1856-27

2007 Summer College on Plasma Physics

30 July - 24 August, 2007

Explosions/expansions of nanoplasmas

Silva O. Louís

Instituto Superior Tecnico
Centro de Fisica de Plasmas
Av. Rovisco Pais
1049-001 LISBON
PORTUGAL

Explosions/expansions of nanoplasmas

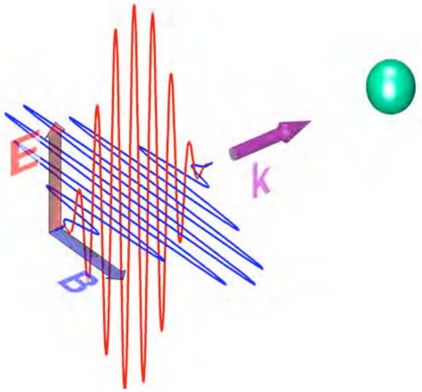
Luís O. Silva

Fabio Peano, Joana L. Martins, Ricardo A. Fonseca

GoLP/Centro de Física dos Plasmas

Instituto Superior Técnico, Lisbon, Portugal

http://cfp.ist.utl.pt/golp/



Outline

- Nanoplasmas
  - ★ motivation and pure Coulomb explosions
- Shock shells and the control of cluster explosions
  - ★ double pump technique
- Kinetics of the expansions/explosions of spherical hot plasmas
  - ★expansion/explosion
- Summary

Ultra intense laser-matter interactions

laser sources

IR technology:

- wavelength ~ 1 μm
- pulse duration ~10 fs – 1 ps
- intensity up to 10^{21} – 10^{22} W/cm^2
- spot size at focus ~ 20 μm

VUV/x-ray technology:

- wavelength ~ 1 – 100 nm
- pulse duration as low as 10 fs
- intensity up to 10^{18} – 10^{19} W/cm^2
- spot size at focus ~ 50 nm – 1 μm

targets

gaseous targets

- radiation can propagate through medium
- poor energy absorption

cluster jets

nm-μm size plasmas

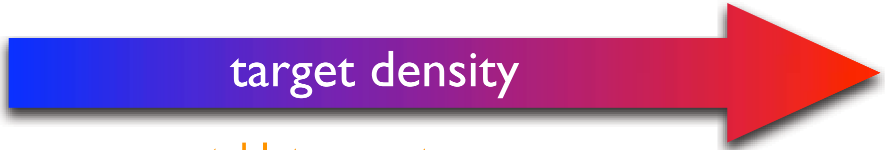
solid targets

- radiation cannot propagate through medium
- medium/high energy absorption

$\omega_{pe} < \omega_L$

$n_{pe} < n_{cr}$

underdense



$\omega_{pe} > \omega_L$

$n_{pe} > n_{cr}$

overdense

electron acceleration

tabletop neutron sources

ion acceleration (keV - MeV)

x-ray production
(keV and long lived sources)

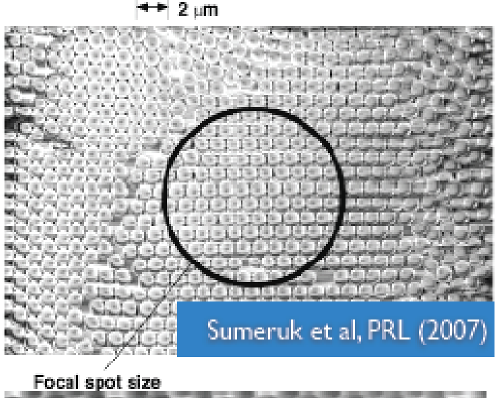
nucleosynthesis

ion acceleration (+MeV)

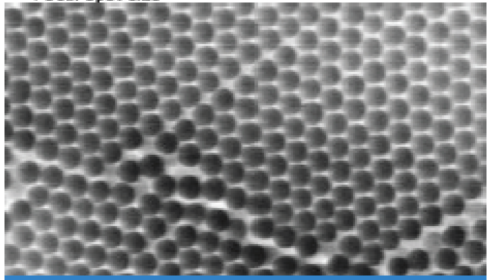
fast ignition for nuclear fusion

Clusters and nano/microstructured targets: nanoplasmas

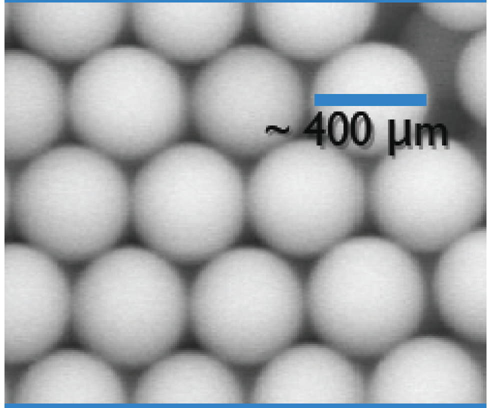
- Ultra intense lasers [IR] in cluster/nano-sized targets
  - ★ very fast (tunnel) ionization/hot electron population = *nanoplasma* (T. Ditmire)
  - ★ quiver motion of e- comparable to target size
  - ★ Ability to control properties of target/ design targets for radiation generation/ ion acceleration



Sumeruk et al, PRL (2007)



http://www.microspheres-nanospheres.com/



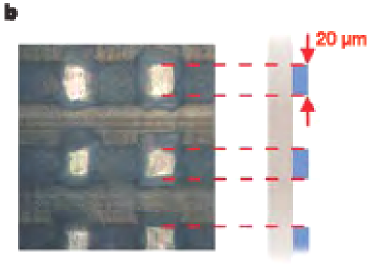
http://www.microspheres-nanospheres.com/

Vol 439|26 January 2006|doi:10.1038/nature04492 nature

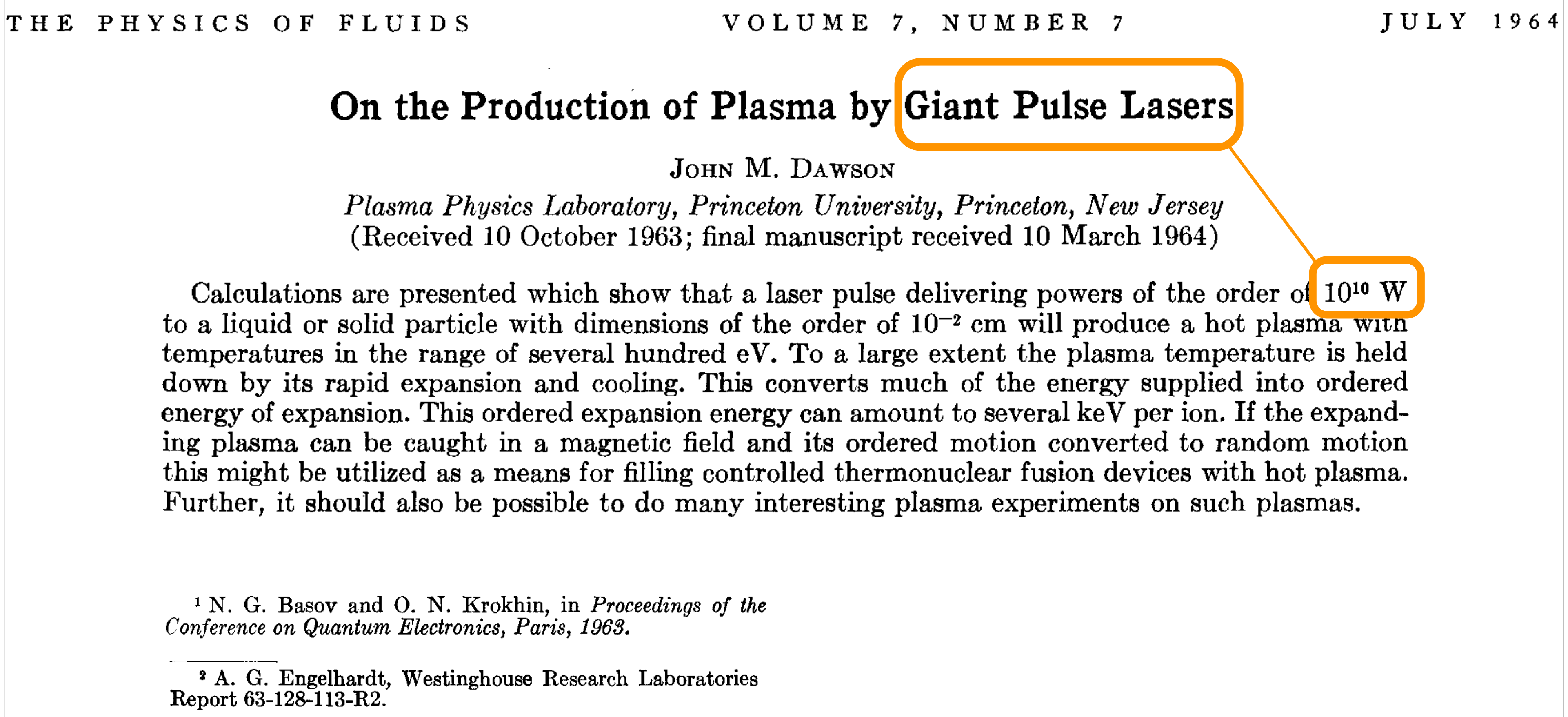
LETTERS

Laser-plasma acceleration of quasi-monoenergetic protons from microstructured targets

H. Schwoerer[1], S. Pfotenhauer[1], O. Jäckel[1], K.-U. Amthor[1], B. Liesfeld[1], W. Ziegler[1], R. Sauerbrey[1], K. W. D. Ledingham[1,2,3] & T. Esirkepov[4,5]



Interaction of lasers with sub-mm scale solids



THE PHYSICS OF FLUIDS VOLUME 7, NUMBER 7 JULY 1964

On the Production of Plasma by Giant Pulse Lasers

John M. Dawson
Plasma Physics Laboratory, Princeton University, Princeton, New Jersey

(Received 10 October 1963; final manuscript received 10 March 1964)

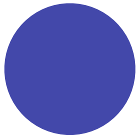
Calculations are presented which show that a laser pulse delivering powers of the order of 10^{10} W to a liquid or solid particle with dimensions of the order of 10^{-2} cm will produce a hot plasma with temperatures in the range of several hundred eV. To a large extent the plasma temperature is held down by its rapid expansion and cooling. This converts much of the energy supplied into ordered energy of expansion. This ordered expansion energy can amount to several keV per ion. If the expanding plasma can be caught in a magnetic field and its ordered motion converted to random motion this might be utilized as a means for filling controlled thermonuclear fusion devices with hot plasma. Further, it should also be possible to do many interesting plasma experiments on such plasmas.

[1] N. G. Basov and O. N. Krokhin, in *Proceedings of the Conference on Quantum Electronics, Paris, 1963.*

---

[2] A. G. Engelhardt, Westinghouse Research Laboratories Report 63-128-113-R2.

