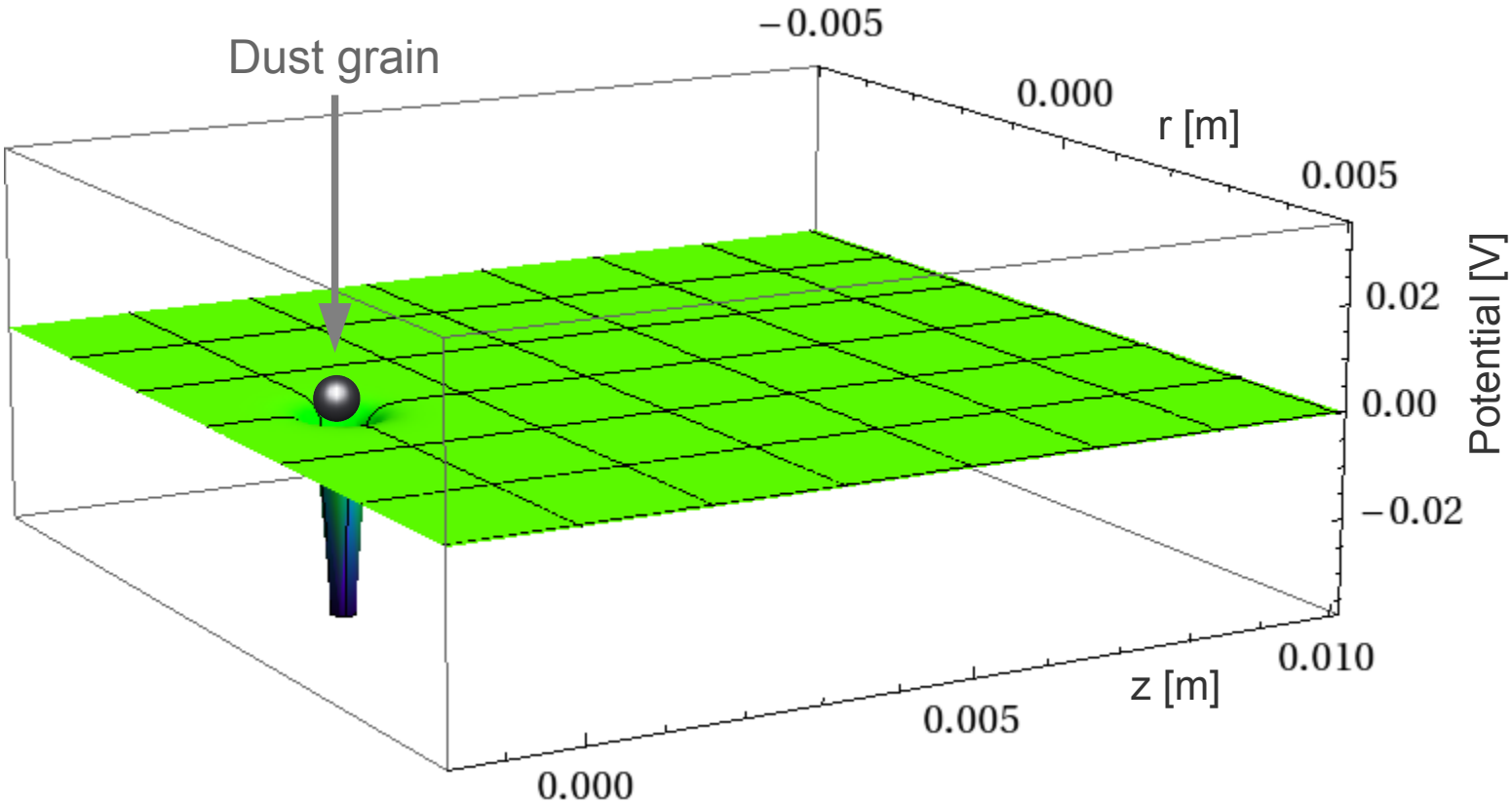


$$Z(z) = i\sqrt{\pi}w(z)$$

$$w(z) = \exp(-z^2)\mathrm{Erfc}(-iz) = \frac{i}{\pi}\int_{-\infty}^{\infty}\frac{exp(-t^2)}{z-t}dt$$

M. Lampe, G. Joyce, et al., Phys. Plasmas **7**, 3851 (2000)

No ion flow: Yukawa Potential



Statically screened Coulomb (Yukawa) potential

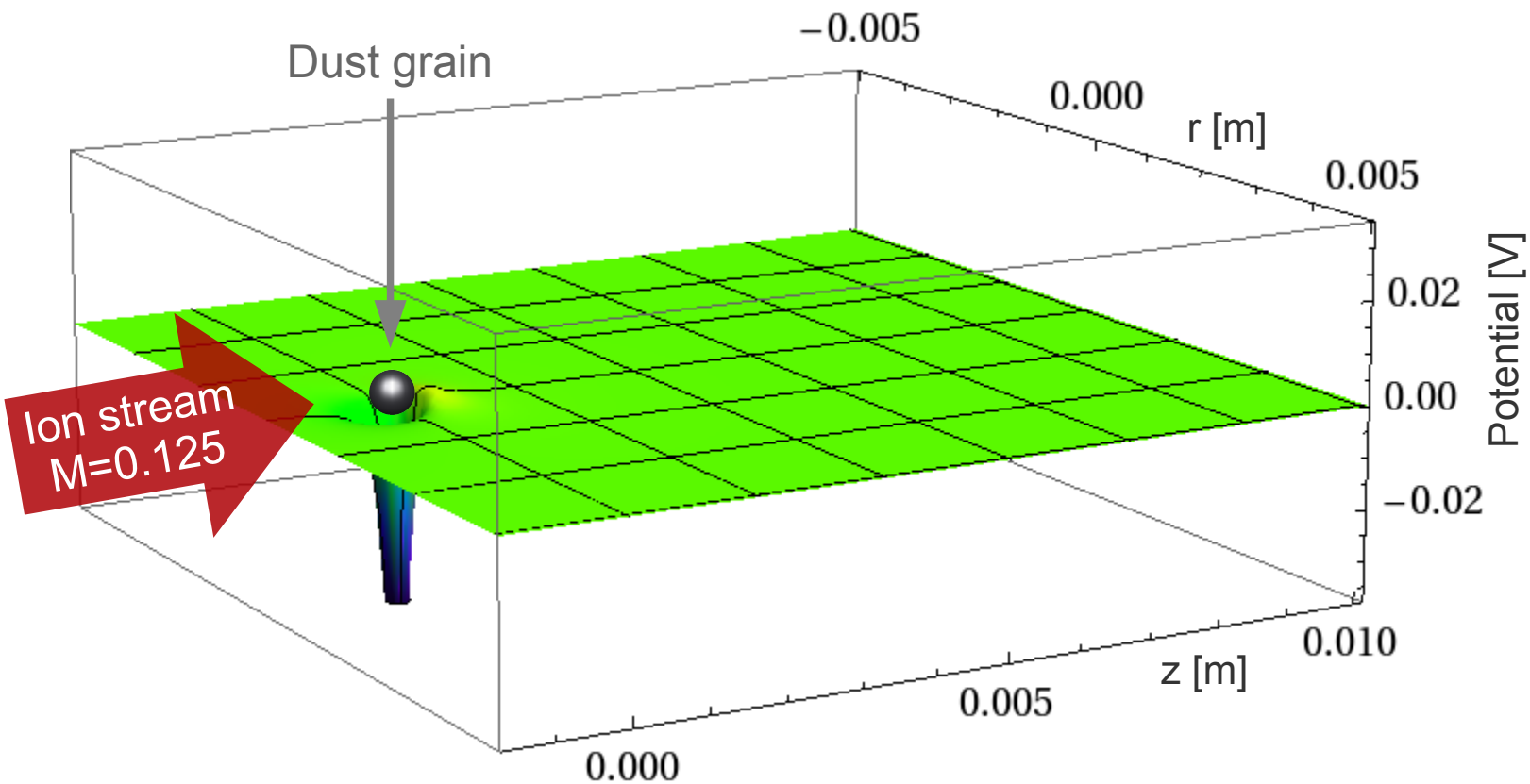
$$\frac{(Ze)^2 e^{-\kappa \cdot |r_i - r_j|}}{|r_i - r_j|}$$

$$\kappa = \frac{1}{\lambda_D}$$

$$\lambda_D^2 = \sum_a \frac{k_B T_a}{e^2 n_a}$$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, $T_e=2.585eV$ (30 000K), $T_e/T_i=30$, $\upsilon_{in}=0.1\omega_{pi}$, $\lambda_{De}=0.845mm$

Potential for Streaming Ions: M=0.125



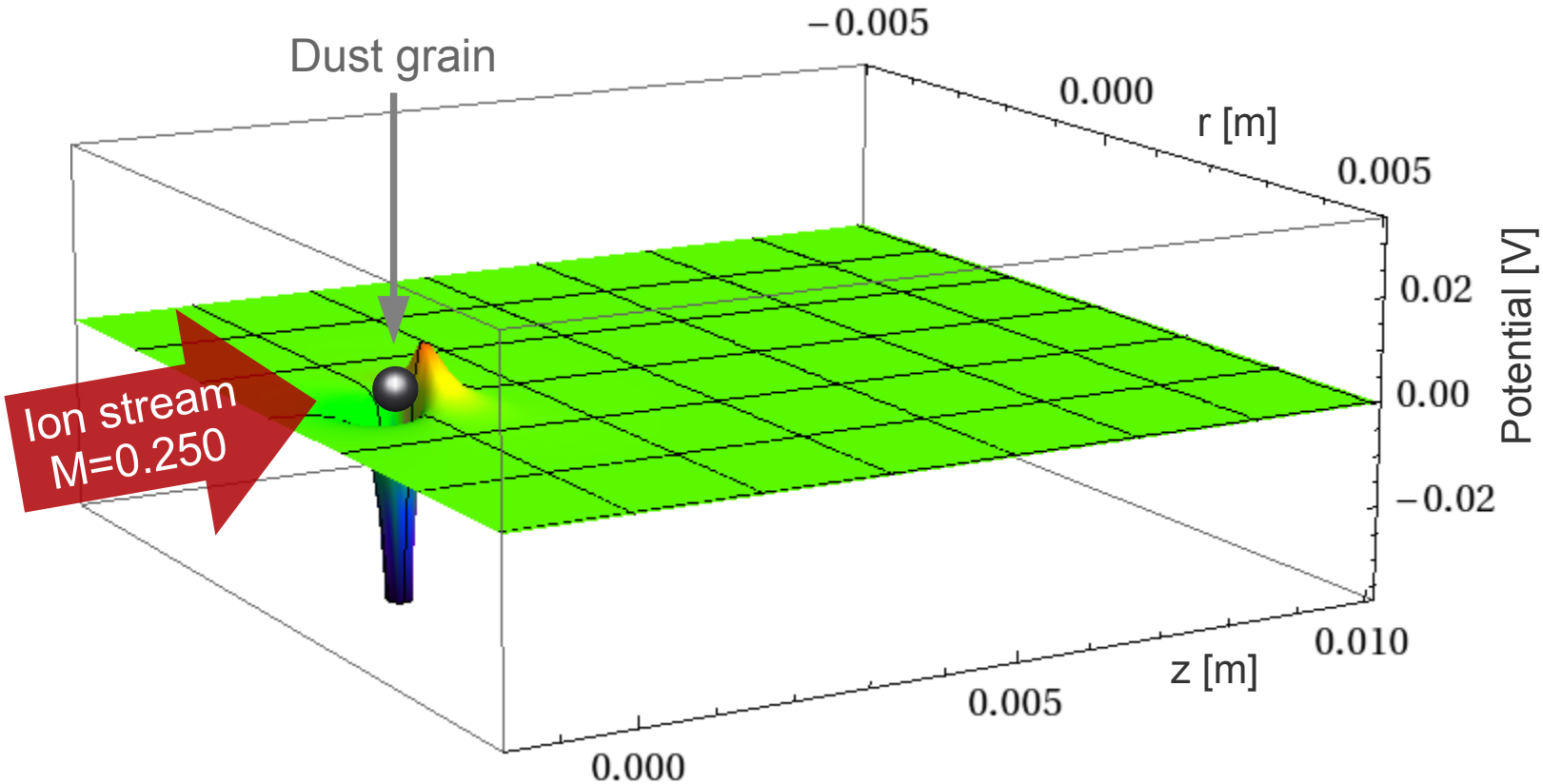
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 2.5mV @ z=0.47mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=0.250



