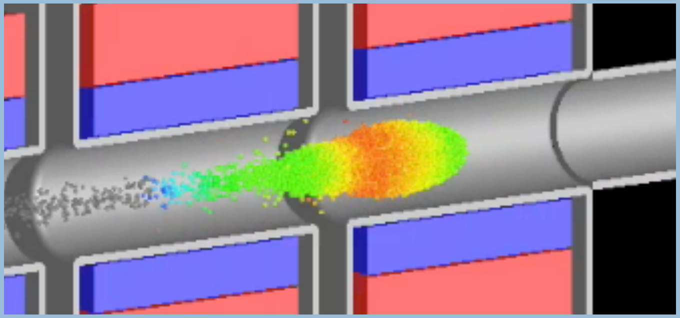
HEDLP / Inertial Fusion Energy
Simulation of intense beams for heavy-ion-fusion science



Ion beam in the NDCX-II accelerator

Alex Friedman

LLNL Fusion Energy Program
and
Heavy Ion Fusion Science Virtual National Laboratory

Large Scale Computing and Storage Requirements for Fusion Energy Sciences
An FES / ASCR / NERSC Workshop
Rockville, MD, August 3-4, 2010

Fusion Energy Program

The Heavy Ion Fusion Science Virtual National Laboratory

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The Heavy Ion Fusion Science VNL (HIFS-VNL) is part of a worldwide ion-driven HEDP community with centers in Germany, Russia, and Japan.

Outline

- ➡ Introduction to the HIFS-VNL research program
- Intense ion beam physics
  - NDCX-II physics design
  - Beam-plasma interactions
  - Warp code plans and requirements
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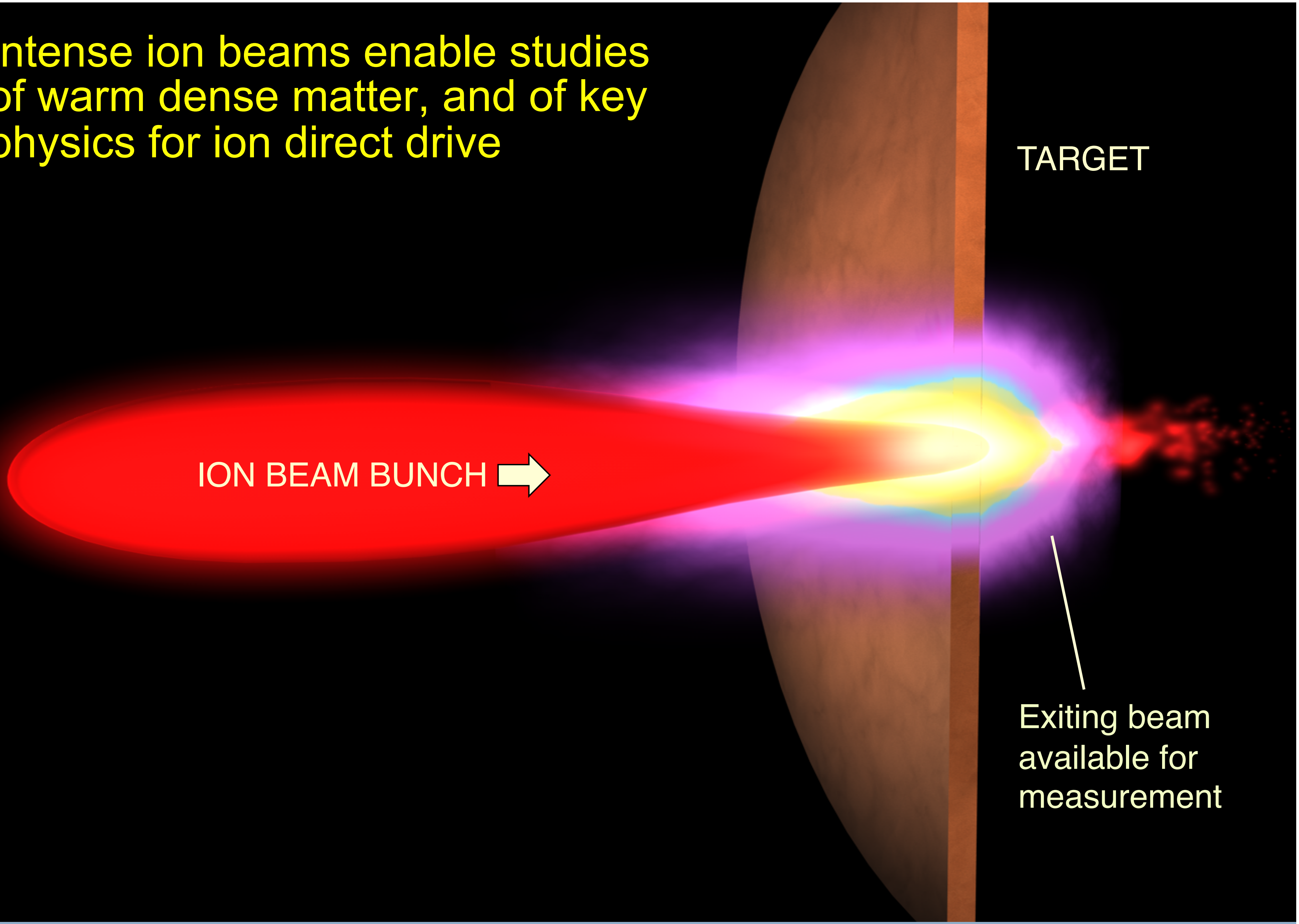
- Final comments