Radiation-cluster interaction: dynamic picture

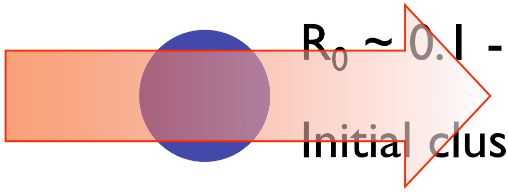


R_0 ~ 0.1 - 100 nm

Initial cluster radius

Radiation-cluster interaction: dynamic picture

Radiation hits cluster



$R_0 \sim 0.1 - 100$ nm

Initial cluster radius

XUV - X ray

$a_0 \sim 10^{-3} - 10^{-4}$

$E_0 \sim$ 100's eV - 10 KeV

$\tau_{laser} \sim 100$ fs

IR light

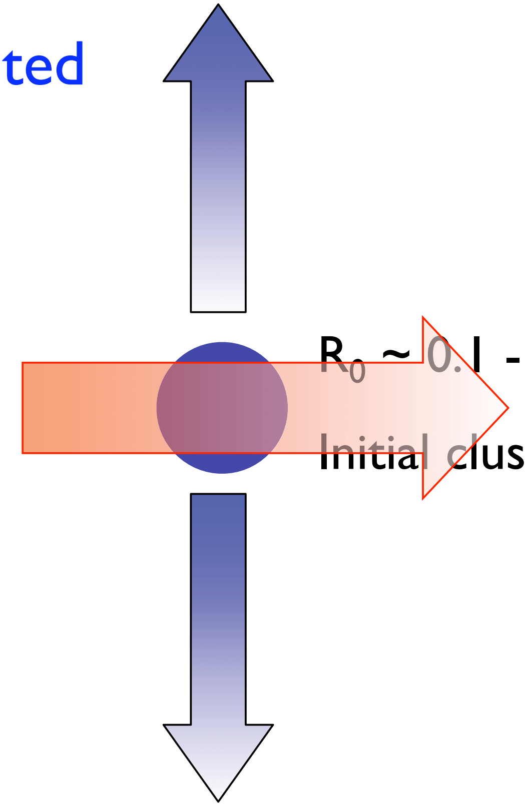
$a_0 \sim 0.01 - 10$

$\lambda_0 \sim 1 \mu m$

$\tau_{laser} \sim 10 - 100$ fs

Radiation-cluster interaction: dynamic picture

Electrons heated/ejected

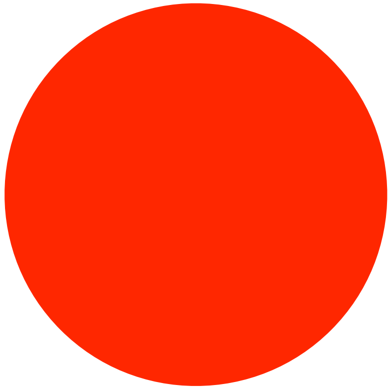


$R_0 \sim 0.1 - 100$ nm

Initial cluster radius

Radiation-cluster interaction: dynamic picture

Ion sphere expands/
explodes



Radius of cluster is critical

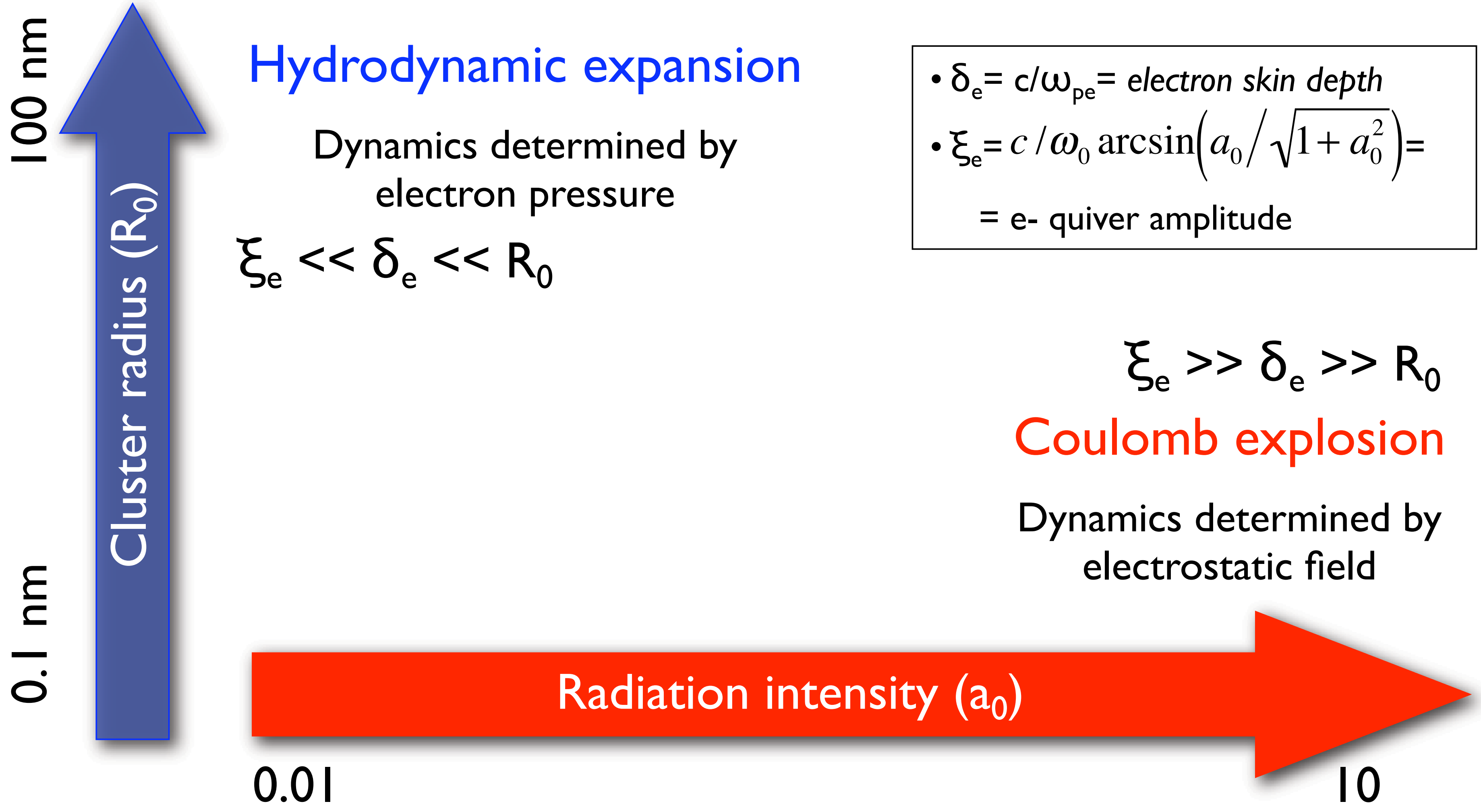
Maximum energy of ions

(for homonuclear D clusters)

$$E_{\max}[\mathrm{KeV}] \approx 6\, n_0\left[10^{22}\,\mathrm{cm}^{-3}\right] R_0^2[10\ \mathrm{nm}]$$

Expansion or explosion? [IR light]

Radius of cluster and radiation intensity (a_0) are the critical parameters



Hydrodynamic expansion

Dynamics determined by
electron pressure

$\xi_e << \delta_e << R_0$

- $\delta_e = c/\omega_{pe}$ = *electron skin depth*
- $\xi_e = c/\omega_0 \arcsin\left(a_0 / \sqrt{1 + a_0^2}\right) =$

  = e- quiver amplitude

$\xi_e >> \delta_e >> R_0$

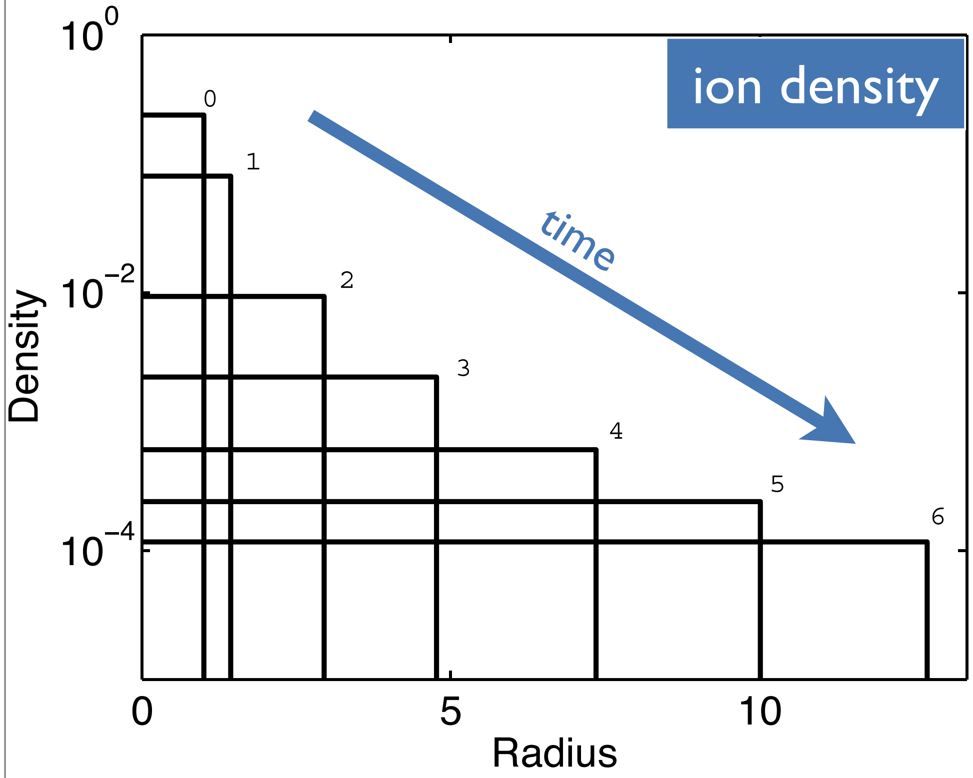
Coulomb explosion

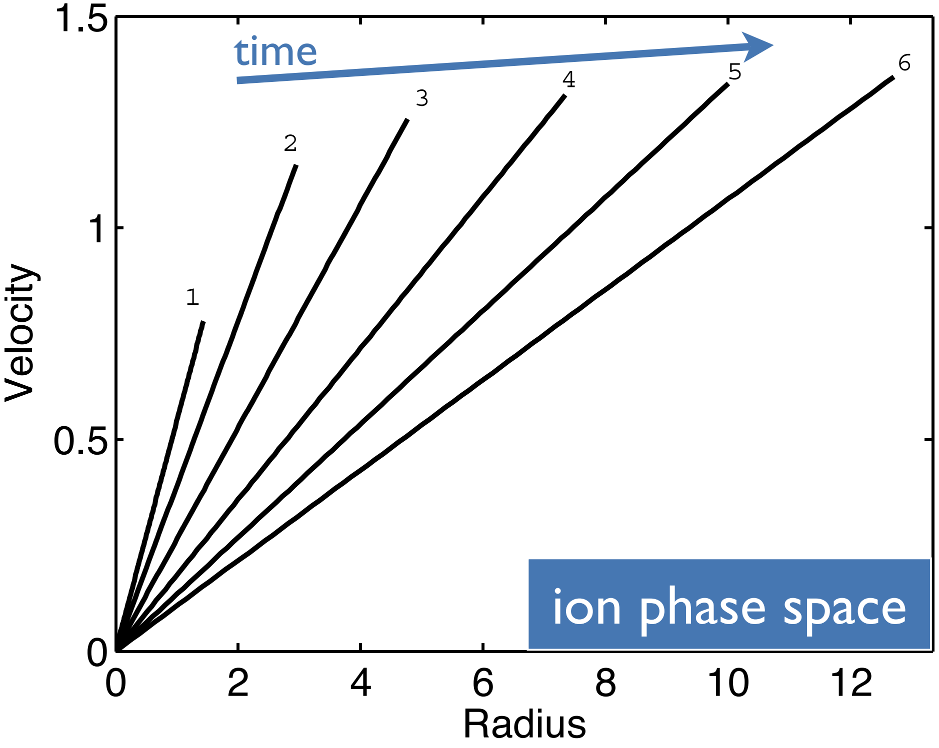
Dynamics determined by
electrostatic field

Coulomb explosions of nanoplasmas

Dynamics of a pure ion sphere

If all electrons are instantaneously stripped from cluster: sphere of ions





Theoretical model provides relevant information

$$r = \mathrm{r}/R_0,\ \tau = t/t_0,\ Q(r) = N(r)/N_0 \qquad t_0 = \sqrt{\frac{mR_0^3}{e^2N_0}}$$

$$m\frac{d^2\mathrm{r}}{dt^2} = eE(\mathrm{r})$$

Newton's equation of motion

$$\frac{1}{\mathrm{r}^2}\frac{d\left(\mathrm{r}^2E\right)}{d\mathrm{r}} = 4\pi en(\mathrm{r})$$

Poisson's equation

$$E = \frac{eN(\mathrm{r})}{\mathrm{r}^2}$$

Spherical symmetry

R0 = initial cluster radius

Q(r) = charge enclosed in a sphere of radius r

(normalized to total charge in the cluster)

r0 = initial position of ion

v0 = 0 = initial velocity of all ions

If no ion overtaking then $Q\left(r(r_0,\tau)\right) = Q(r_0)$

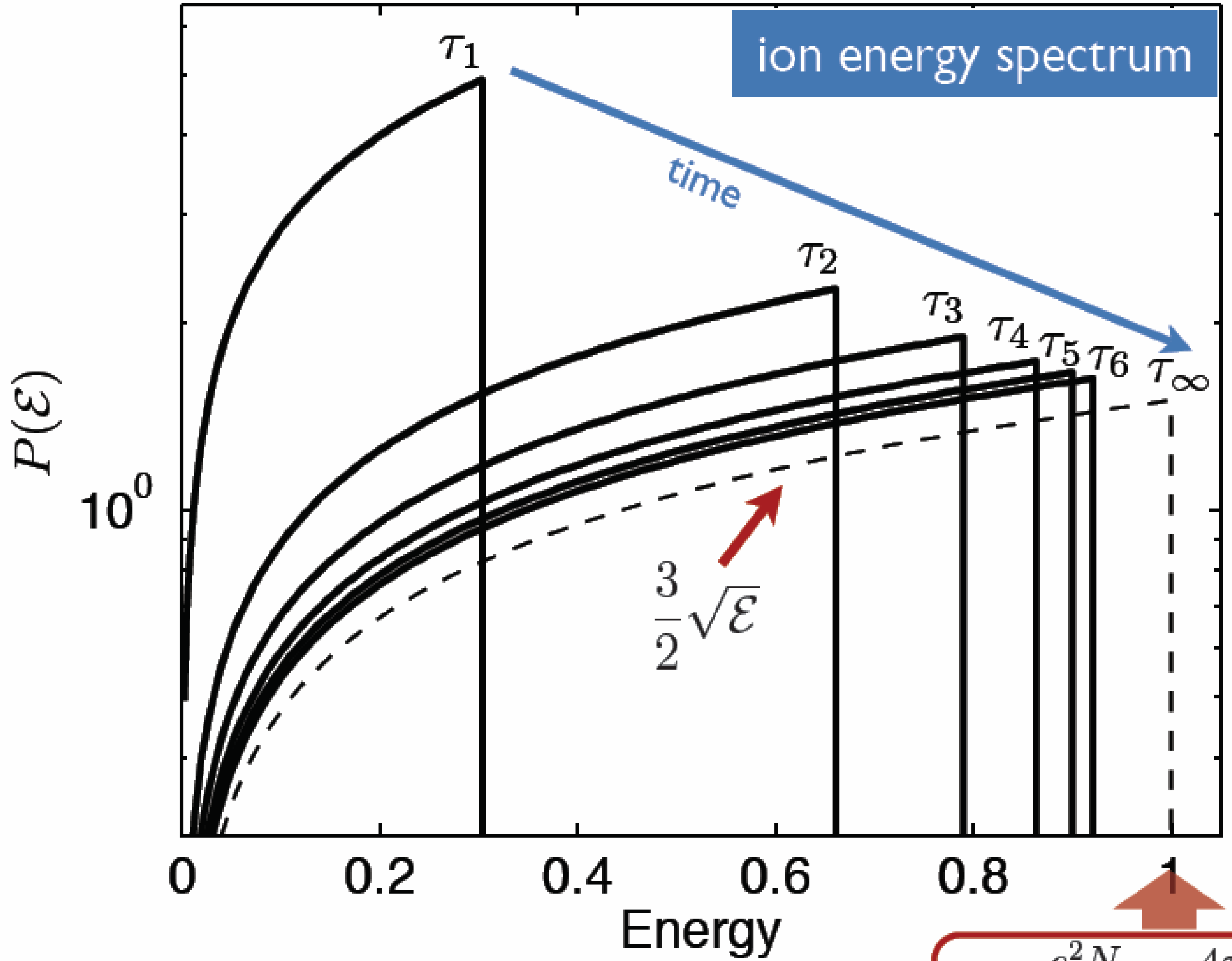
$$\frac{d\left(v^2/2\right)}{d\tau} = -Q_0(r_0)\frac{d}{d\tau}\left(\frac{1}{r}\right) \qquad \frac{1}{2}v^2 = Q_0(r_0)\left[\frac{1}{r_0} - \frac{1}{r}\right]$$

Energy conservation

$$\xi = r/r_0 \qquad \frac{d\xi}{d\tau} = \sqrt{\frac{2Q_0(r_0)}{r_0^3}}\sqrt{\frac{\xi-1}{\xi}} \qquad \sqrt{\xi}\sqrt{\xi-1} + \log\left|\sqrt{\xi}+\sqrt{\xi-1}\right| = \tau\sqrt{\frac{2Q_0(r_0)}{r_0^3}}$$

Solution eq. motion

Energy spectrum of pure Coulomb explosions



$$P(\mathcal{E}) = \frac{dQ}{d\mathcal{E}} = \frac{1}{v}\frac{dQ}{dv}$$

$$\mathcal{E}_0 = \frac{e^2 N_0}{R_0} = \frac{4\pi}{3} n_0 e^2 R_0^2.$$

Shock shells and control of nanoplasmas

Can the plasma expansions be controlled?

strong influence of electron dynamics on the expansion [1,2]

laser features determine amount of energy delivered to electrons

possibility of controlling plasma expansions using appropriately-shaped laser pulses

applications requiring accurate expansion control:

- production of intracluster nuclear reactions, via generation of large-scale shock shells [3]
- three-dimensional imaging of biological samples through diffraction of ultrashort x-ray pulses [4]

[1] F. Peano, R. A. Fonseca, and L. O. Silva, Phys. Rev. Lett. 94, 033401 (2005).
[2] F. Peano, F. Peinetti, R. Mulas, G. Coppa, L. O. Silva, Phys. Rev. Lett. 96, 175002 (2006).
[3] F. Peano, R. A. Fonseca, J. L. Martins, and L. O. Silva, Phys. Rev. A 73, 053202 (2006).
[4] R. Neutze et al., Nature 406, 752 (2000); H. Wabnitz et al., Nature 420, 482 (2002).