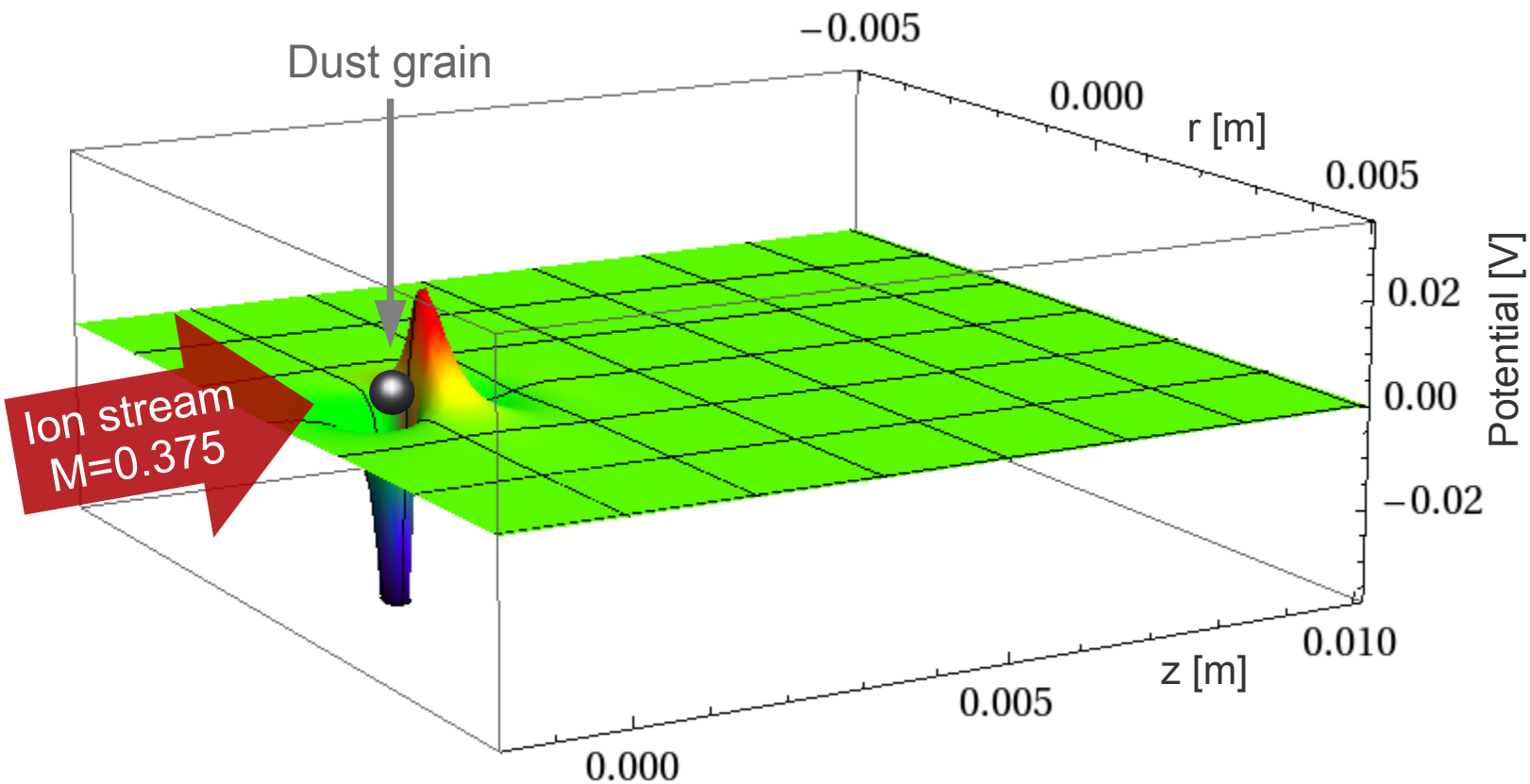
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 10.9mV @ z=0.29mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=0.375



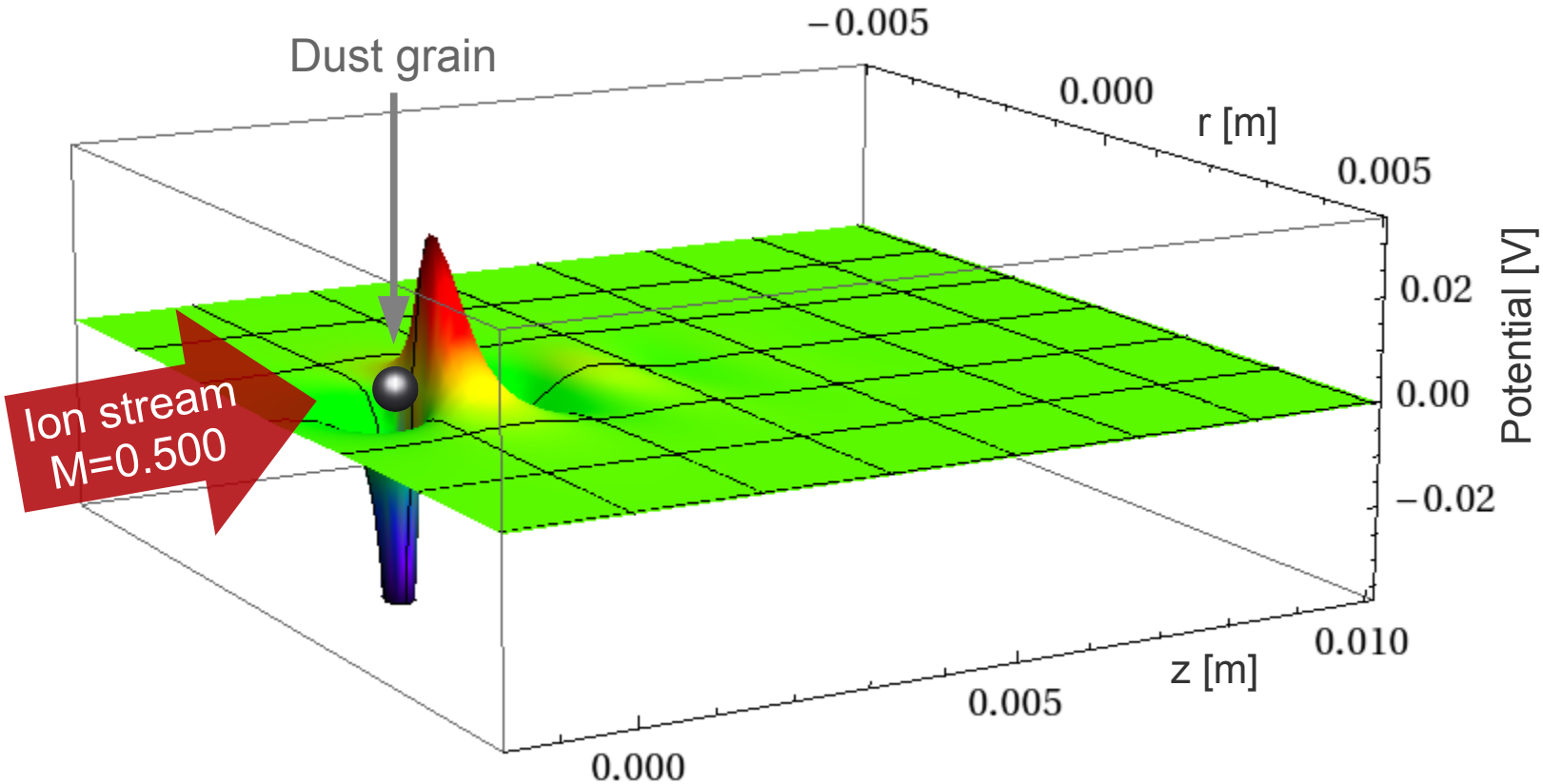
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 21.7mV @ z=0.39mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=0.500



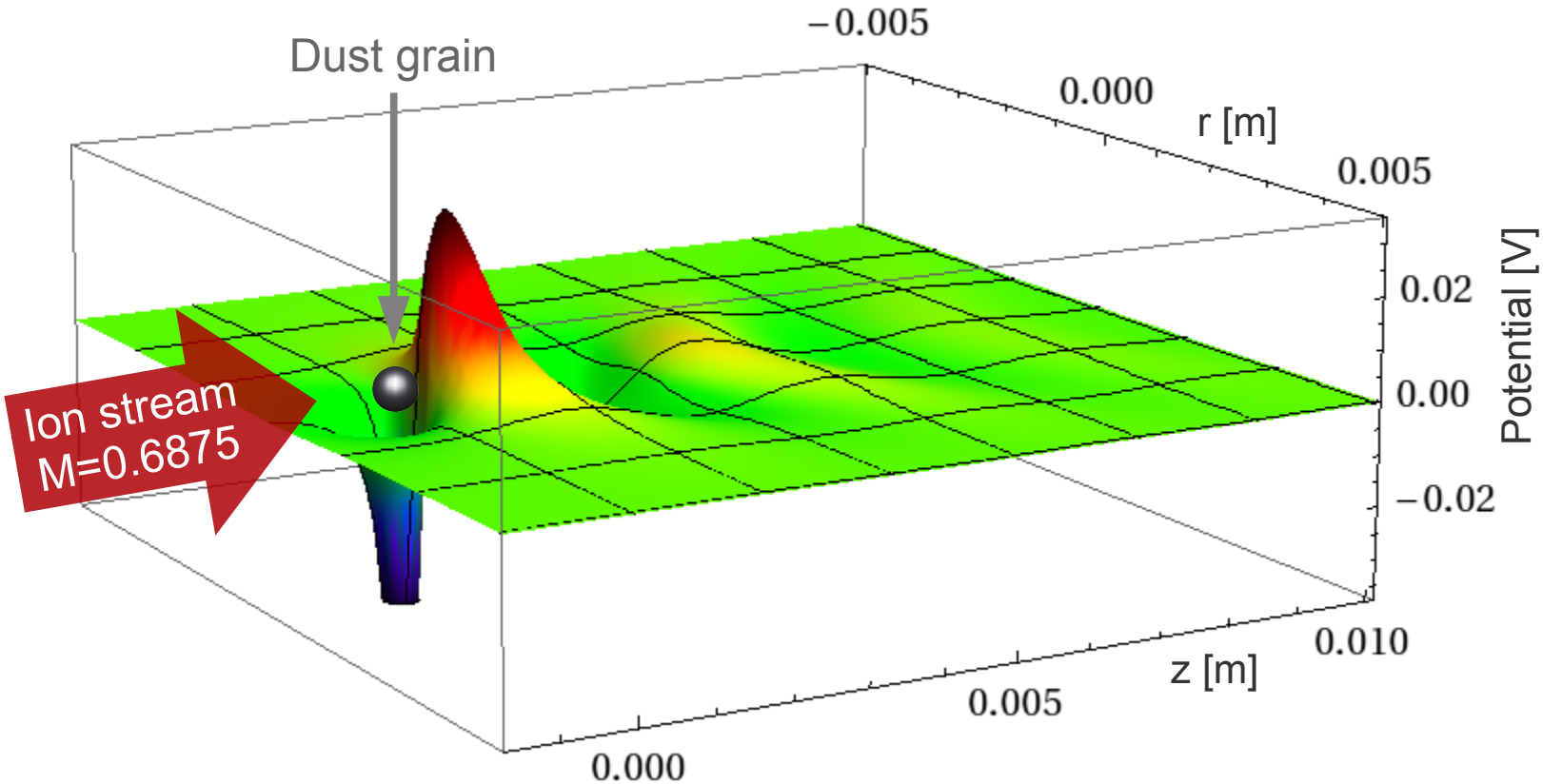
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 31.2mV @ z=0.46mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=0.6875