Uniform vs. nonuniform explosions

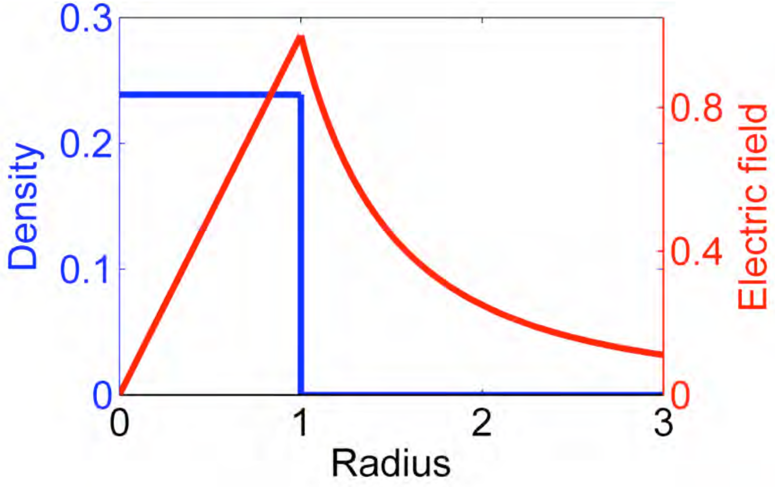
Shocks occur when the initial density profile is nonuniform [1]

uniform density profile:

- Force is maximum at the boundary
- No overtaking between ions

⇓

expansion is uniform

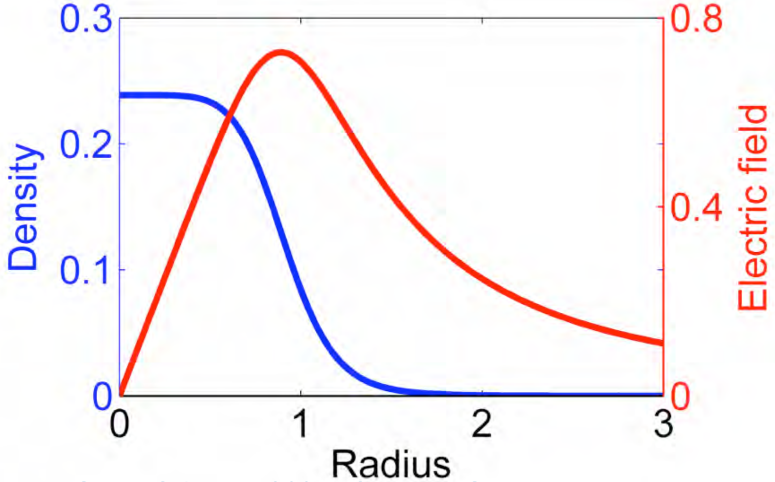


nonuniform density profile:

- force is maximum within the cluster
- inner ions overtake outer ions

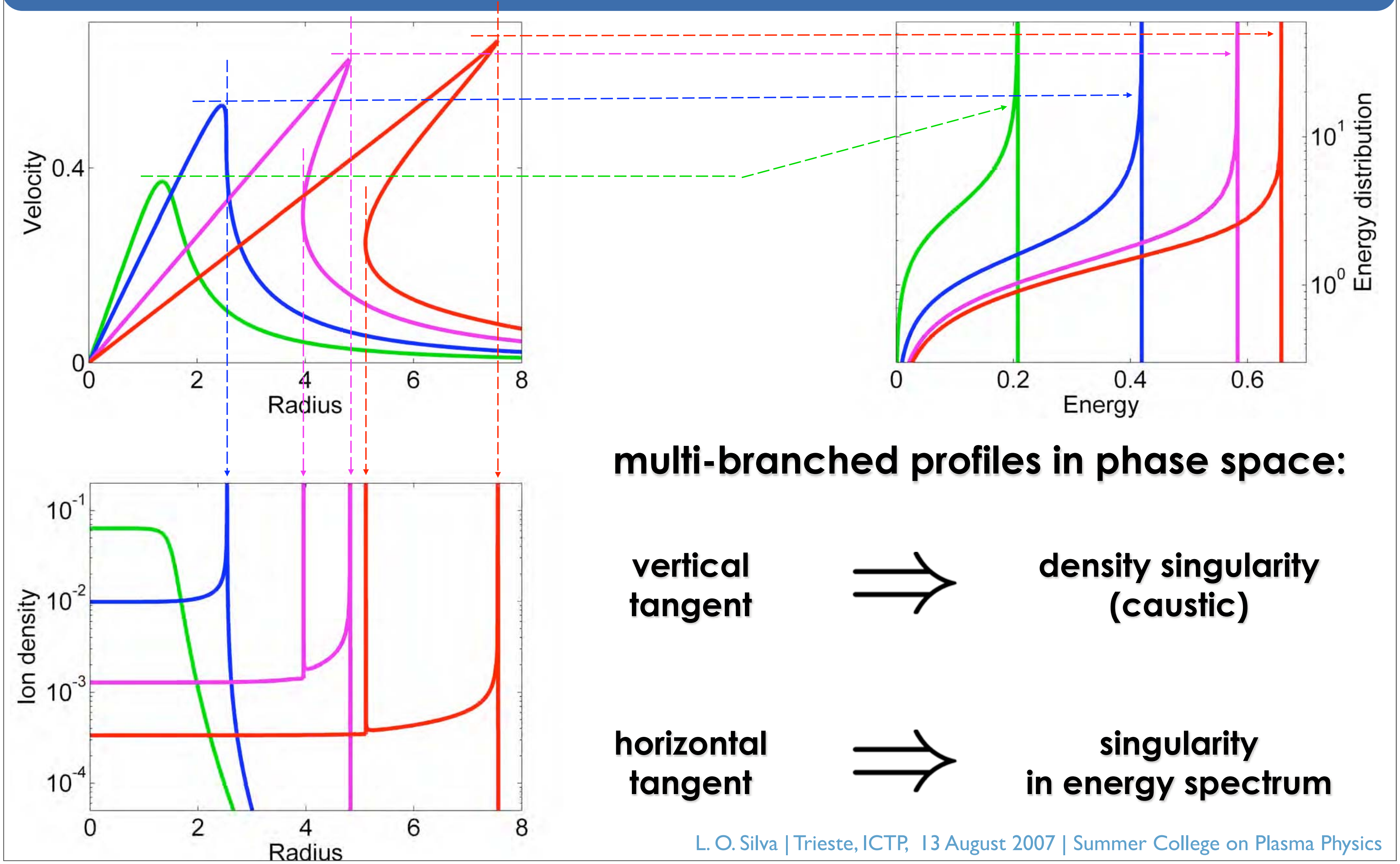
⇓

shock shell form



[1] A. E. Kaplan et al, Phys. Rev. Lett. 91, 143401 (2003).

Shock shell structure



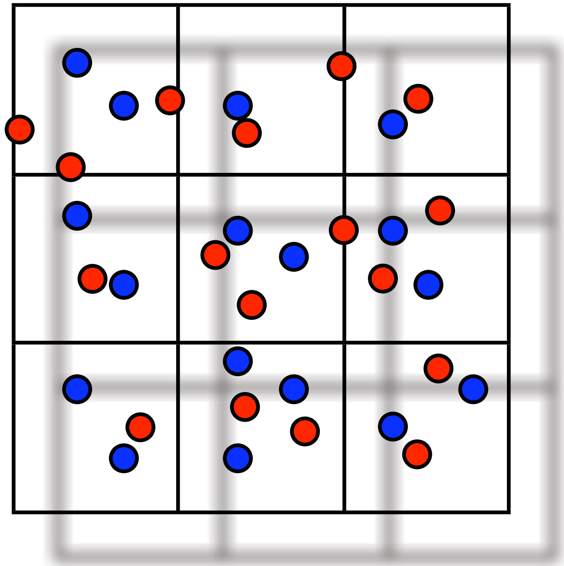
multi-branched profiles in phase space:

vertical tangent ⇒ **density singularity (caustic)**

horizontal tangent ⇒ **singularity in energy spectrum**

Particle-in-cell simulations

Solving Maxwell's equations on a grid with self-consistent charges and currents due to charged particle dynamics



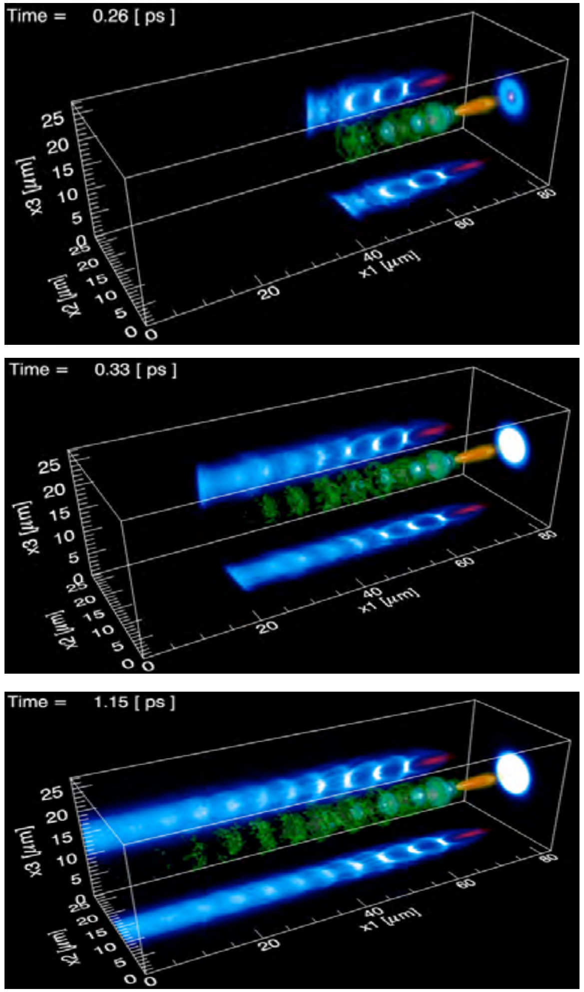
State-of-the-art

~ 10^9 particles

~ $(500)^3$ cells

RAM ~ 0.5 TByte
Run time: hours to months
Data/run ~ 1 TByte

One-to-one simulations of plasma based accelerators & cluster dynamics
Weibel/two stream instability in astrophysics, fast igniton



Particle-in-cell (PIC) - (Dawson, Buneman, 1960's)
Maxwell's equation solved on simulation grid
Particles pushed with Lorentz force

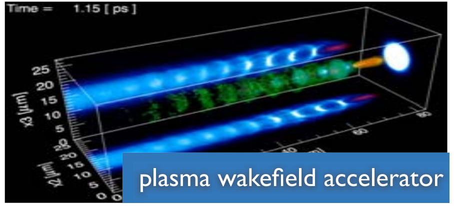
osiris 2.0

osiris.framework

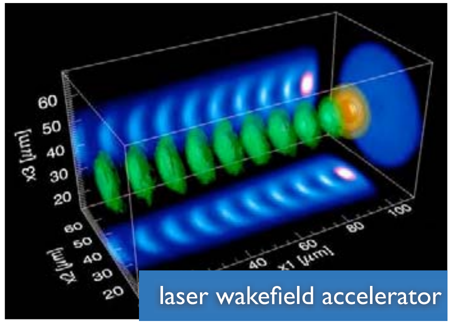
- Massivelly parallel particle-in-cell code
- Visualization and data analysis infrastructure
- Developed by the *osiris.consortium*
  - ⇒ UCLA + IST + USC

New in version 2.0

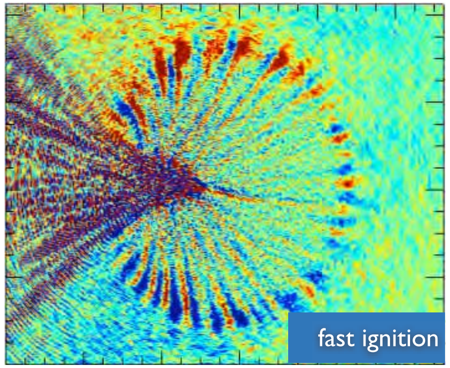
- Bessel/Hermite-Laguerre beams
- Relativistic binary collisions module
- Impact and tunnel ionization (ADK model)
- Dynamic load balancing
- Parallel I/O
- Advanced particle tracking
- High-order deposition schemes

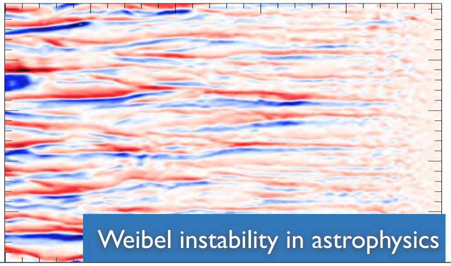


plasma wakefield accelerator



laser wakefield accelerator


fast ignition


Weibel instability in astrophysics

Self-consistent PIC simulations [IR light]

Laser:

- λ_0 = 820 nm
- τ_{laser} = 35 fs
- a_0 = 2

Cluster:

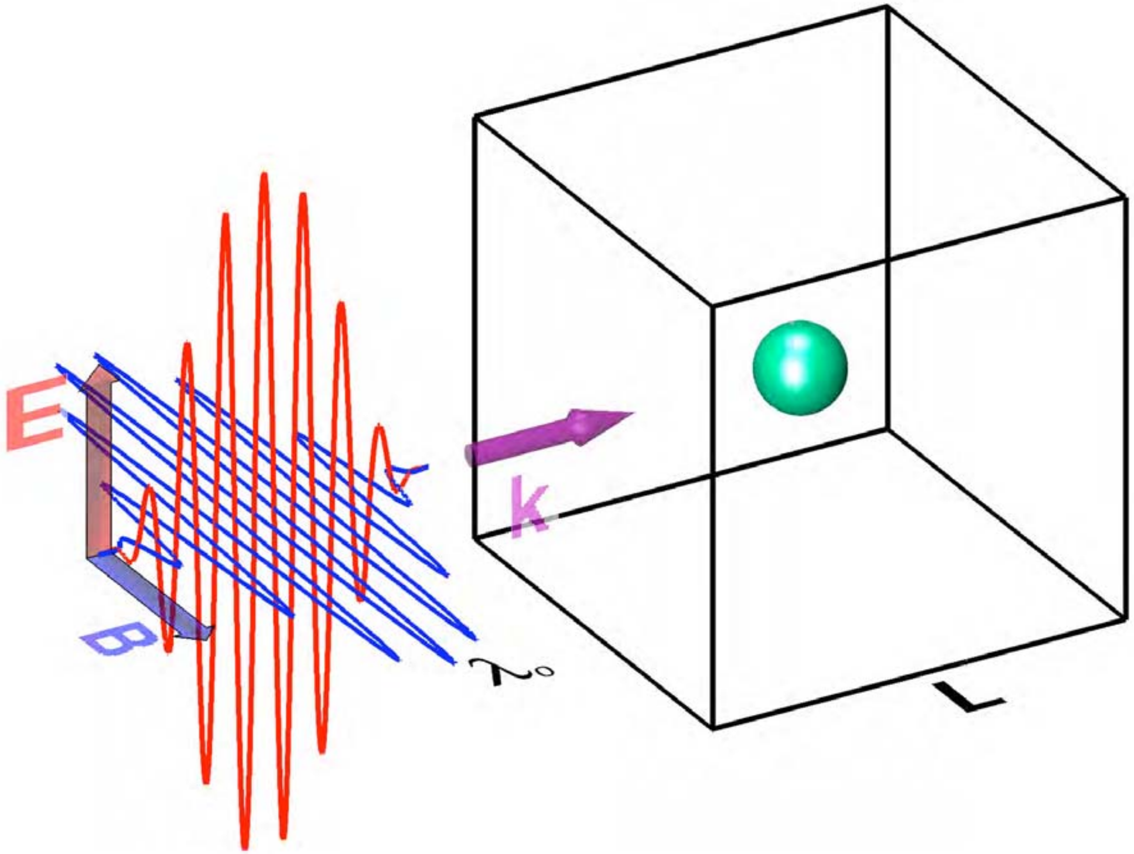
- R_0 = 32 nm
- $n_0 = 4.5\ 10^{22}\ cm^{-3}$

Simulation box:

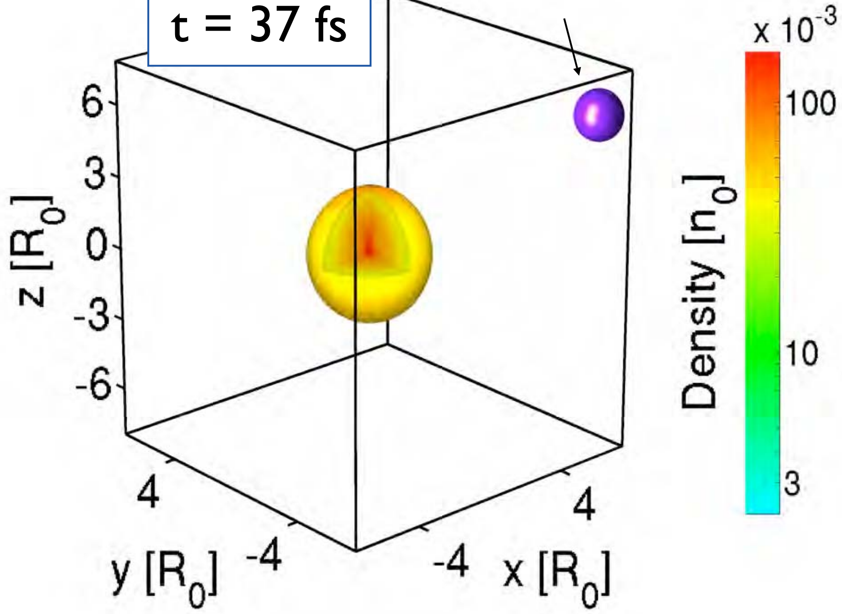
- L = 820 nm
- 336 x 336 x 336 cells

Particles:

- $N = 4.75\ 10^6$ part./species

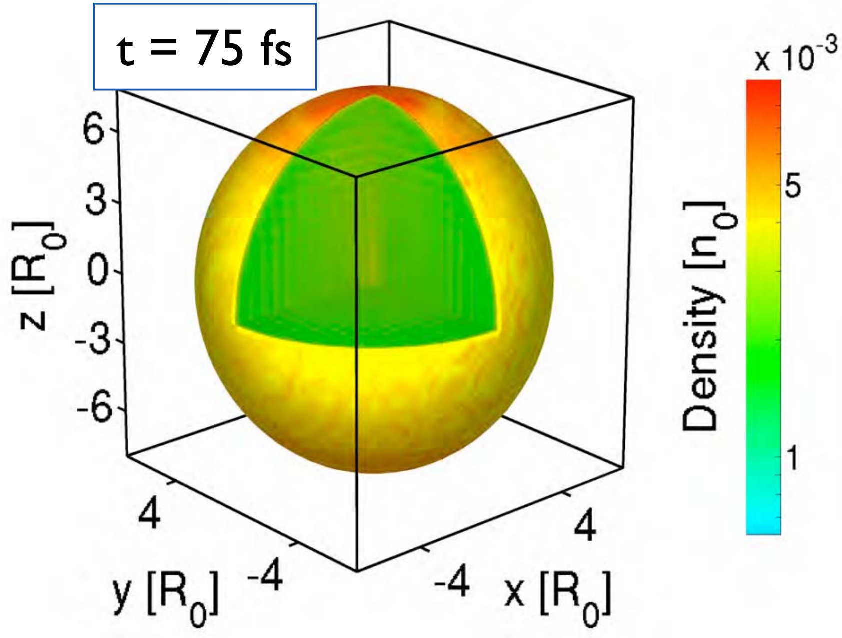


e$^-$ dynamics leads to formation of very small scale shock shells

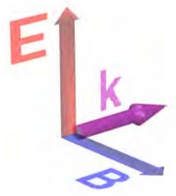


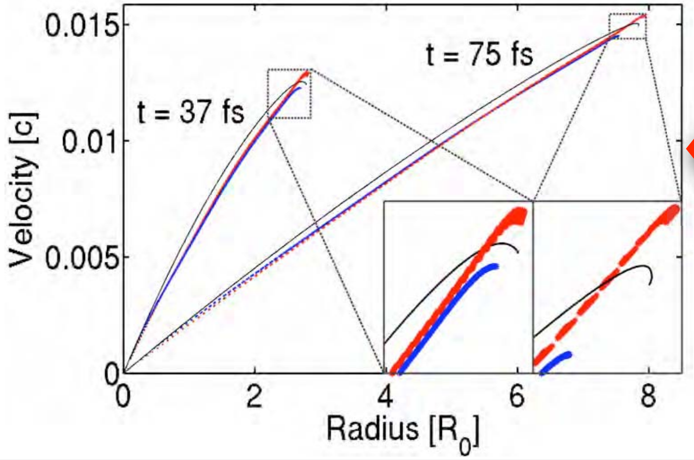
t = 37 fs

initial dimension of cluster



t = 75 fs





Small scale shock shell

Intra cluster relative velocity of ions is very small

How to induce and to control large scale shock shells using sequential pulses

Double pulse technique

- A weak radiation pulse drives a slow hydrodynamic expansion

  leads to smoothly decreasing plasma density profile

- After a time delay Δt, a strong radiation pulse removes/strongly heats all the electrons from the cluster core

- First expansion in the hydrodynamic regime

$$\mathrm{v}_{\mathrm{exp}} = \sqrt{k_B T_e / m_i}$$

IR Light

$$k_B T_e \sim \boxed{\tau_{\mathrm{las}} I_{\mathrm{las}}} / L\bar{n}, \qquad \bar{n} \sim 10^{19}\ \mathrm{cm}^{-3}$$

Laser energy transferred to e- in length L, with an average e^- density n

$$R_0 \sim 10\ \mathrm{nm},\ \mathrm{I} \sim 10^{15}\ \mathrm{W/cm}^2$$

$$k_B T_e \sim 0.1 - 1\ \mathrm{KeV},\ v_{\mathrm{exp}} \sim 0.1\ \mathrm{nm/fs} \rightarrow \qquad \Delta t \sim 100\ \mathrm{fs}$$

Double pulse: simulation parameters [IR light]

Lasers:

- λ_0 = 820 nm
- $\tau_{laser,1}$ = 35 fs, $\tau_{laser,2}$ = 20 fs
- a_1 = 0.05, a_2 = 2.5
- Δt = 170 fs

Clusters:

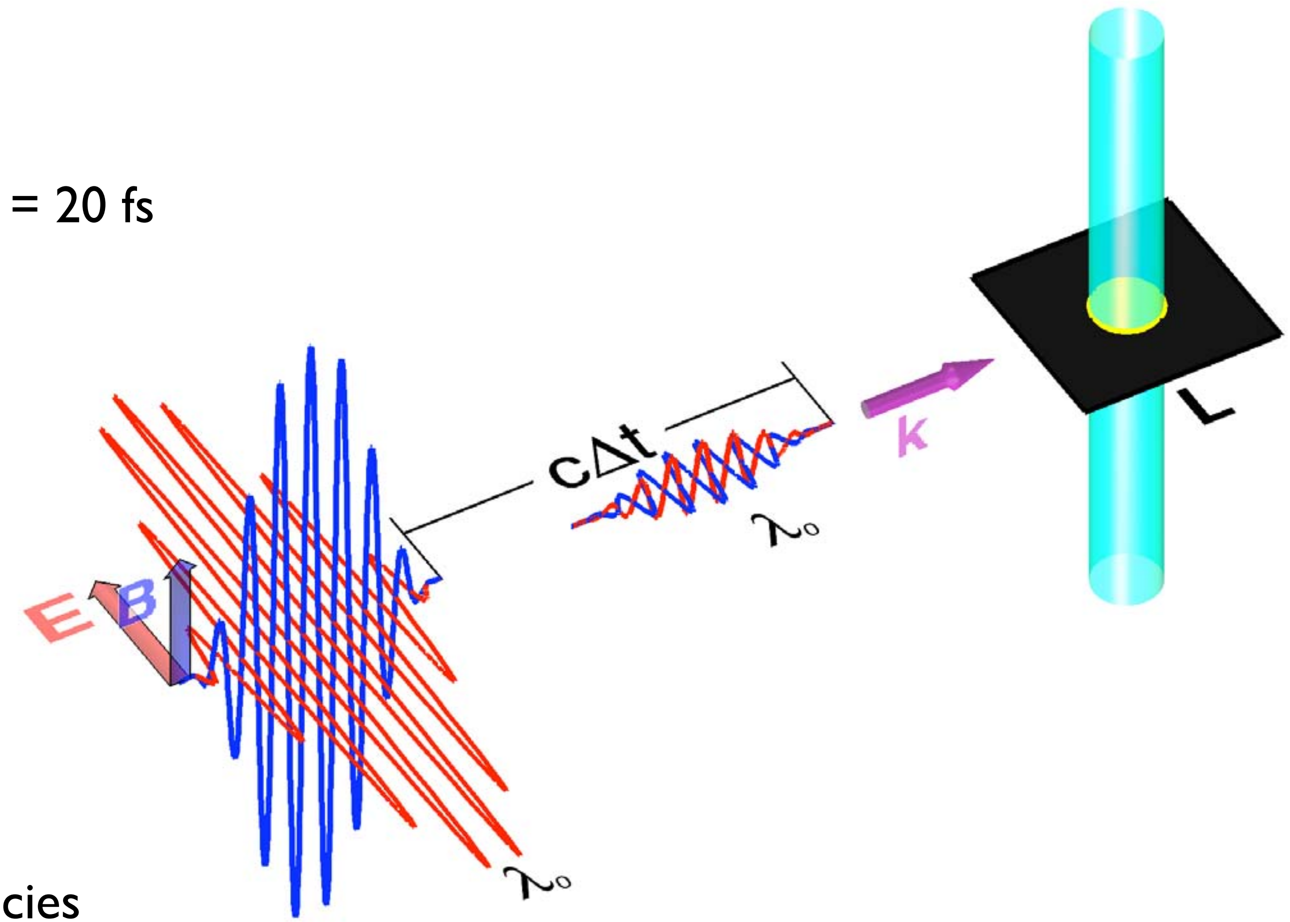
- R_0 = 32 nm
- $n_0 = 4.5\ 10^{22}\ cm^{-3}$

Simulation box:

- L = 1 μm
- 840 x 840 cells

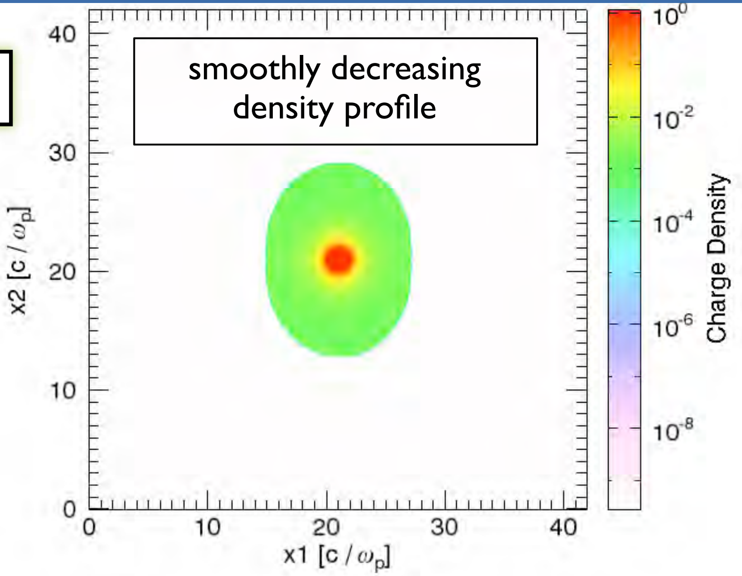
Particles

- $N = 1.2\ 10^6$ part./species



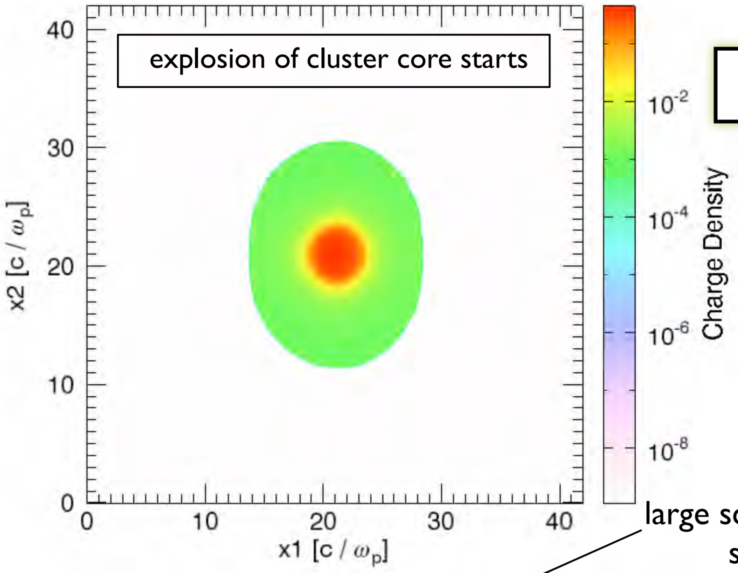
Ion density (after Δt)