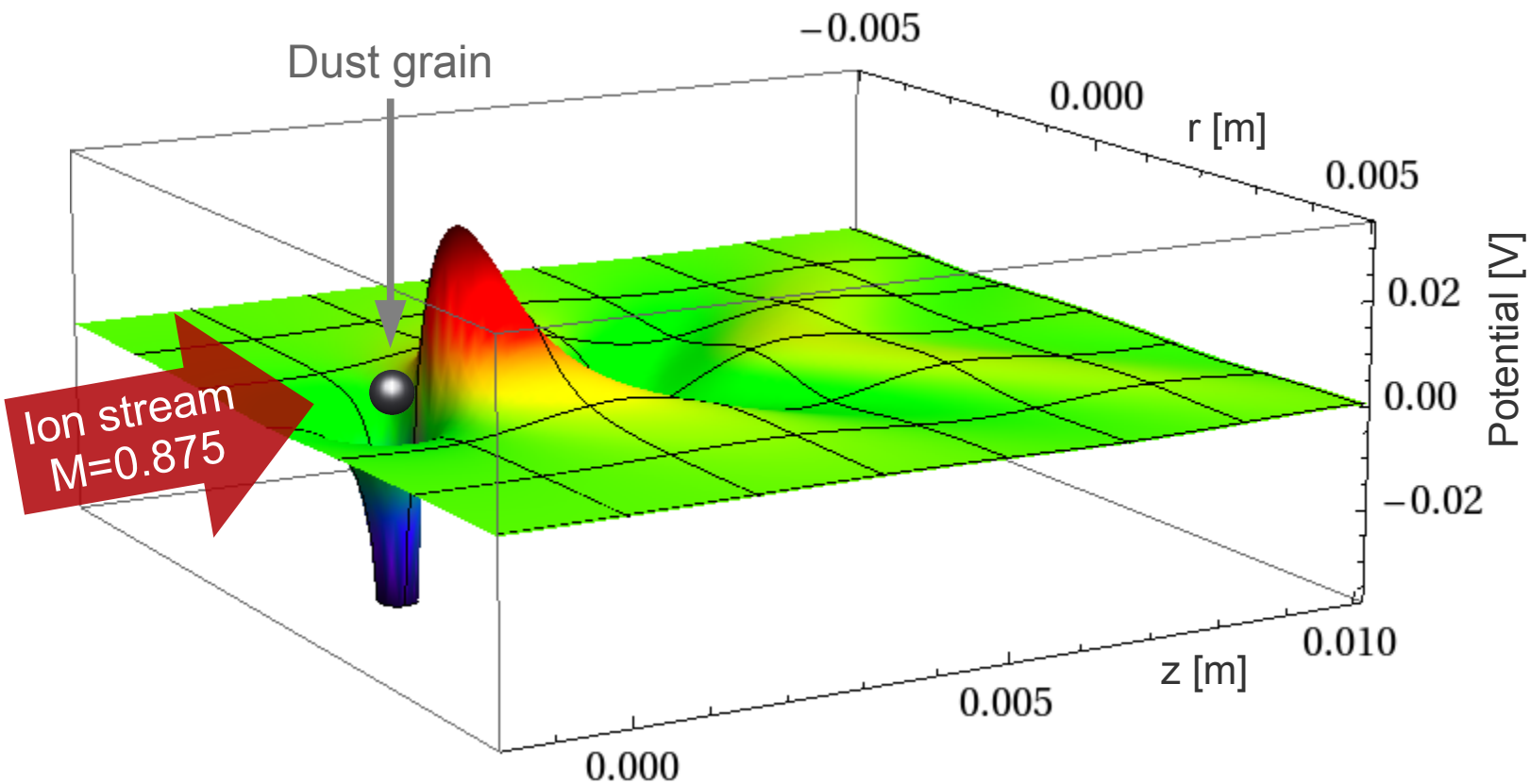
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 35.3mV @ z=0.64mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=0.875



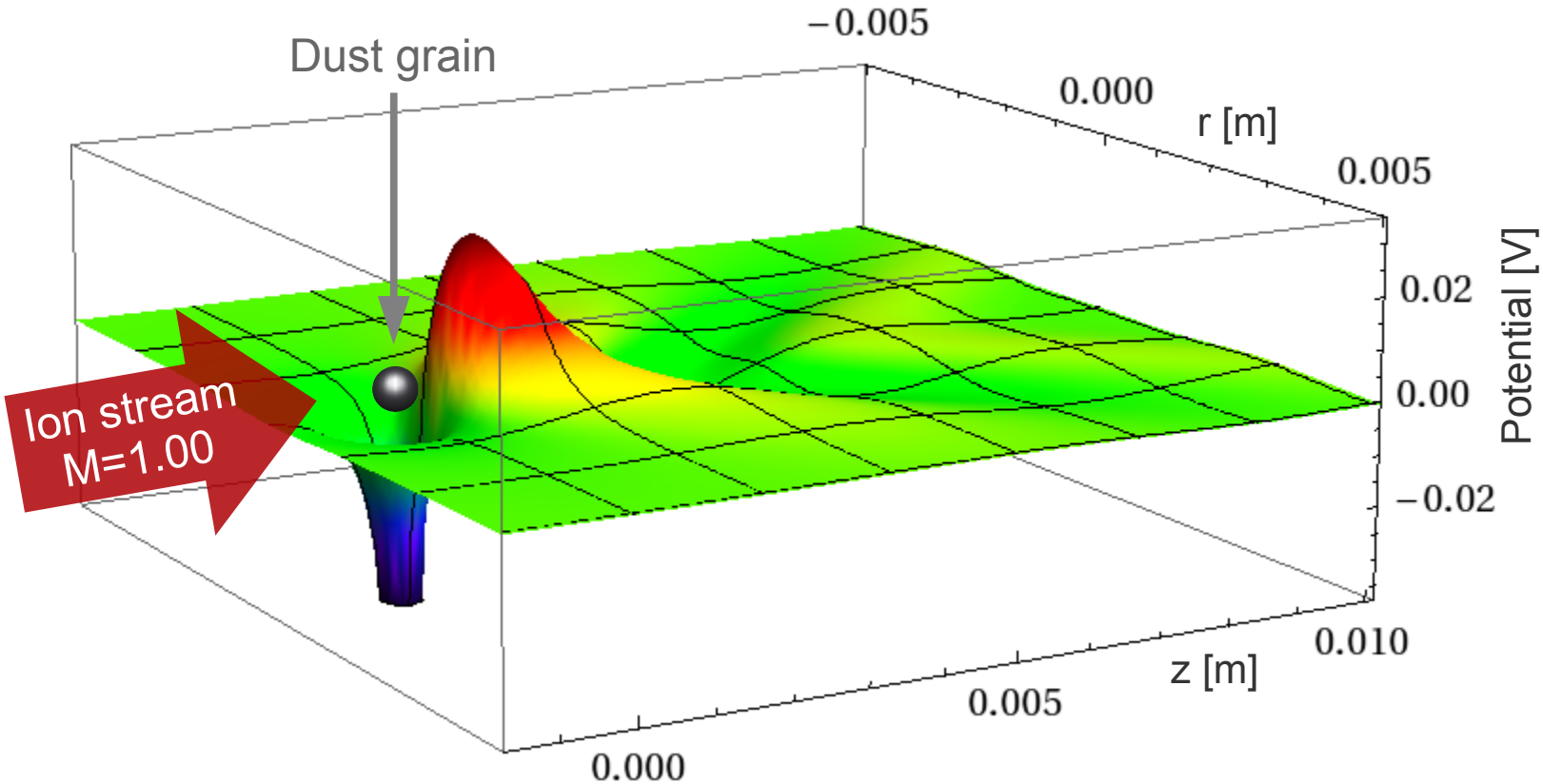
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 32.7mV @ z=0.85mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=1.00



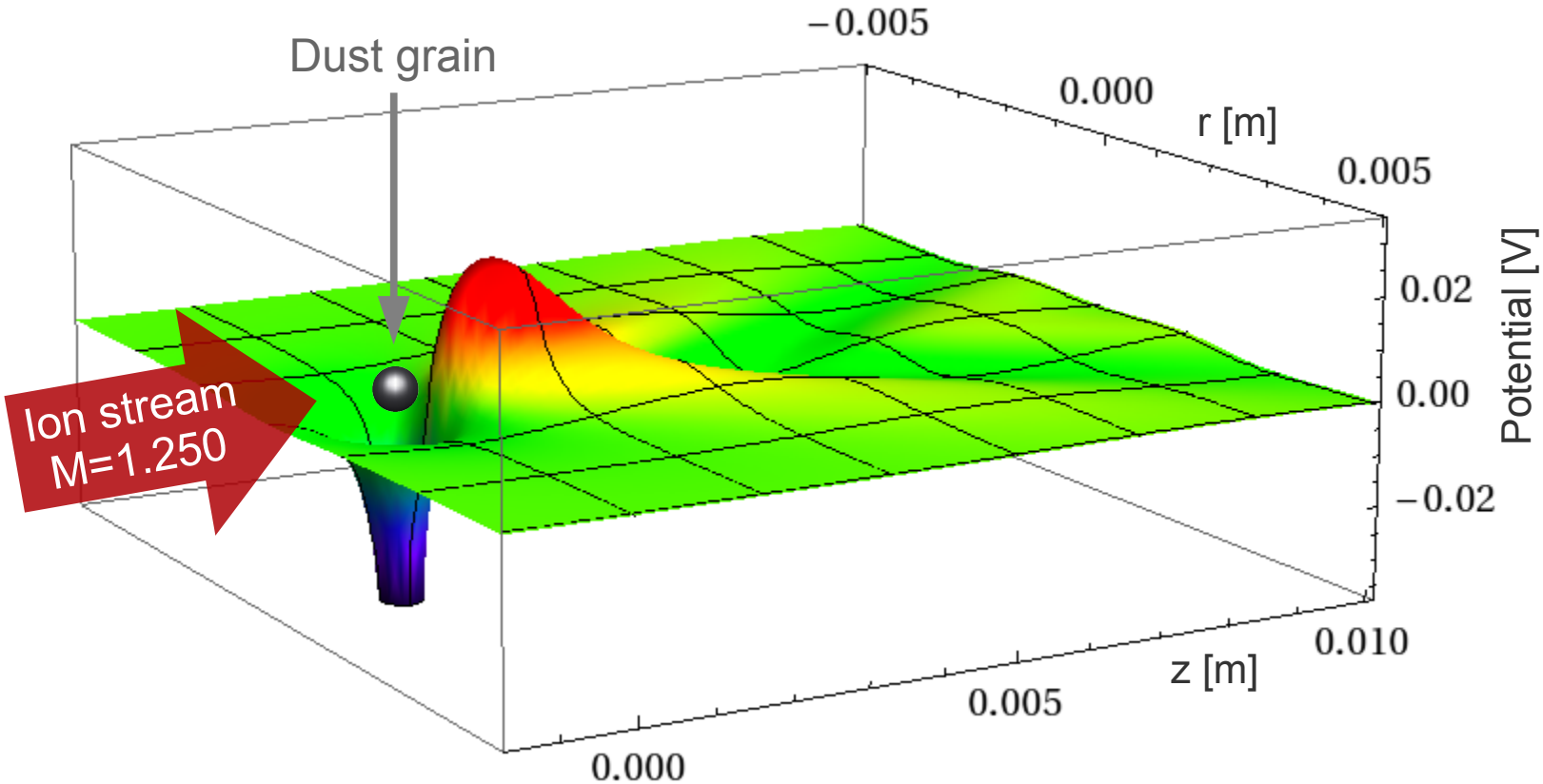
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 29.9mV @ z=0.97mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=1.250