168 fs



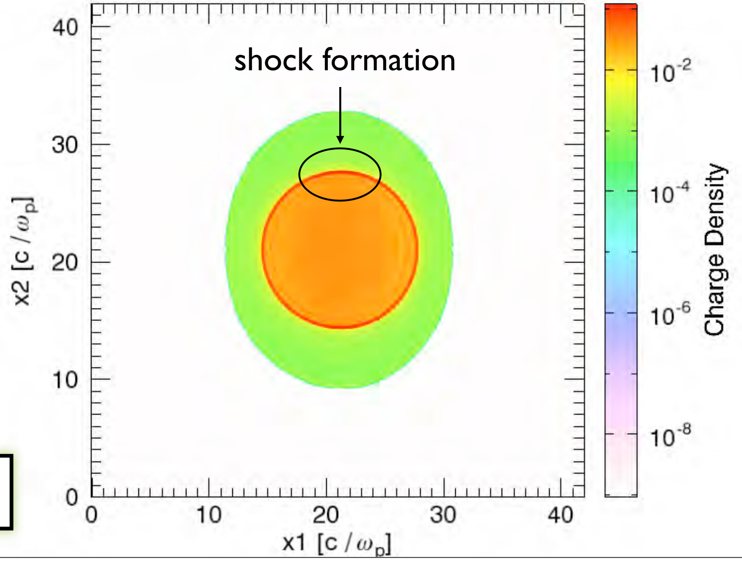
smoothly decreasing density profile

206 fs



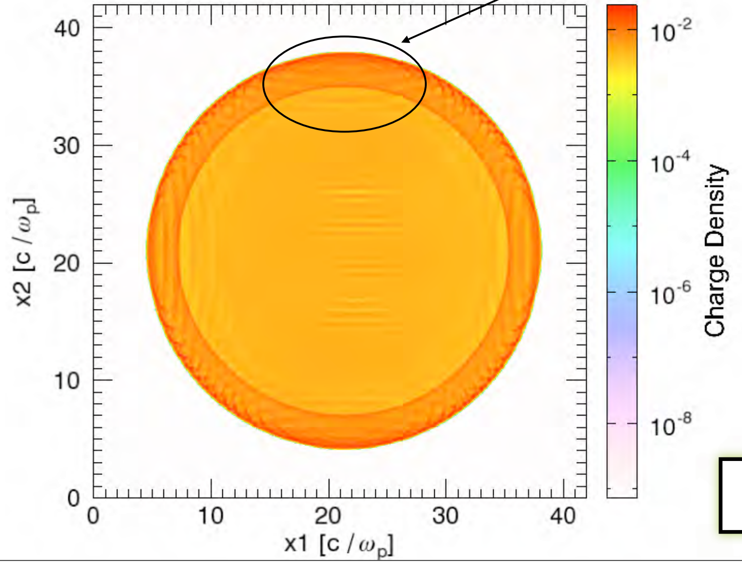
explosion of cluster core starts

187 fs



shock formation

237 fs



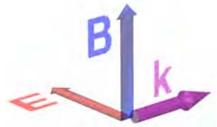
large scale shock shell

Evolution of the ion phase space

large scale shock shells can be driven by double [laser] pulse technique

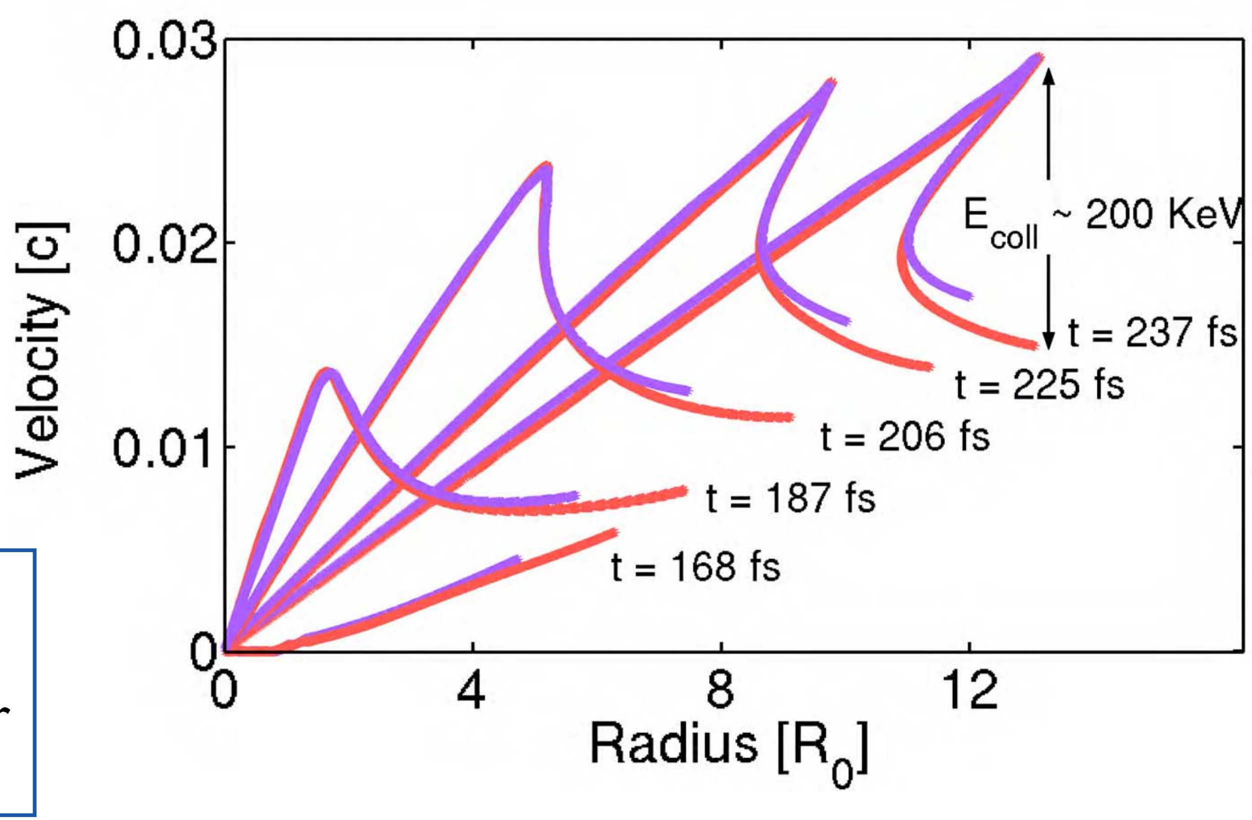
High relative velocities can be controlled and tuned by varying Δt

For D cluster, intra cluster neutron yield can be comparable to inter cluster neutron yield



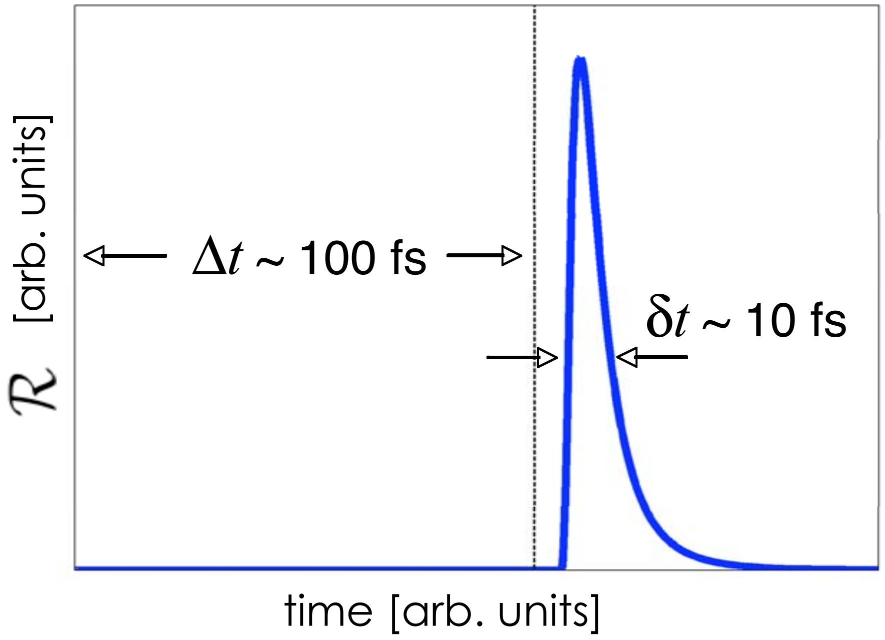
● Laser polarization direction

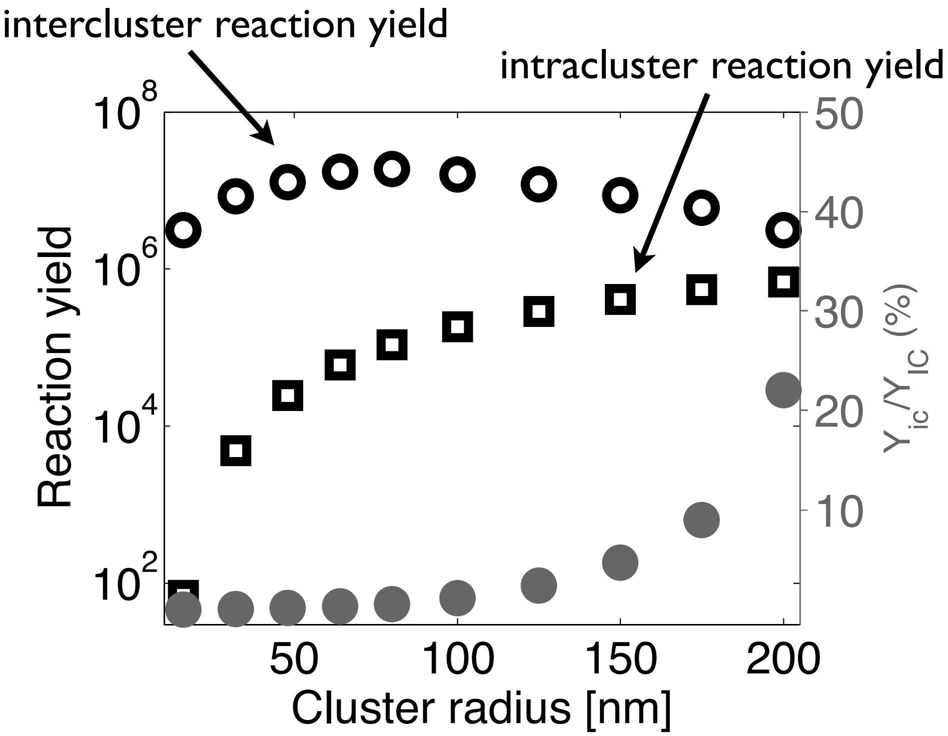
● Propagation direction



Neutron production from intracluster reactions*

Intracluster reactions lead to short burst of fusion neutrons





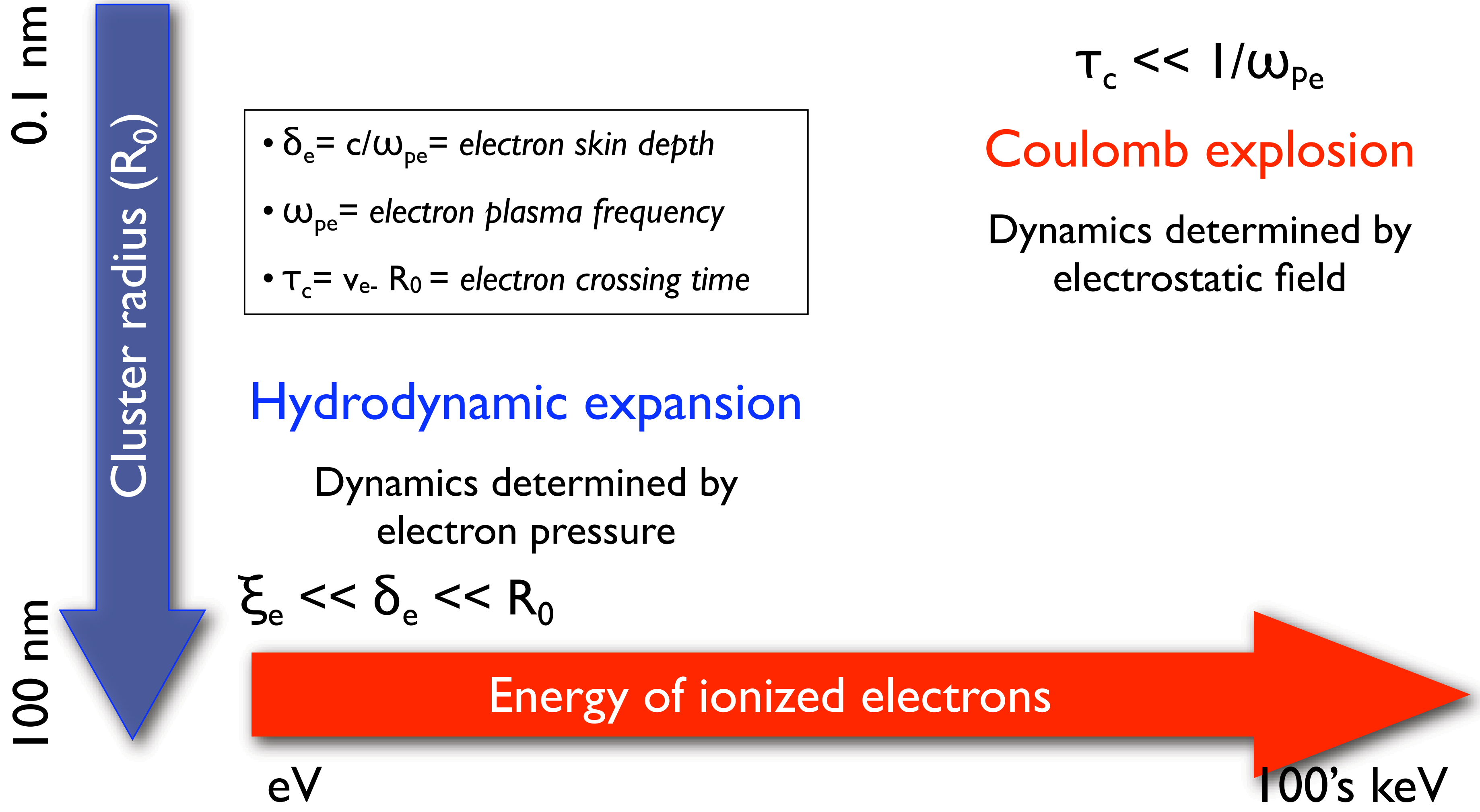
For very large clusters, intracluster nuclear reactions can be comparable to intercluster reactions

* Peano et al, Phys. Rev. A 73, 053202 (2006)

Control of nanoplasmas with VUV light

Expansion or explosion? [VUV light ↑]