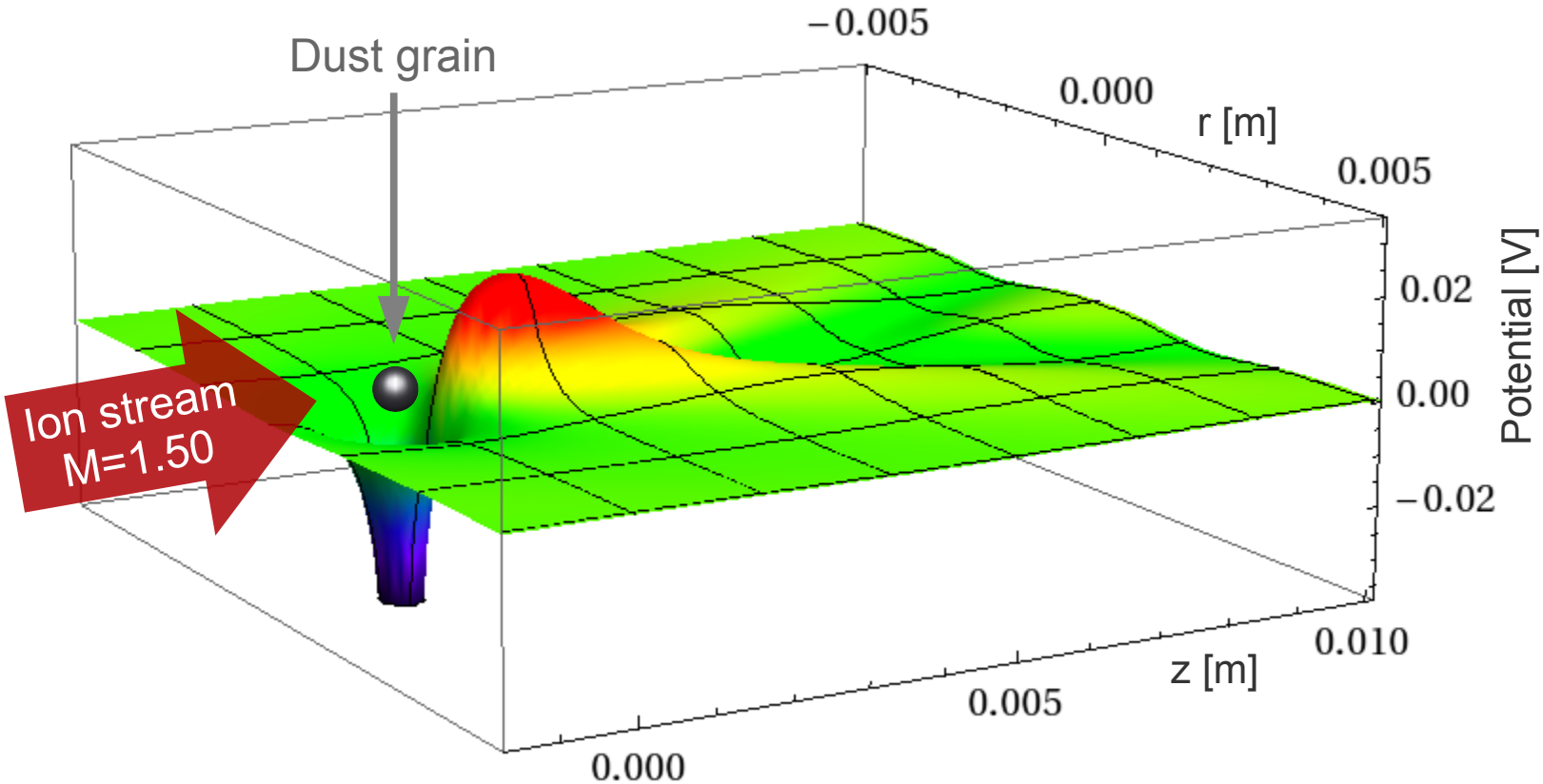
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 25.1mV @ z=1.22mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=1.50



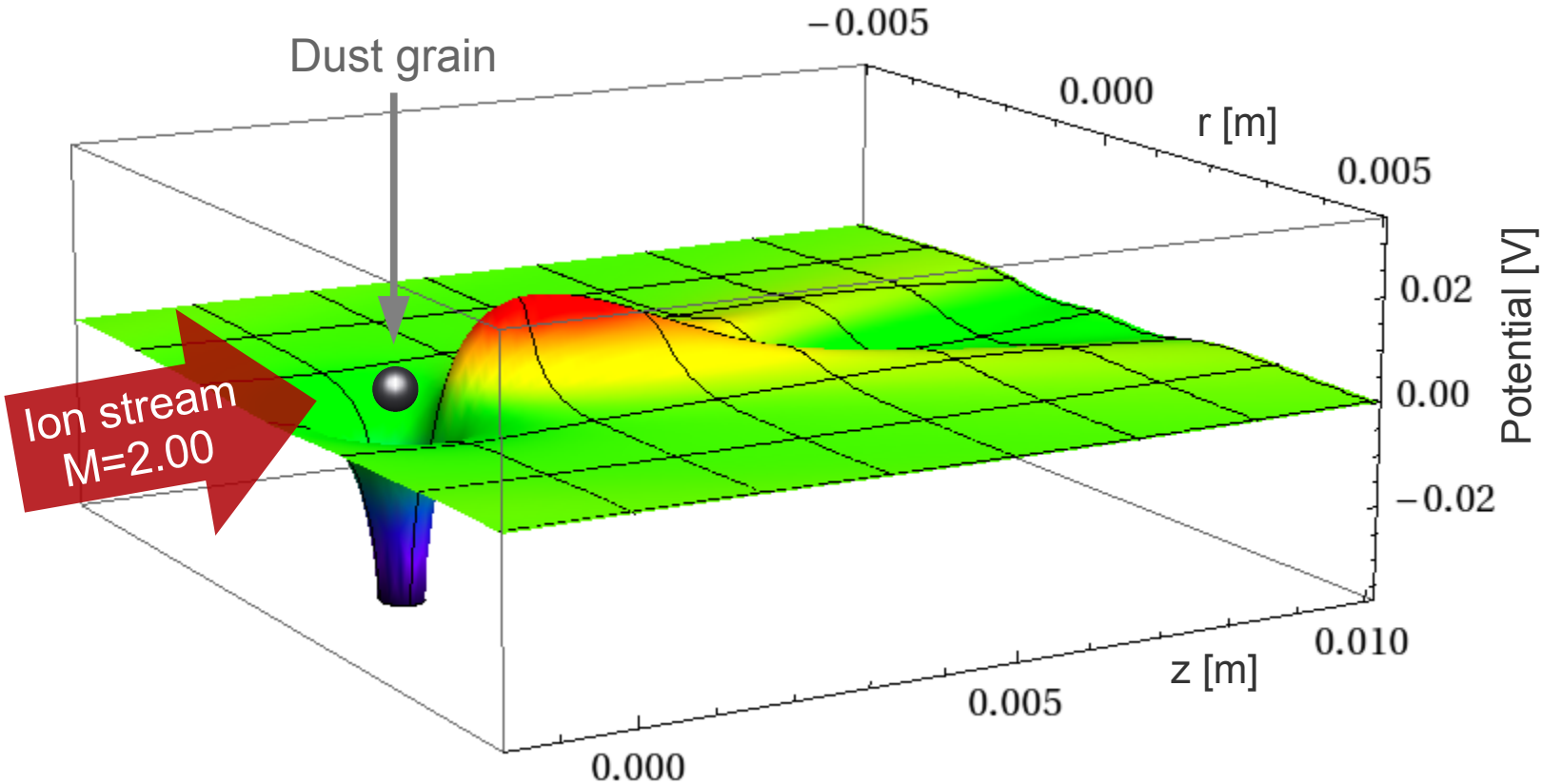
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 21.7mV @ z=1.43mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Potential for Streaming Ions: M=2.00



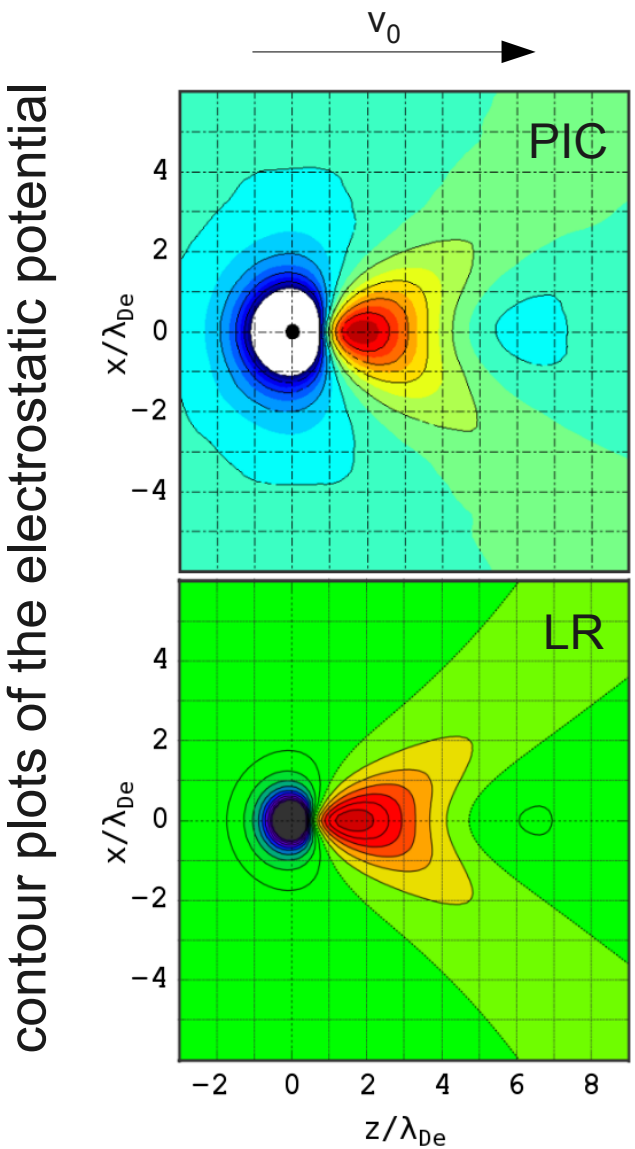
Dynamically screened Coulomb potential: 'wake' potential
(first peak height: 17.0mV @ z=1.84mm)

P. Ludwig, W.J. Miloch, H. Kählert, M. Bonitz, New J. Phys. (2012)

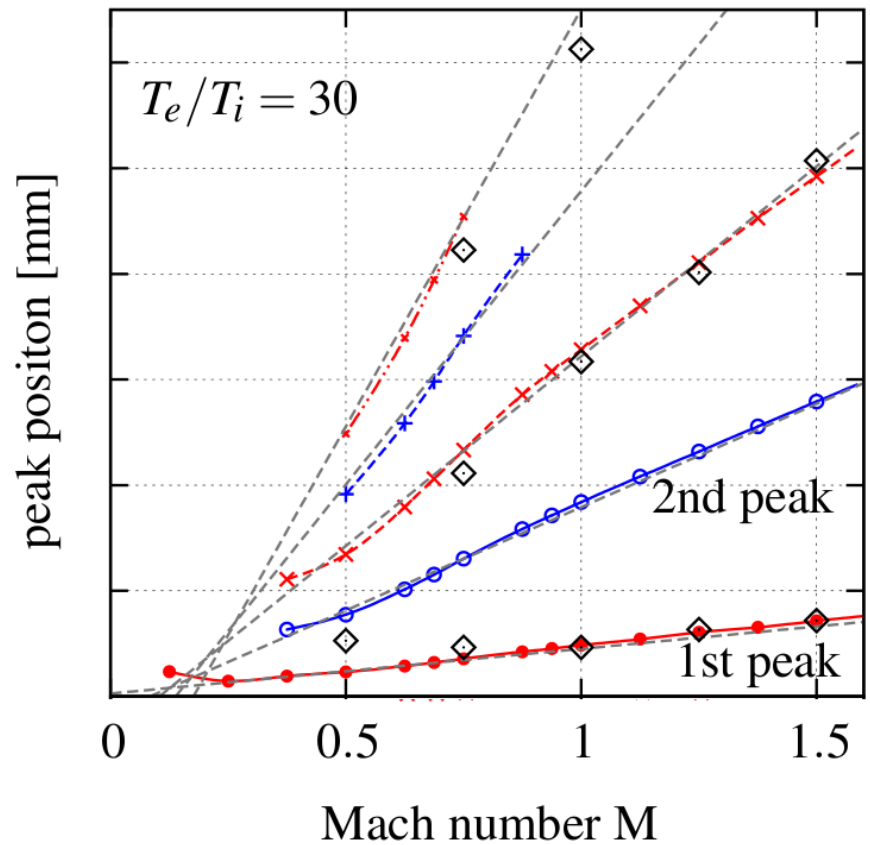
Mach number $M \equiv \frac{u_i}{c_s}$, sound (Bohm) speed $c_s \equiv \sqrt{\frac{k_B T_e}{m_i}}$

Plasma parameters (Argon): $n=2\times10^8 cm^{-3}$, T_e=2.585eV (30 000K), T_e/T_i=30, $\upsilon_{in}=0.1\omega_{pi}$, λ_{De}=0.845mm

Linear Dielectric Response ansatz validated against full nonlinear 3D Particle-in-Cell (PIC) simulations



3D PIC by W. Miloch (top) vs LR results (bottom) for M=1.5, T_e/T_i=10, and collision freq. υ_{in}=0.



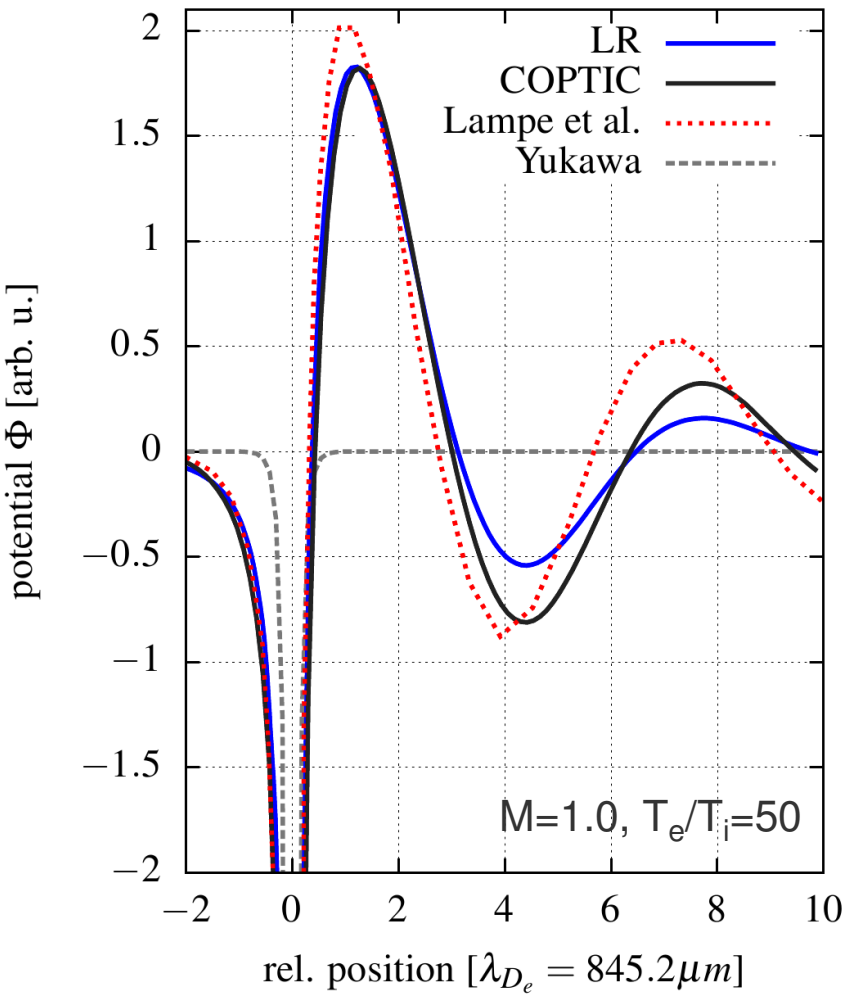
LR results: Peak positions of the wake potential as function of Mach number M. Red (blue) lines correspond to a positive (negative) space charge.

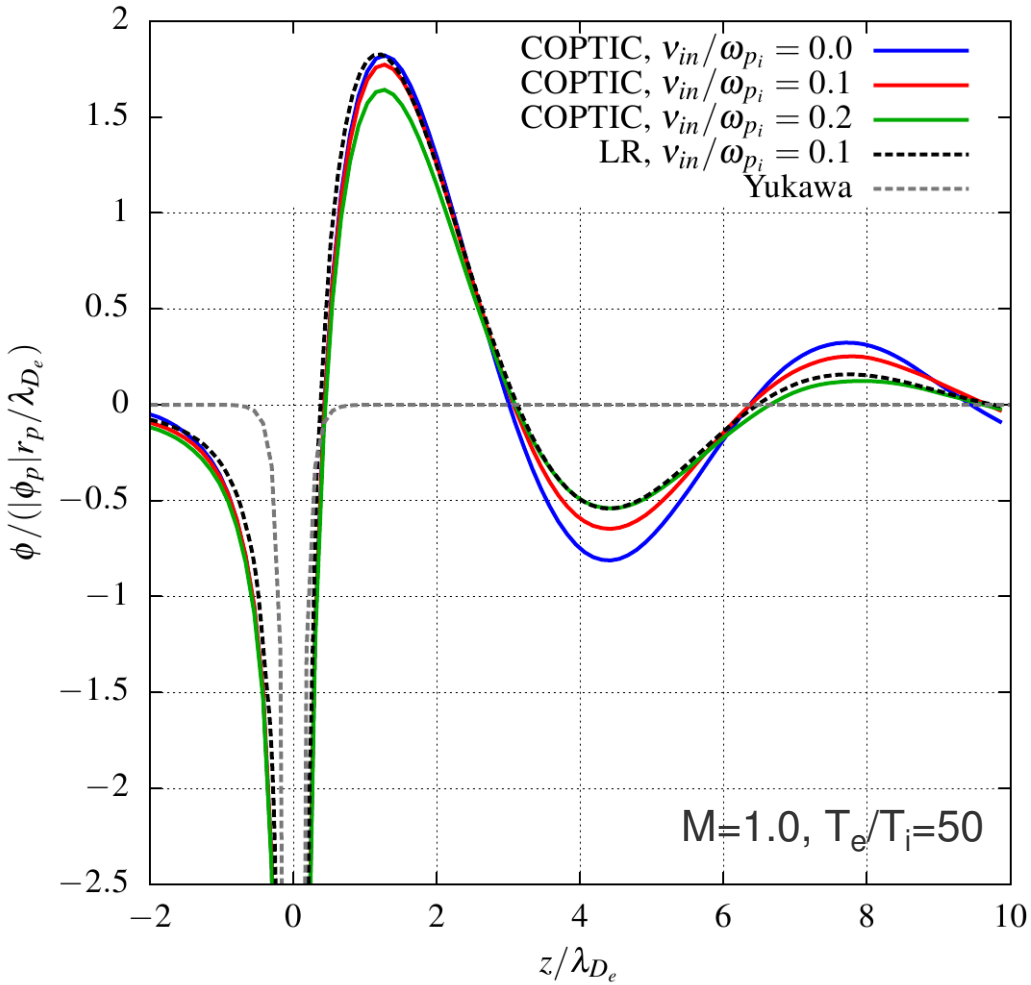
Diamonds: 3D PIC results for the wake maxima (collisionless plasma, W. Miloch)

P. Ludwig, W.J. Miloch, H. Kählert, and M. Bonitz, New J. Phys. (2012)

Linear Dielectric Response ansatz validated against full nonlinear 3D Particle-in-Cell (PIC) simulations

Potential cuts through the grain along the flow direction





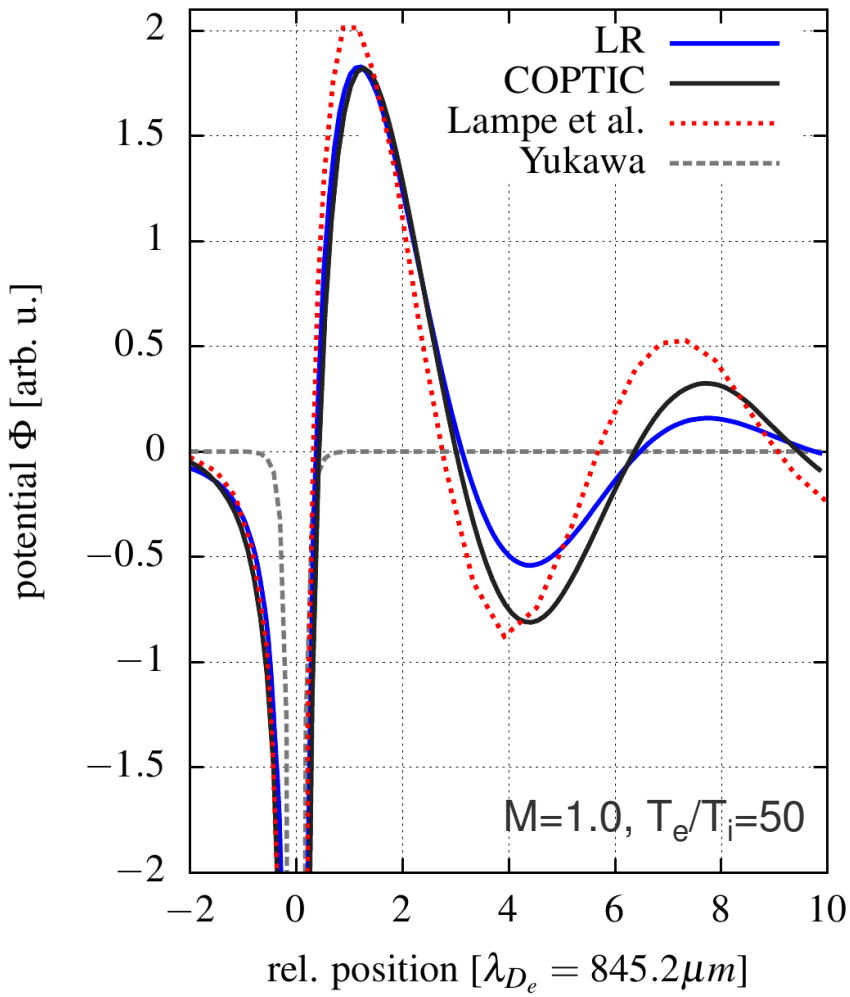
LR: finite damping included υ_{in}=0.1,
COPTIC: collsionless PIC*
Lampe *et al.*: collisionless LR