Radius of cluster and ionization dynamics (T_e) are the critical parameters



- $\delta_e = c/\omega_{pe}$ = *electron skin depth*
- ω_{pe} = *electron plasma frequency*
- $\tau_c = v_{e-} R_0$ = *electron crossing time*

$$\tau_c << 1/\omega_{Pe}$$

Coulomb explosion

Dynamics determined by
electrostatic field

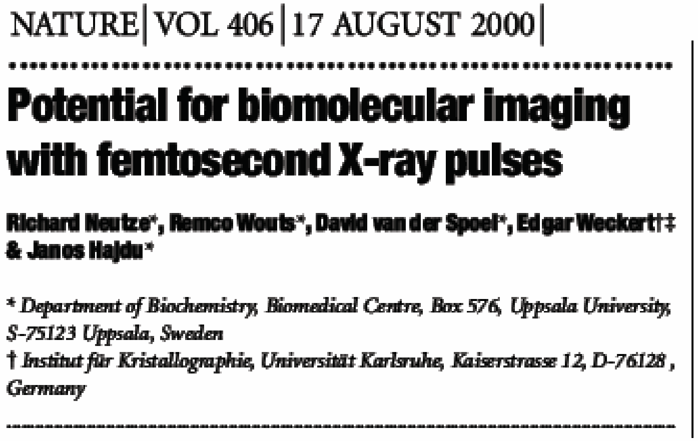
Hydrodynamic expansion

Dynamics determined by
electron pressure

$$\xi_e << \delta_e << R_0$$

Explosion of biosamples with intense XUV/X-ray sources

Intense XUV/X-ray sources @ DESY and @ SLAC coming online soon

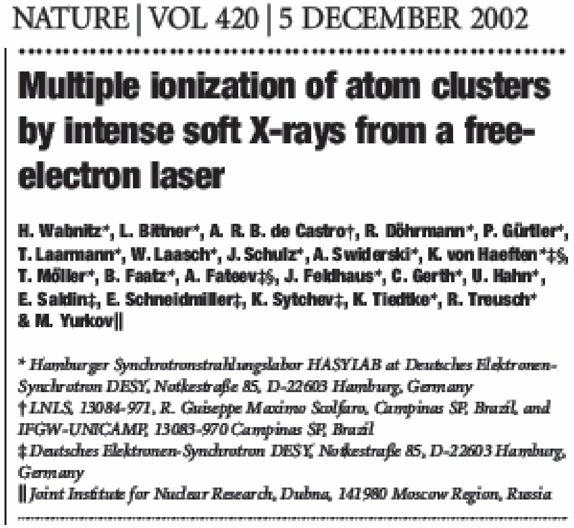


NATURE | VOL 406 | 17 AUGUST 2000 |

Potential for biomolecular imaging with femtosecond X-ray pulses

Richard Neutze*, Remco Wouts*, David van der Spoel*, Edgar Weckert†‡ & Janos Hajdu*

** Department of Biochemistry, Biomedical Centre, Box 576, Uppsala University, S-75123 Uppsala, Sweden*
† Institut für Kristallographie, Universität Karlsruhe, Kaiserstrasse 12, D-76128 , Germany

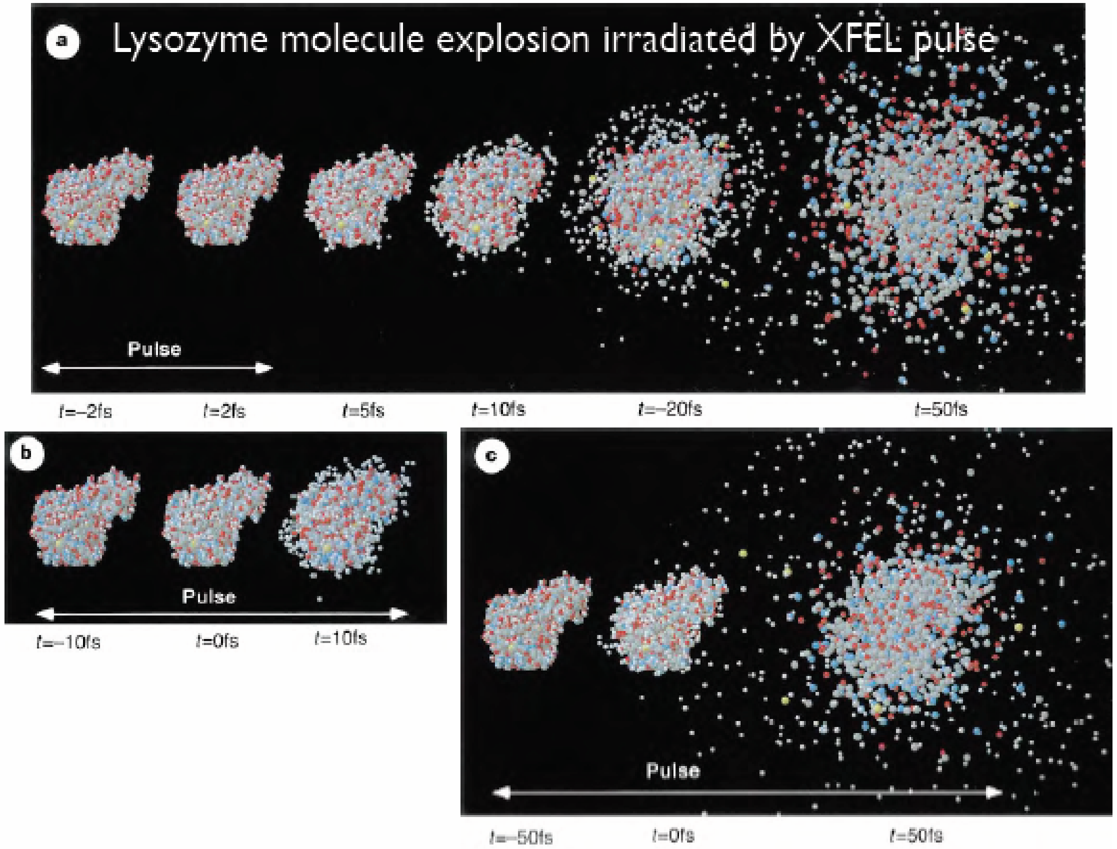


NATURE | VOL 420 | 5 DECEMBER 2002

Multiple ionization of atom clusters by intense soft X-rays from a free-electron laser

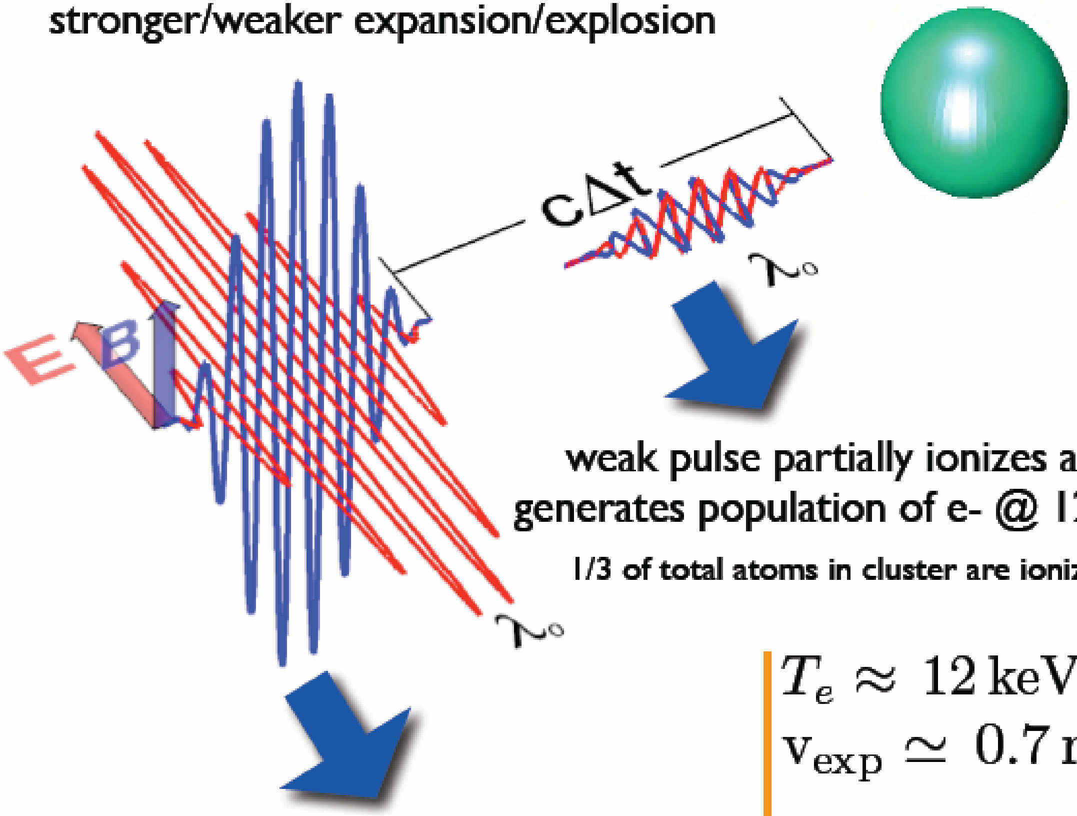
H. Wabnitz*, L. Bittner*, A. R. B. de Castro†, R. Döhrmann*, P. Gürtler*, T. Laarmann*, W. Laasch*, J. Schulz*, A. Swiderski*, K. von Haeften*‡§, T. Möller*, B. Faatz*, A. Fateev‡§, J. Feldhaus*, C. Gerth*, U. Hahn*, E. Saldin‡, E. Schneidmiller‡, K. Sytchev‡, K. Tiedtke*, R. Treusch* & M. Yurkov||

** Hamburger Synchrotronstrahlungslabor HASYLAB at Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, D-22603 Hamburg, Germany*
† LNLS, 13084-971, R. Guiseppe Maximo Scolfaro, Campinas SP, Brazil, and IFGW-UNICAMP, 13083-970 Campinas SP, Brazil
‡ Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, D-22603 Hamburg, Germany
|| Joint Institute for Nuclear Research, Dubna, 141980 Moscow Region, Russia



How to drive shock shells in clusters with XFEL?

Fraction of ionized atoms determines stronger/weaker expansion/explosion



weak pulse partially ionizes and generates population of e- @ 12 keV

1/3 of total atoms in cluster are ionized

after $\boxed{\Delta t}$, strong pulse ionizes and generates population of e- @ 12 keV

2/3 of total atoms in cluster are ionized

$$T_e \approx 12\,\mathrm{keV}$$

$$\mathrm{v_{exp}} \simeq 0.7\,\mathrm{nm/fs}$$

R_0 = 30 nm → $R_{cluster}$ = 5 R_0

Δt ~ 150 fs

Radiation:

- E_0 = 12.4 keV

Cluster (D):

- R_0 = 32 nm
- $n_0 = 10^{22}$ cm^{-3}

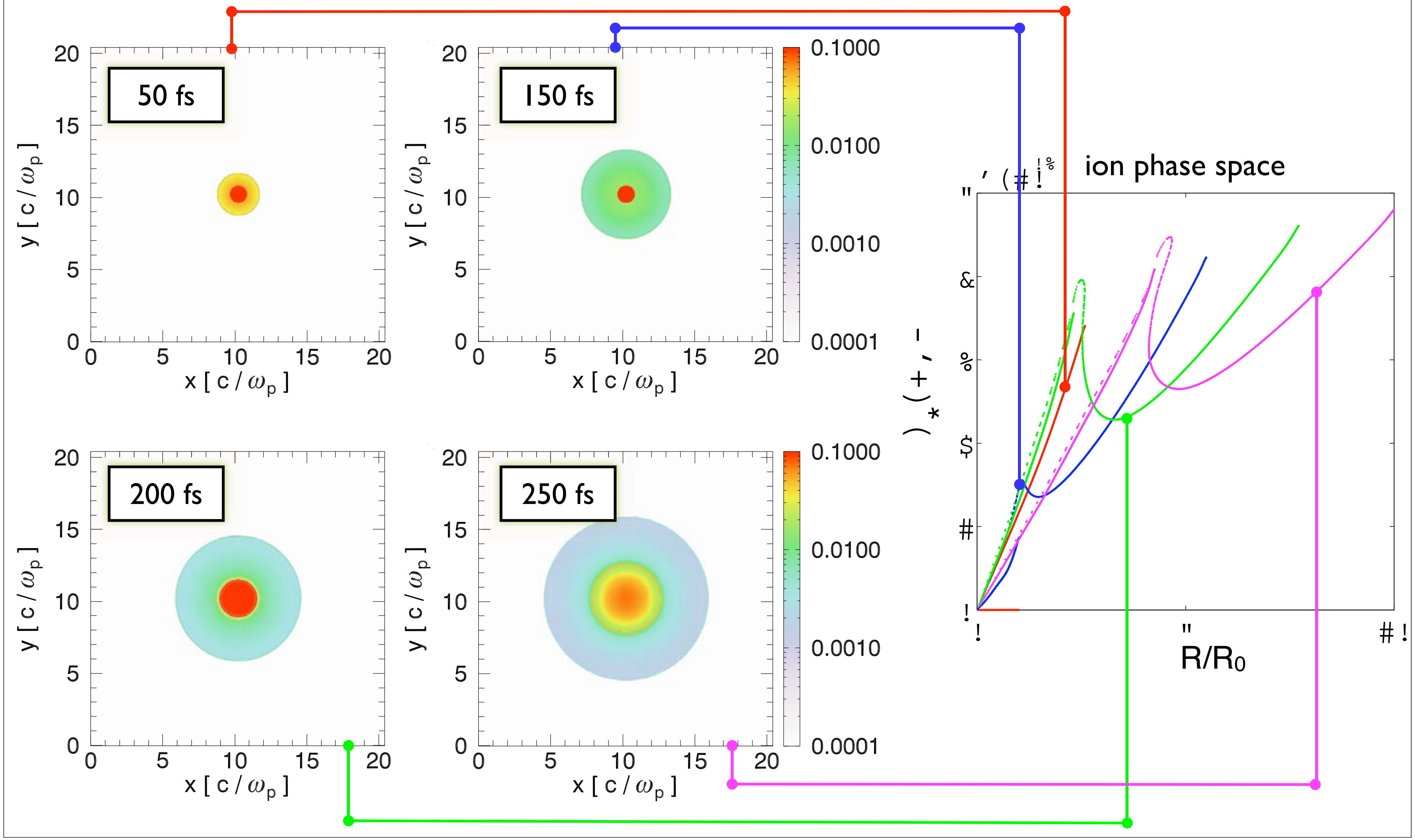
Simulation box:

- L_{box} ~ 1200 nm
- 256 x 256 x 256 cells
- 512 x 512 cells

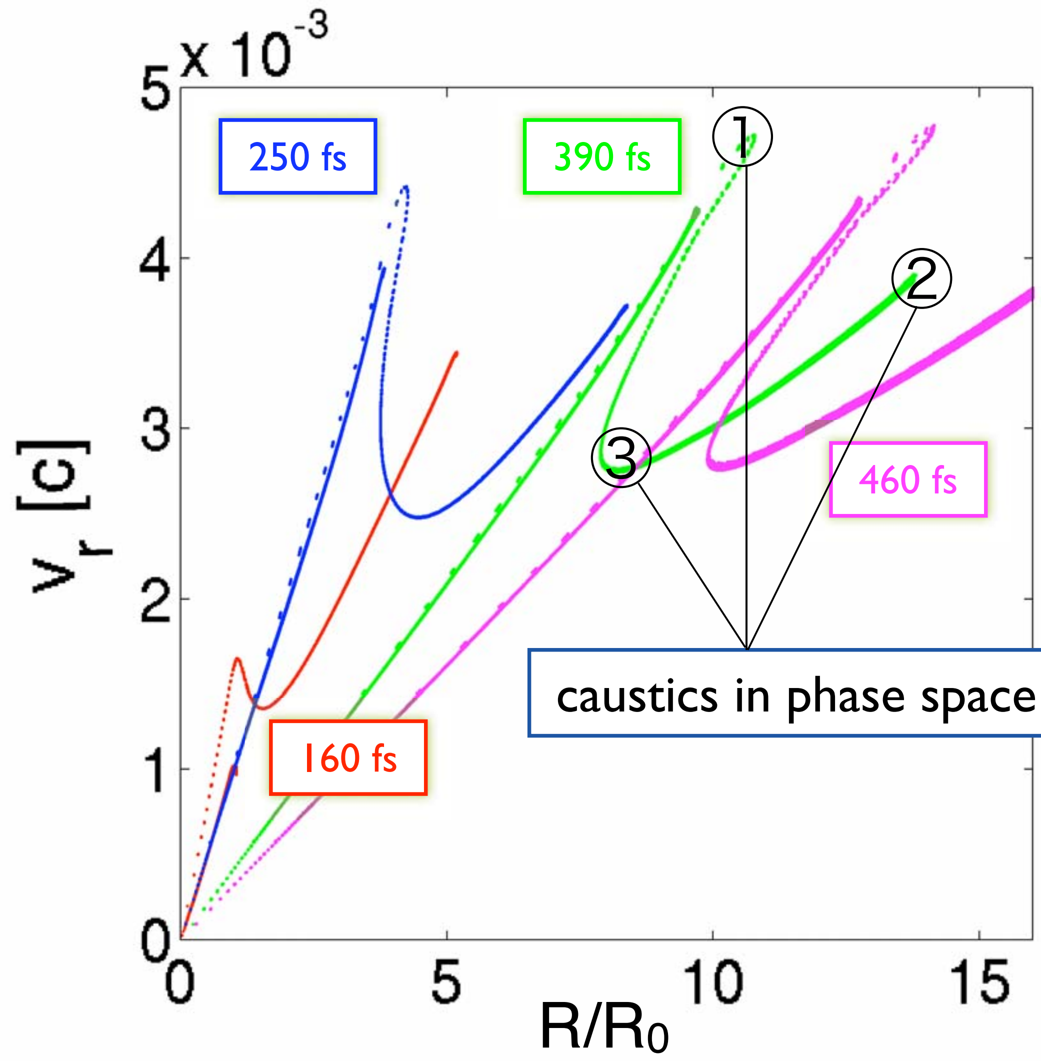
Particles:

- $\#_{3D}$/cell = 125 part./spec.
- $\#_{2D}$/cell = 100 part./spec.

Ion density and phase space evolution [2D]



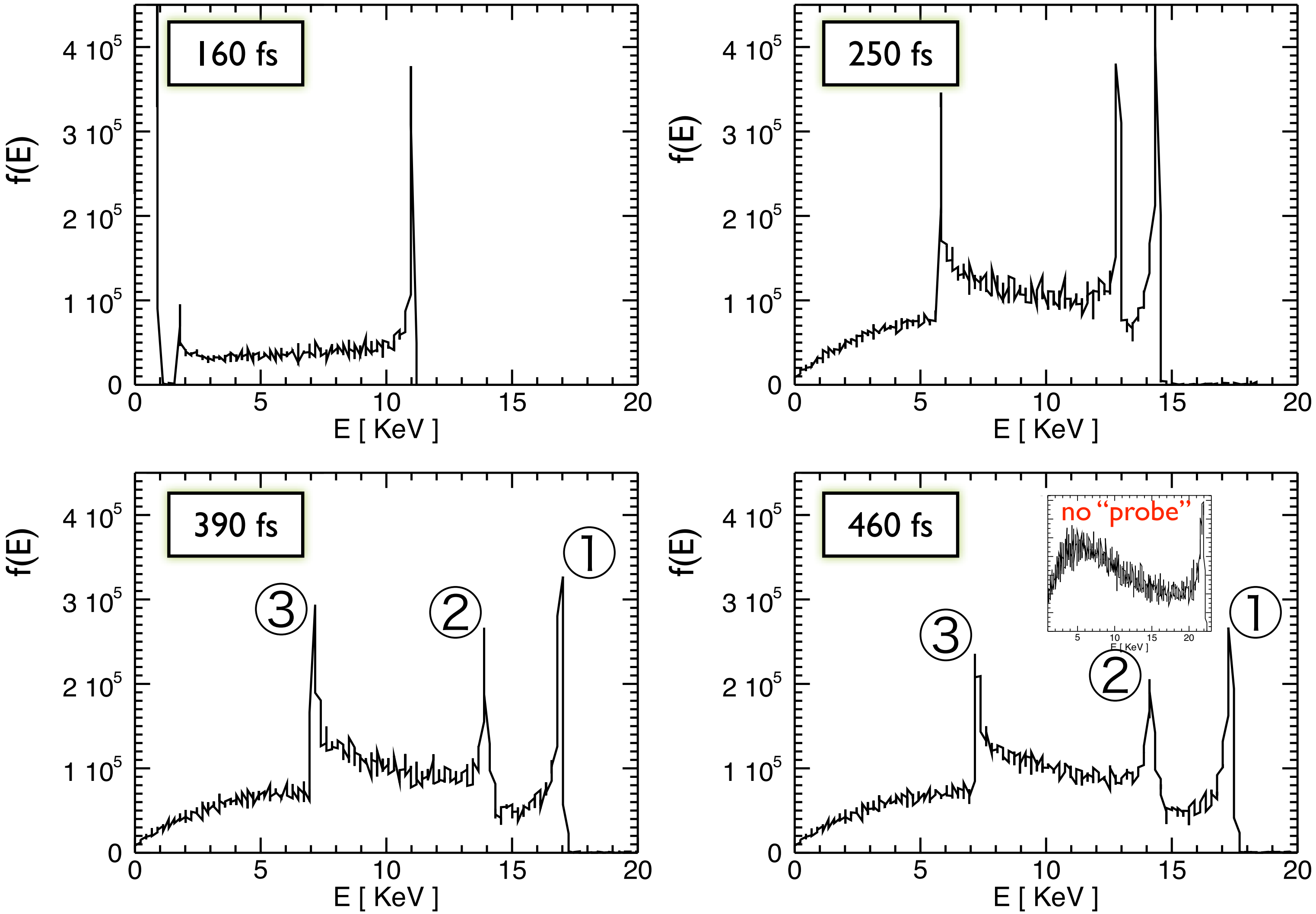
Evolution of ion phase space [3D]



$\Delta t \sim 150$ fs

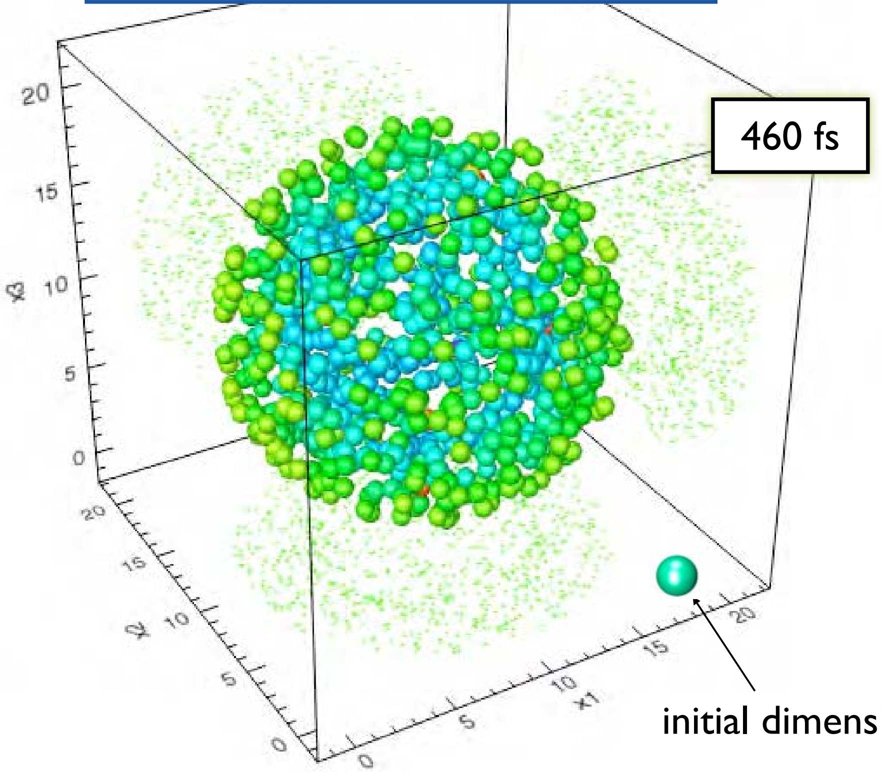
caustics in phase space ⇒ bunching in energy

Clear signature of shock shells in ion spectrum



Highest (& inner) energy ions overtake slower (& outer) ions

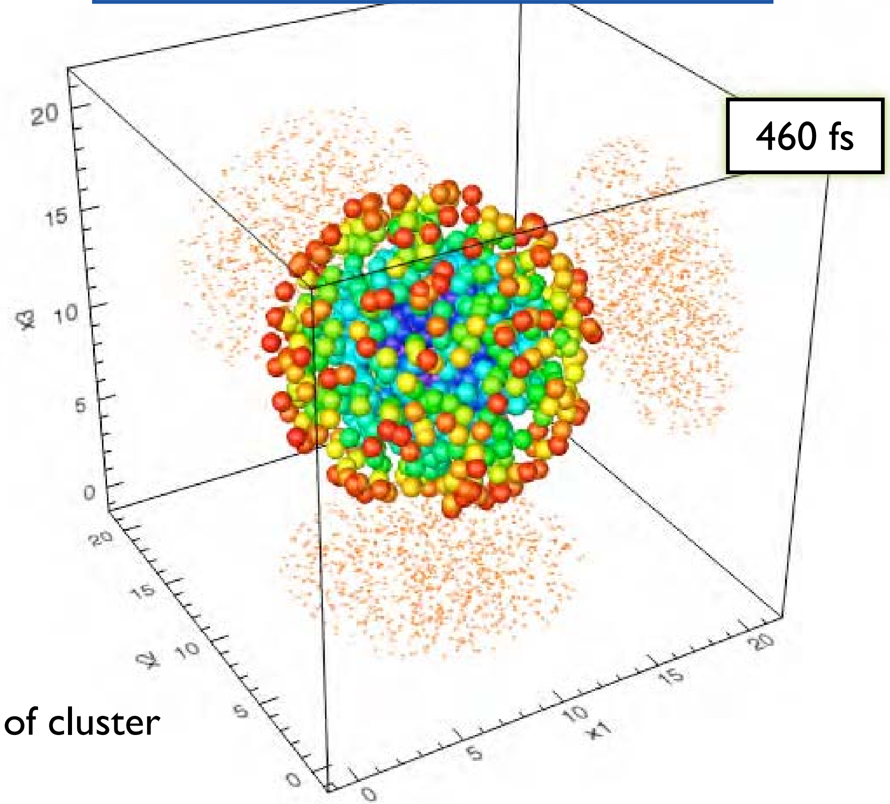
Ions ionized by weak beam



460 fs

initial dimension of cluster

Ions ionized by strong beam



460 fs

similar explosion physics as with IR light
different physics to control explosion

Kinetics of the expansion/explosion of nanoplasmas

The Vlasov-Poisson (VP) model

cgs units

$$\begin{cases} \dfrac{\partial f_{\mathrm{e}}}{\partial t} = -\mathbf{v}\dfrac{\partial f_{\mathrm{e}}}{\partial \mathbf{x}} - \dfrac{e}{m}\dfrac{\partial \Phi}{\partial \mathbf{x}}\dfrac{\partial f_{\mathrm{e}}}{\partial \mathbf{v}} \\ \dfrac{\partial f_{\mathrm{i}}}{\partial t} = -\mathbf{v}\dfrac{\partial f_{\mathrm{i}}}{\partial \mathbf{x}} + \dfrac{Ze}{M}\dfrac{\partial \Phi}{\partial \mathbf{x}}\dfrac{\partial f_{\mathrm{i}}}{\partial \mathbf{v}} \\ \nabla^2 \Phi = 4\pi e\left(\displaystyle\int f_{\mathrm{e}} d\mathbf{v} - Z\int f_{\mathrm{i}} d\mathbf{v}\right) \end{cases}$$

units

mass: m

charge: e

time: $\sqrt{\dfrac{m R_0{}^3}{e^2 N_0}}$

length: R_0

initial radius of the cluster

total number of electrons

dimensionless units

$$\begin{cases} \dfrac{\partial \hat{f}_{\mathrm{e}}}{\partial \hat{t}} = -\hat{\mathbf{v}}\dfrac{\partial \hat{f}_{\mathrm{e}}}{\partial \hat{\mathbf{x}}} - \dfrac{\partial \hat{\Phi}}{\partial \hat{\mathbf{x}}}\dfrac{\partial \hat{f}_{\mathrm{e}}}{\partial \hat{\mathbf{v}}} \\ \dfrac{\partial \hat{f}_{\mathrm{i}}}{\partial \hat{t}} = -\hat{\mathbf{v}}\dfrac{\partial \hat{f}_{\mathrm{i}}}{\partial \hat{\mathbf{x}}} + Z\dfrac{m}{M}\dfrac{\partial \hat{\Phi}}{\partial \hat{\mathbf{x}}}\dfrac{\partial \hat{f}_{\mathrm{i}}}{\partial \hat{\mathbf{v}}} \\ \hat{\nabla}^2 \hat{\Phi} = 4\pi\left(\displaystyle\int \hat{f}_{\mathrm{e}} d\hat{\mathbf{v}} - \int \hat{f}_{\mathrm{i}} d\hat{\mathbf{v}}\right) \end{cases}$$

Dynamics depends on two dimensionless parameters:

$$Z\frac{m}{M}$$

$$\hat{T}_0 = \frac{R_0 k_{\mathrm{B}} T_0}{e^2 N_0} = 3\frac{\lambda_{\mathrm{D},0}^2}{R_0^2}$$