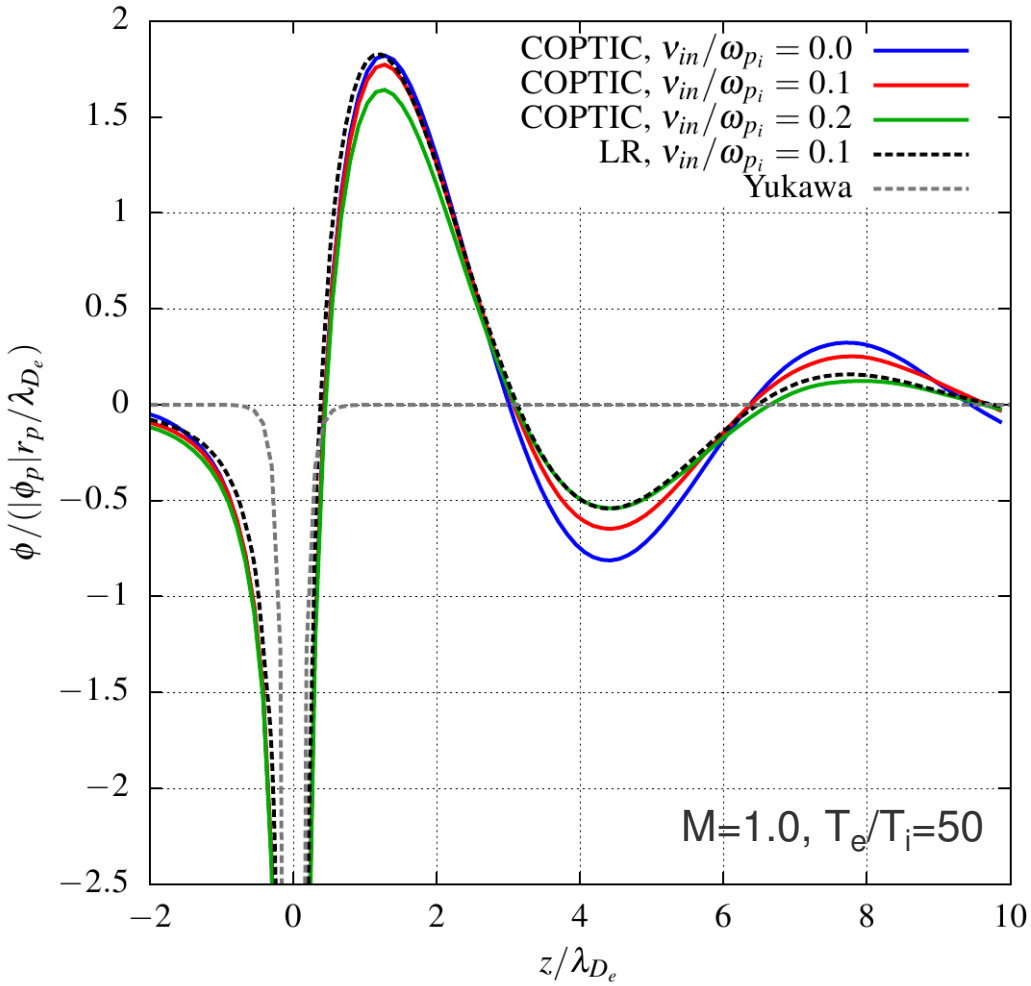
PIC (COPTIC) results* for different collision frequencies vs. Linear Response calculation for υ_{in}=0.1.

* I. Hutchinson, Phys. Plasmas **18**, 032111 (2011)

Linear Dielectric Response ansatz validated against full nonlinear 3D Particle-in-Cell (PIC) simulations

Potential cuts through the grain along the flow direction





LR: finite damping included υ_{in}=0.1,
COPTIC: collsionless PIC*
Lampe *et al.*: collisionless LR

PIC (COPTIC) results* for different collision frequencies vs. Linear Response calculation for υ_{in}=0.1.

Excellent quality of the linear LR results → accurate N-particle-dynamics

* I. Hutchinson, Phys. Plasmas **18**, 032111 (2011)

N-particle simulation of a realistic plasma
Multiscale approach

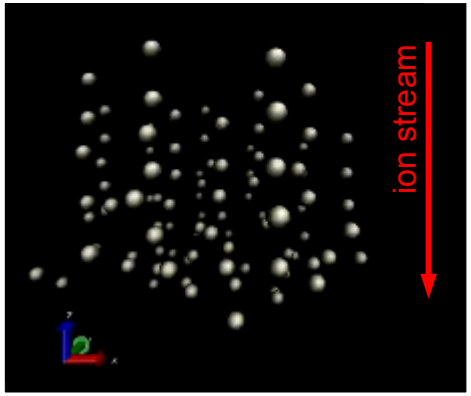
Langevin dynamics scheme for correlated dust:

$$m_d \ddot{\mathbf{r}}_k = -\nabla V_k^{\text{eff}}(\mathbf{r},t) - \omega_0^2 m_d \mathbf{r}_k - \nu_{dn} m_d \dot{\mathbf{r}}_k + \mathbf{f}_k(t)$$

$$V_k^{\text{eff}}(\mathbf{r},t) = \sum_{l \neq k}^{N_d} q_d \Phi_l(\mathbf{r},t) \qquad \Phi_i(\mathbf{r},t) = \int \frac{d^3k}{2\pi^2} \frac{q}{k^2} \frac{e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{v}_i t)}}{\epsilon^{\mathrm{l}}(\mathbf{k}, \mathbf{k}\cdot\mathbf{v}_i)}$$

friction coefficient, Gaussian random force, and plasma temperature are related by the fluctuation-dissipation theorem

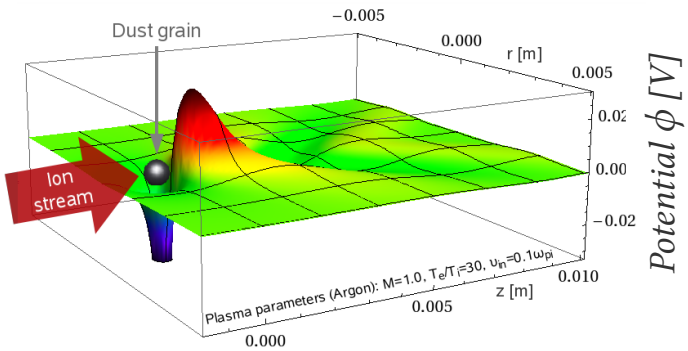
$$\langle \mathbf{f}_i^\alpha(t) \mathbf{f}_j^\beta(t') \rangle = 2m\nu_{dn} k_B T \delta_{ij} \delta_{\alpha\beta} \delta(t-t'), \ \alpha, \beta \in \{x, y, z\}$$



Dust chains in a streaming ion-electron plasma

Approximations:

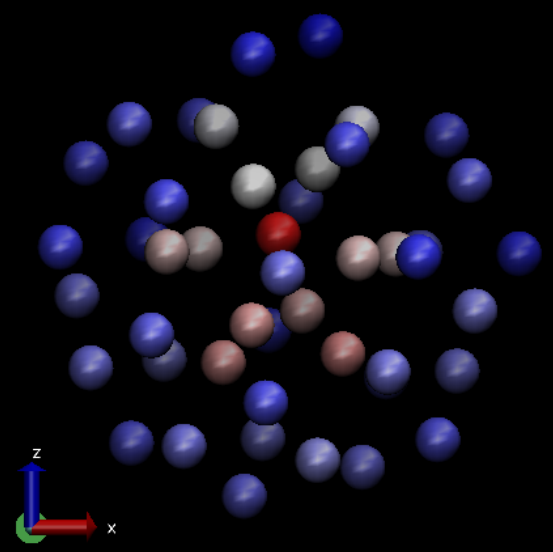
1. neutrals in thermal equilibrium
2. average over particle (d) plasma period → stationary e-i flow
3. Fokker-Planck approximation for d-n interaction
4. weak d-i and d-e coupling → lineare response for e-i dynamics



Multiscale Dust Dynamics Simulations

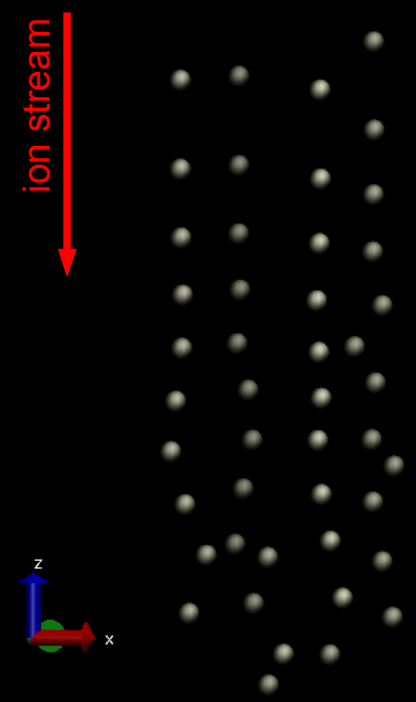
Snapshots, 46 particles in a trap

M=0.01



N=46

M=1.0



Simulation parameters

Electrons: $n_e=n_i=1.0E14/m^3$, $T_e=2.5eV$, $\lambda_{De}(T_e,n_e)=1175.41\mu m$

Ions (Argon, Z=1): temperature: $T_e/T_i=83.333$ ($T_i=0.03eV=348K$), $\lambda_{Di}(T_i,n_i)=128.76\mu m$

Neutrals: gas pressure: 15Pa, scattering freq.: $\nu_{in}/\omega_i=0.201$, $T_n=T_i$

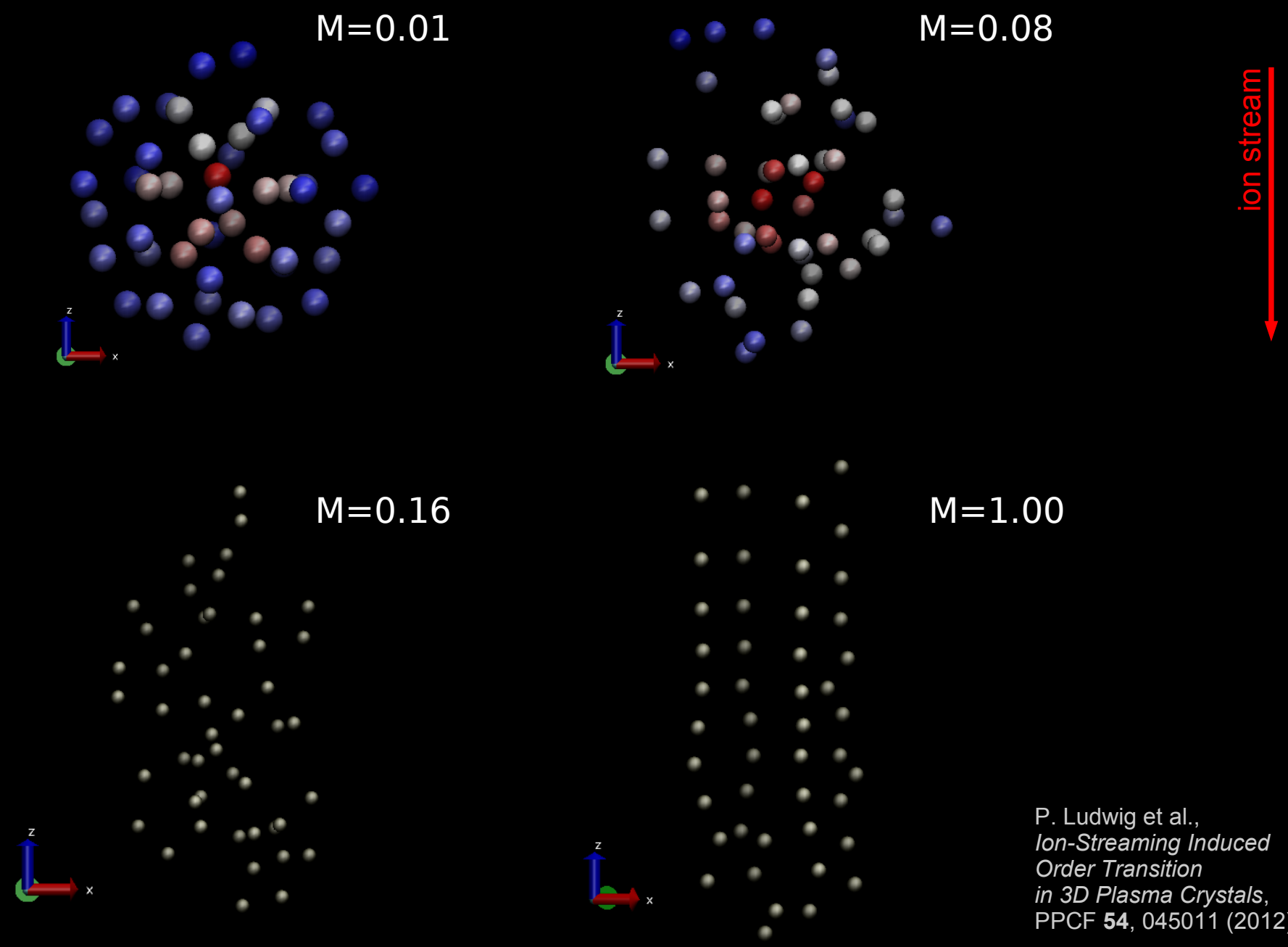
Dust: charge: $Q_d=-6000e_0$, coll. freq.: $\nu_{dn}=19.08Hz$, radius: $R_d=2.43\mu m$, $m_d=9.1E-14kg$

trap: $\omega_0=\omega_z=7.0Hz$, $c_s=\mathrm{sqrt}(k_BT_e/m_i)=2460m/s$, $\lambda_{D,tot}^{-2}=\lambda_{De}^{-2}+\lambda_{Di}^{-2}=128.00\mu m$, $\lambda_{D\alpha}=\mathrm{sqrt}(\varepsilon_0 k_B T_\alpha/(n_\alpha q_\alpha^2))$

P. Ludwig et al., *Ion-Streaming Induced Order Transition in 3D Plasma Crystals*, Plas. Phys. Control. Fusion **54**, 045011 (2012)

Multiscale Dust Dynamics Simulations

Snapshots, 46 particles in a trap

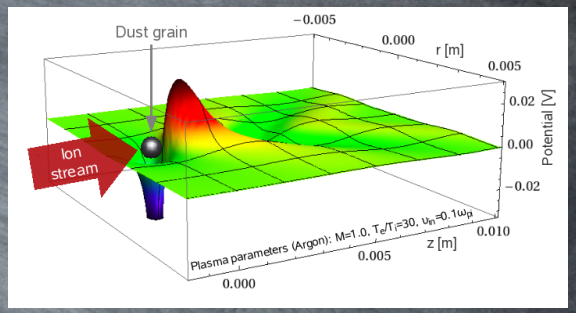


P. Ludwig et al.,
Ion-Streaming Induced Order Transition in 3D Plasma Crystals,
PPCF **54**, 045011 (2012)

Quo vadis?

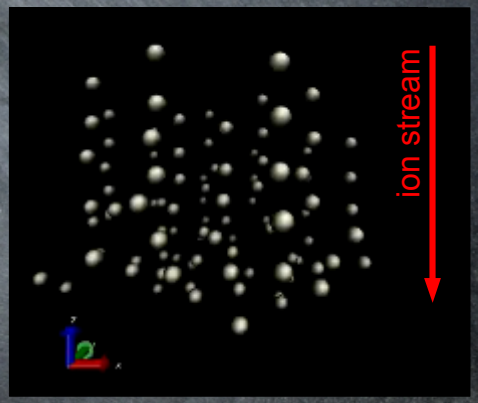
1. Initial code development and high precision computation of the <u>classical</u> wake potential
   → Linear response approach validated by self-consist. nonlinear 3D PIC simulations (Miloch, Hutchinson)

   Ludwig et al., 'On the Wake Structure in Streaming Complex Plasmas', New Journal of Physics (2012)



2. Implementation and test of our multiscale Langevin Dynamics code; first results for the collective particle dynamics in the presence of a streaming plasma background (proof of concept)
   → test system: classical complex (dusty) plasmas
   → (moderate) plasma streaming can trigger structural instabilities / phase transitions

   Ludwig et al., 'Ion-Streaming Induced Order Transition in 3D Dust Clusters', Plas. Phys. Control. Fusion (2012)



3. Computation of the dynamically screened ion potential using a quantum (Mermin) dielectric function
   → any degeneracy
   → appropriate inclusion of collisional effects and local-field corrections of electron coupling interactions
   → check: tdDFT reference calculation of a streaming ion in a degenerate electron gas?!

4. Large-scale MD simulations of unconfined dense quantum plasmas (PBC)

Many thanks for your attention!

Bonitz, Horing, Ludwig (eds.), 'Introduction to Complex Plasmas', Springer 2010

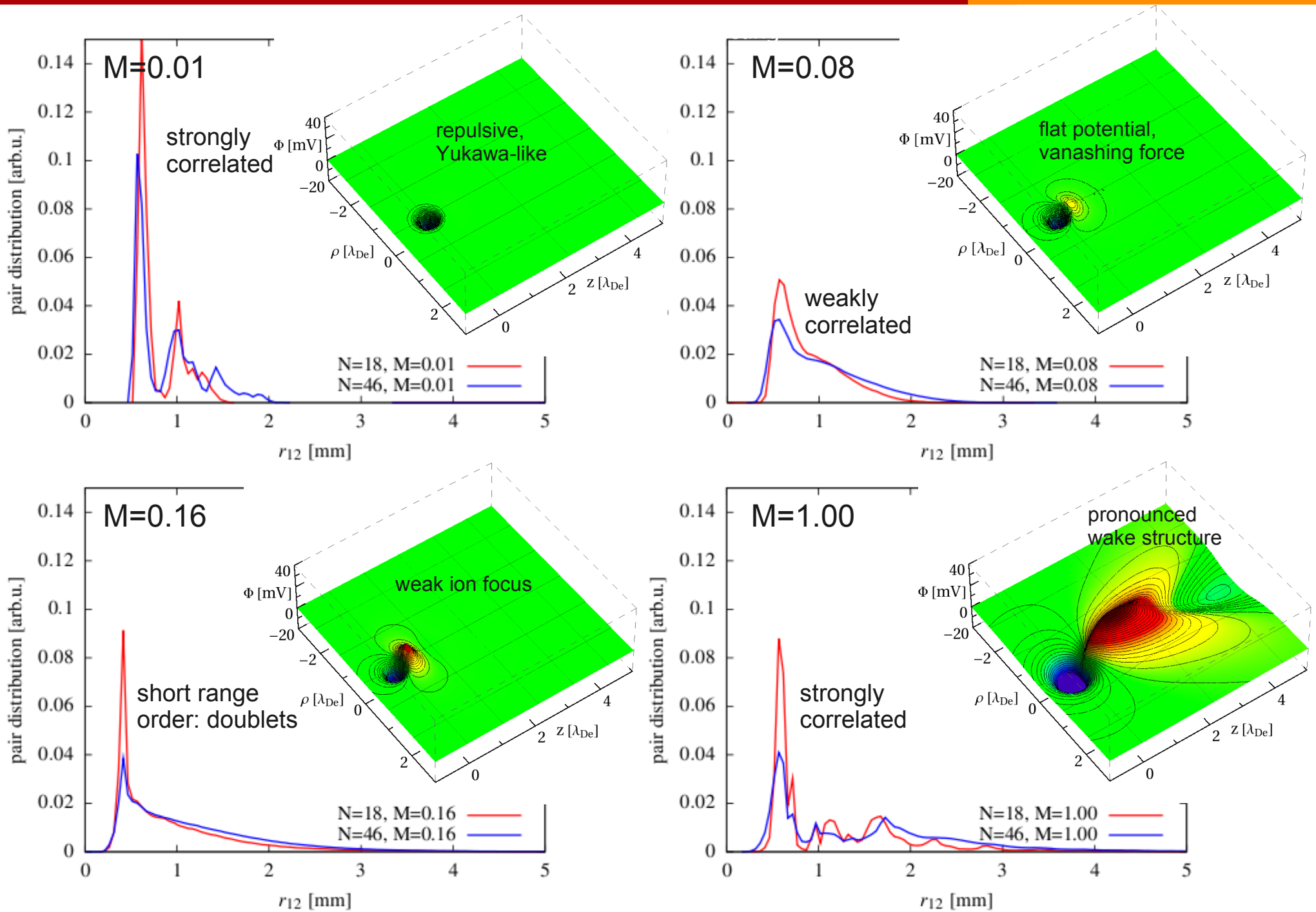
Ludwig et al., 'Tuning Correlations in Multi-Component Plasmas',
Plas. Phys. Control. Fusion (2010)

Ludwig et al., 'Ion-Streaming Induced Order Transition in 3D Dust Clusters',
Plas. Phys. Control. Fusion (2012)

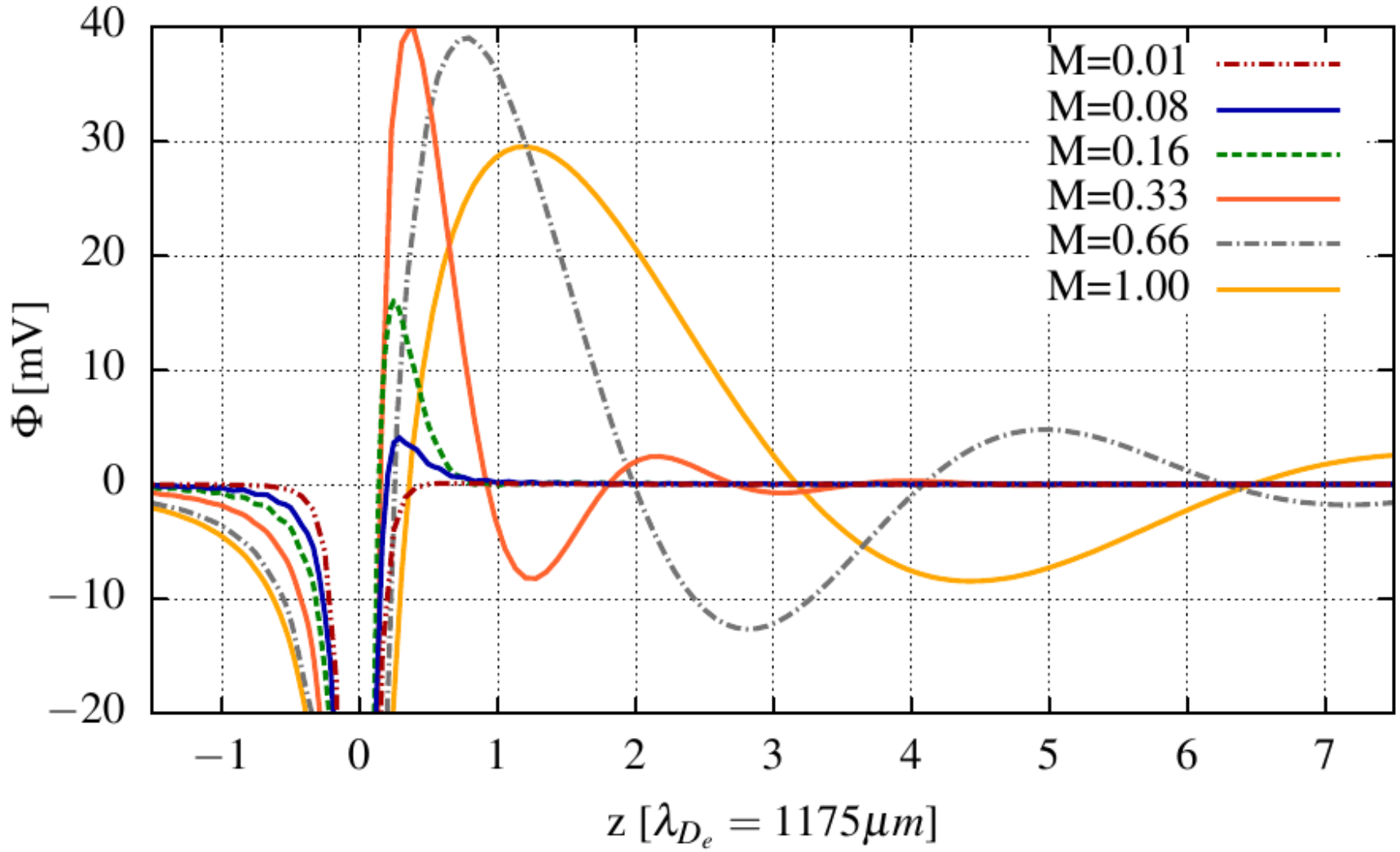
Ludwig et al., 'On the Wake Structure in Streaming Complex Plasmas',
New Journal of Physics (2012)

http://dr-ludwig.com

Pair distribution function
(thermally averaged)