Initial conditions (dimensionless units):

$$\hat{f}_{\mathrm{i}}\left(\hat{\mathbf{x}}, \hat{\mathbf{v}}, t=0\right) = \frac{3}{4\pi}\delta\left(\hat{\mathbf{v}}\right)\Theta\left(1 - |\hat{\mathbf{x}}|\right)$$

cold ions @ t=0

$$\hat{f}_{\mathrm{e}}\left(\hat{\mathbf{x}}, \hat{\mathbf{v}}, t=0\right) = \frac{3}{4\pi}\left(\frac{1}{2\pi\hat{T}_0}\right)^{\frac{3}{2}}\exp\left(-\frac{\hat{\mathbf{v}}^2}{2\hat{T}_0}\right)\Theta\left(1 - |\hat{\mathbf{x}}|\right)$$

hot non relativistic ions @ t=0

Ergodic model*

ion trajectories: $r_i\left(r_0, t\right)$

electron energies: $\epsilon\left(\epsilon_0, t\right)$

ion density: $n_i\left(r, t\right)$

electron density: $n_e\left(r, t\right)$

electrostatic potential: $\Phi\left(r, t\right)$

$$\begin{cases} m_i \dfrac{\partial^2 r_i}{\partial t^2} = -Ze\dfrac{\partial \Phi}{\partial r}(r_i) \\ \dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left(r^2\dfrac{\partial \Phi}{\partial r}\right) = 4\pi e\left(n_e - Zn_i\right) \\ n_i(r_i) = n_{i,0}(r_0)\dfrac{r_0^2}{r_i^2}\Big/\dfrac{\partial r_i}{\partial r_0} \\ n_e = \dfrac{1}{4\pi r^2}\displaystyle\int \rho_0(\epsilon_0)\,\mathscr{P}\left(r, \epsilon; \Phi\right) \mathrm{d}\epsilon_0 \\ \dfrac{\mathrm{d}\epsilon}{\mathrm{d}t} = -e\displaystyle\int \dfrac{\partial \Phi}{\partial t}\mathscr{P}\left(r, \epsilon; \Phi\right) \mathrm{d}r \end{cases}$$

e- phase space volume is conserved

$\rho\left(\epsilon, t\right) \mathrm{d}\epsilon = \rho_0\left(\epsilon_0\right) \mathrm{d}\epsilon_0$

$$\mathscr{P}\left(r, \epsilon; \Phi\right) = \frac{r^2\left(\epsilon + e\Phi\right)^{\frac{1}{2}}}{\int r'^2\left[\epsilon + e\Phi\left(r'\right)\right]^{\frac{1}{2}} \mathrm{d}r'} =$$ **probability density for electrons with energy ϵ to lie at r**

boundary conditions: $\frac{\partial \Phi}{\partial r}(0, t) = 0, \quad \Phi \overset{r\rightarrow\infty}{\longrightarrow} 0$

initial conditions: $n_i(r_i, 0) = n_{i,0}\left(r_0\right), \quad \rho(\epsilon, 0) = \rho_0\left(\epsilon_0\right)$

---

* Peano et al, Phys. Rev. E 75, 066403 (2007)

Energy spectrum of the ions

positive charge buildup within r_i

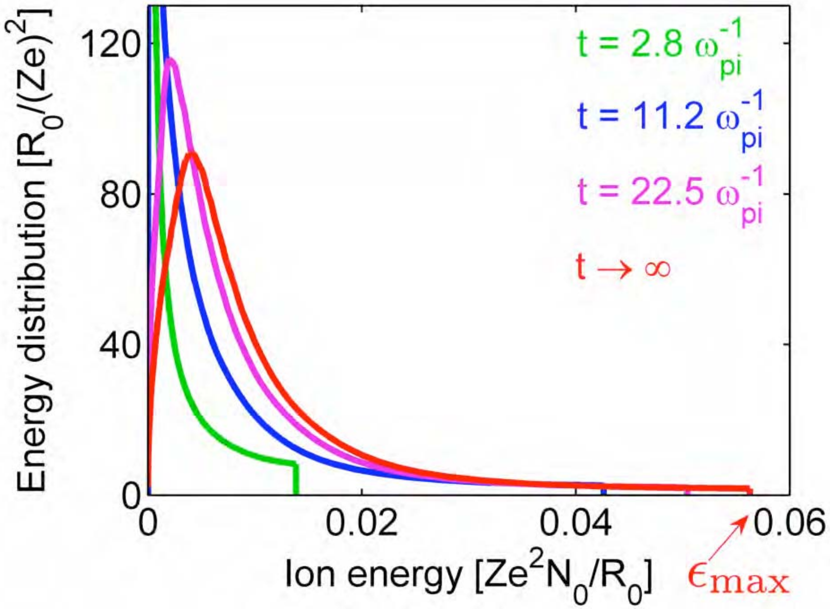
asymptotic ion energy depends
strongly on electron dynamics:

$$\frac{\epsilon_\infty(r_0)}{Ze} = \frac{q(r_0,0)}{r_0} + \int_0^\infty \frac{1}{r_\mathrm{i}(r_0,t)} \frac{\partial q(r_\mathrm{i}(r_0,t),t)}{\partial t} \mathrm{d}t$$

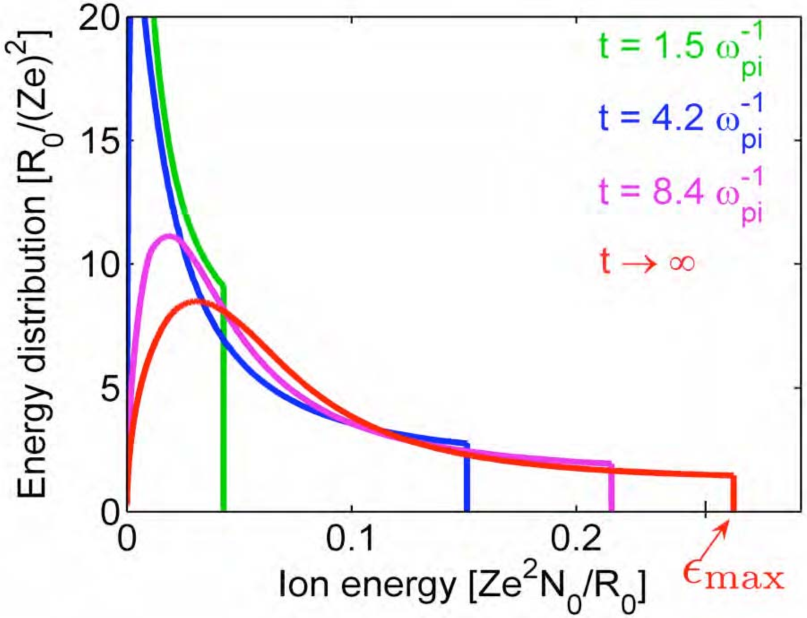
ion-front radius

energy spectra can develop a local maximum far from its cutoff energy

$\hat{T}_0 = 7.2 \times 10^{-3}$



$\hat{T}_0 = 7.2 \times 10^{-2}$

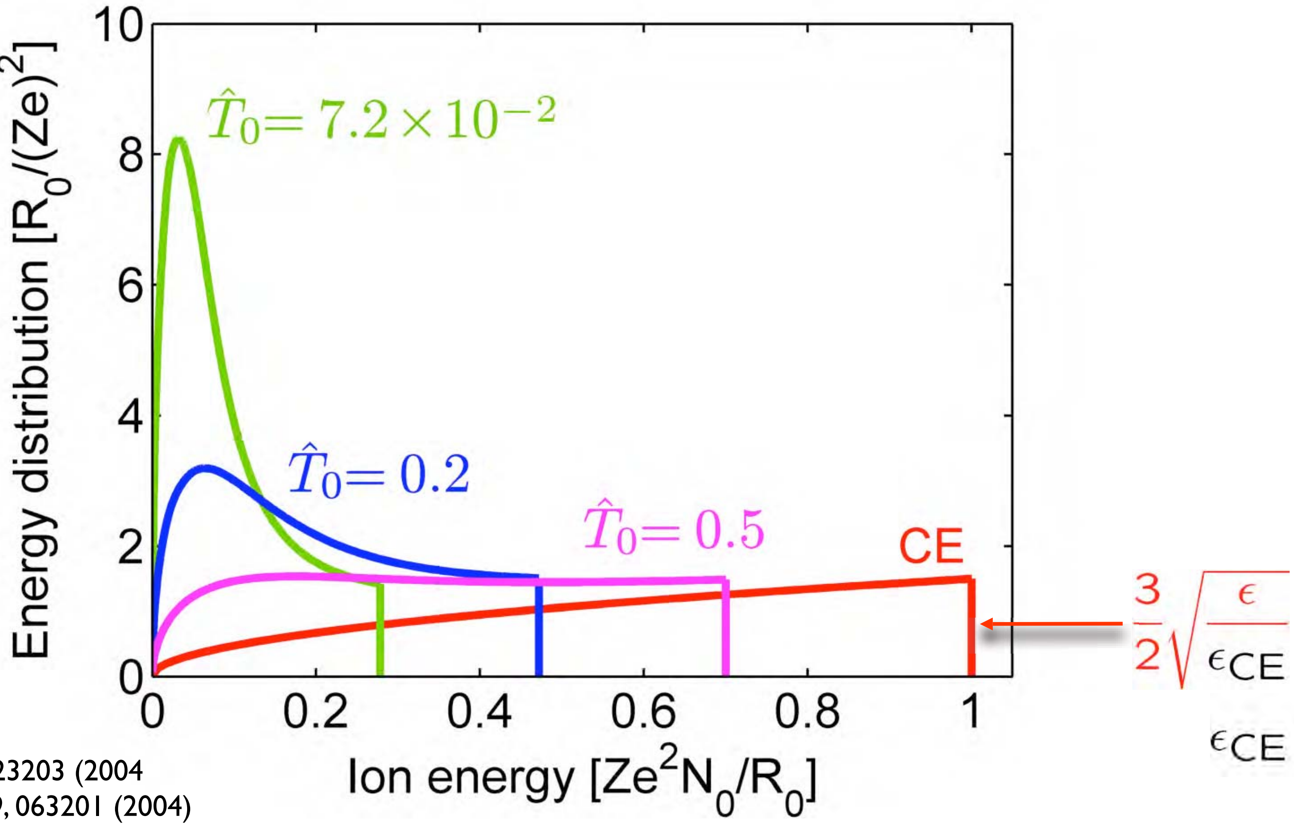


Influence of $\hat{T}_0$ on energy spectrum I

- energy spectra become monotonic at $\hat{T}_0 \simeq 0.5$

$$\Downarrow$$

- transition towards Coulomb Explosion (CE) regime

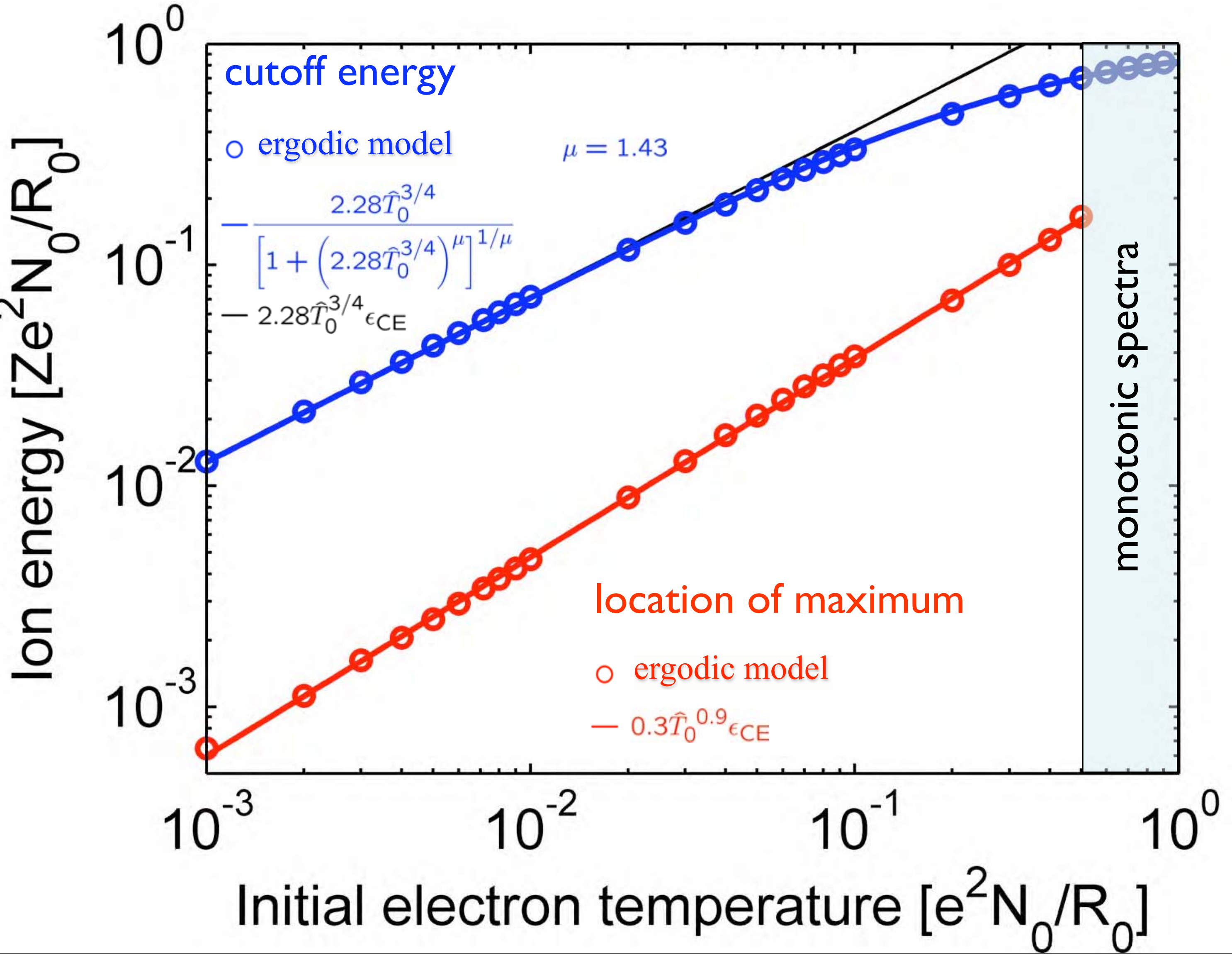


$$\frac{3}{2}\sqrt{\frac{\epsilon}{\epsilon_{CE}}}$$

$$\epsilon_{CE} = \frac{Ze^2 N_0}{R_0}$$

Experimental results:
S. Sakabe et al., Phys. Rev. A 69, 023203 (2004
M. Hirokane et al., Phys. Rev. A 69, 063201 (2004)

Influence of $\hat{T}_0$ on energy spectrum II



Summary

- In clusters, explosion/expansion can be controlled via double pump techniques
- Ability to fine tune ion energy/features of ion spectrum in experiments
- Model to describe expansion/explosion function of λ_D/R_0 (energy deposited on the electrons/R_0^2)
- Nanoplasmas/nanostructured materials provide additional "control knob":
    - radiation generation
    - ion acceleration