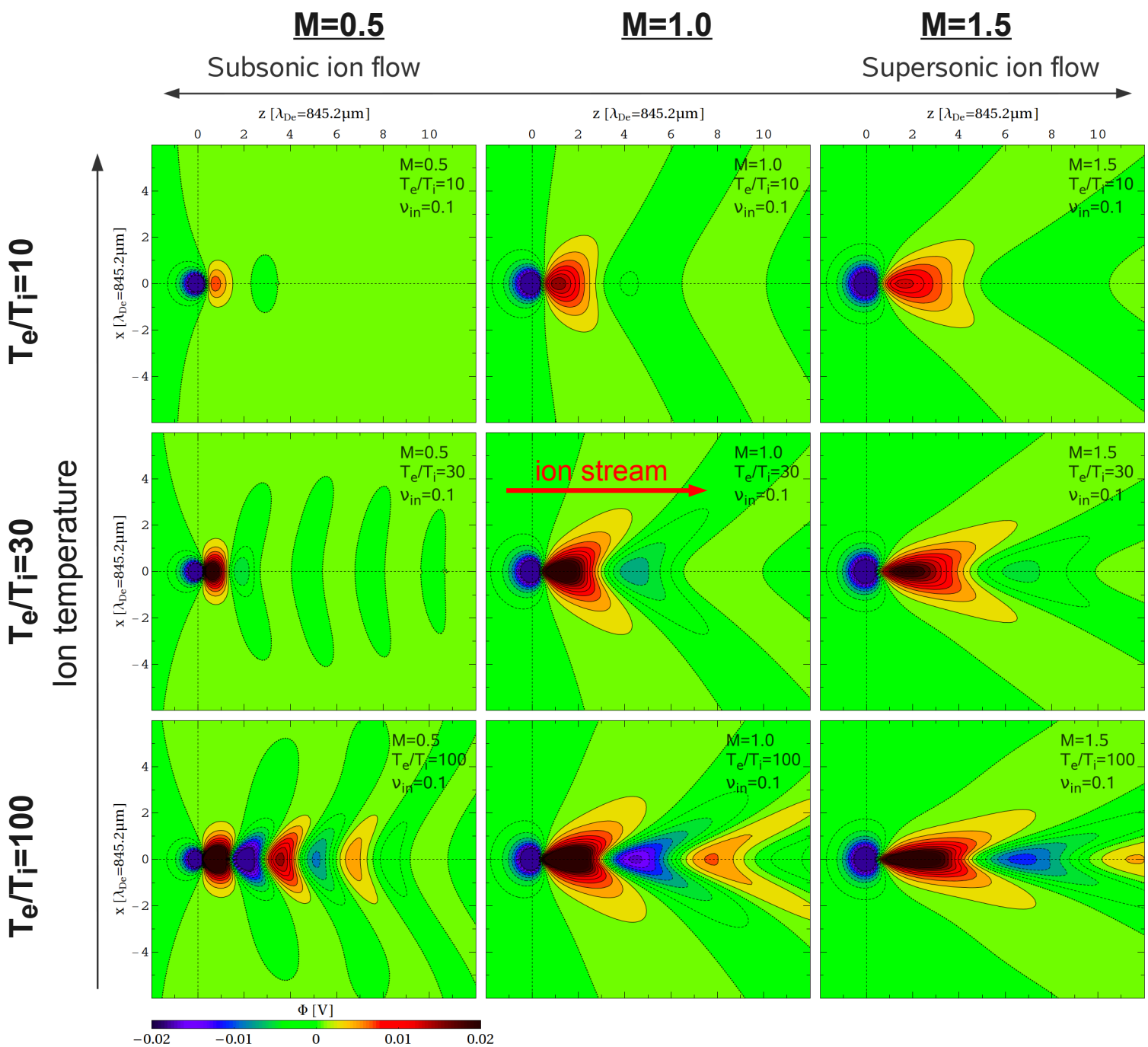


Electrostatic grain potential



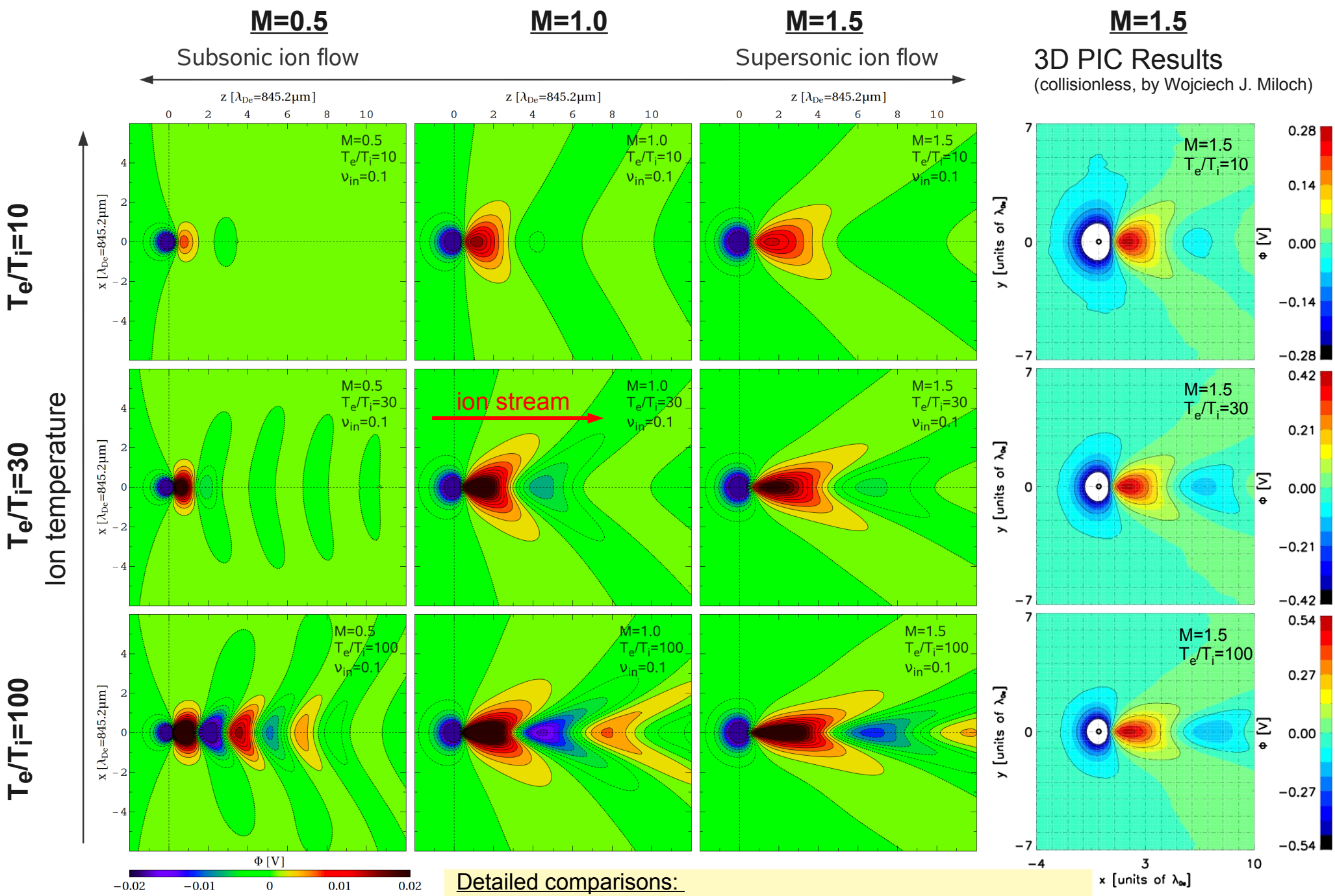
Electrostatic grain potential Φ(r, z) in streaming direction z at the radial position ρ = x = y = 0 [cut through Fig. 1].

Wake Potentials in Streaming Dusty Plasmas



PL, W.J. Miloch, H. Kählert, M. Bonitz, *On the Wake Structure in a Streaming Complex Plasma*, to be published 2011

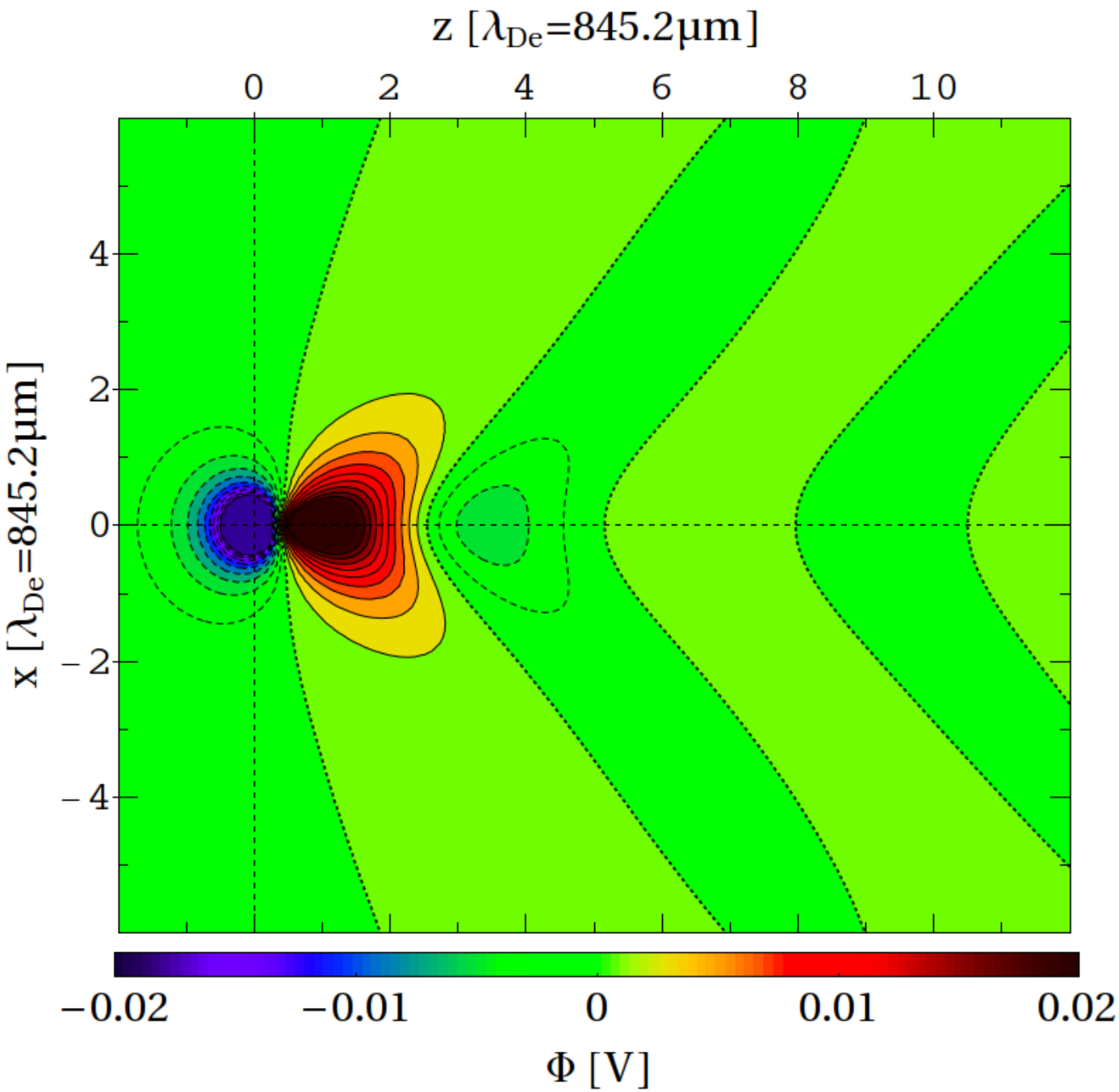
Wake Potentials in Streaming Dusty Plasmas



Detailed comparisons:

- PL, W.J. Miloch, H. Kählert, and M. Bonitz, to be published (2011)
- Hutchinson, Phys. Plas., **18**, 032111 (2011)

Spline Interpolated force fields (1024x1024)



Spline Interpolated force fields (1024x1024)