The HIFS-VNL employs intense ion beams for High Energy Density Physics and Inertial Fusion Energy (IFE) target physics

- Heavy Ion Fusion has long been considered an attractive approach to Inertial Fusion Energy.
- In the early 2000's, the VNL's mission was shifted to exploring HEDP, especially Warm Dense Matter (WDM) physics.
- We're now re-expanding our program beyond WDM physics, into heavy-ion IFE target physics.*
- We're building a new facility, NDCX-II, to support this expanded program

*These research directions were identified in the January 2009 FESAC HEDLP, and November 2009 Research Needs HEDLP, Workshops.

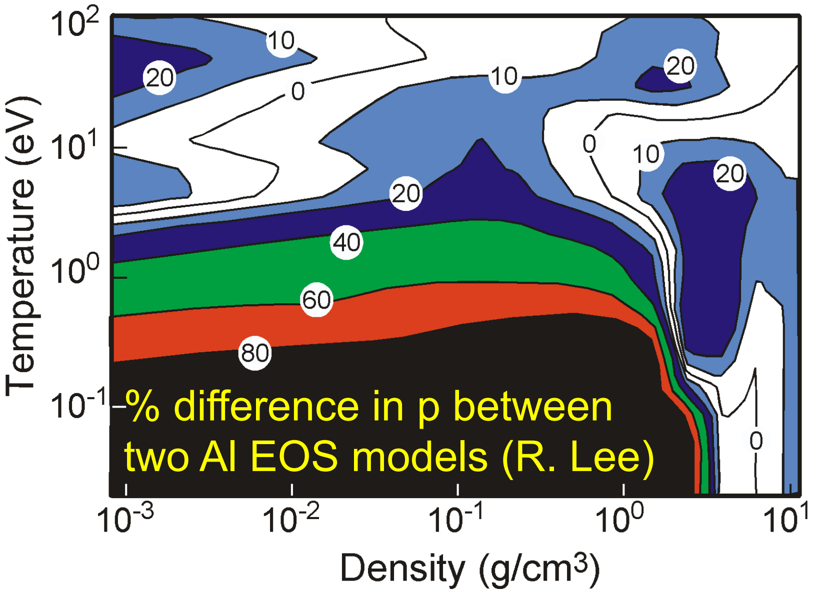
Intense ion beams enable studies of warm dense matter, and of key physics for ion direct drive



Studies of WDM science & IFE target science are complementary

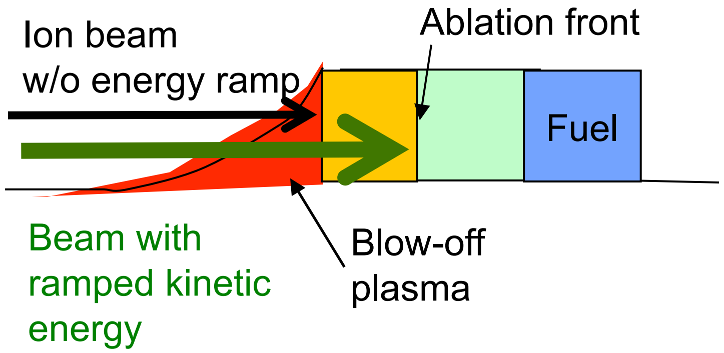
- WDM is of fundamental interest …
  - in the universe, *e.g.*, giant planets
  - In the laboratory, *e.g.*, early stages of IFE targets
  - perhaps for such applications as high power switches

… but is not well understood.



% difference in p between two Al EOS models (R. Lee)

- Heavy-ion-driven IFE is attractive due to driver efficiency, compatibility with liquid walls, robust final optics, and more.
  - Advanced target concepts may lead to simpler / cheaper drivers
  - NDCX-II experiments will explore techniques for highly efficient coupling of beam energy into the target implosion



Ion beam w/o energy ramp

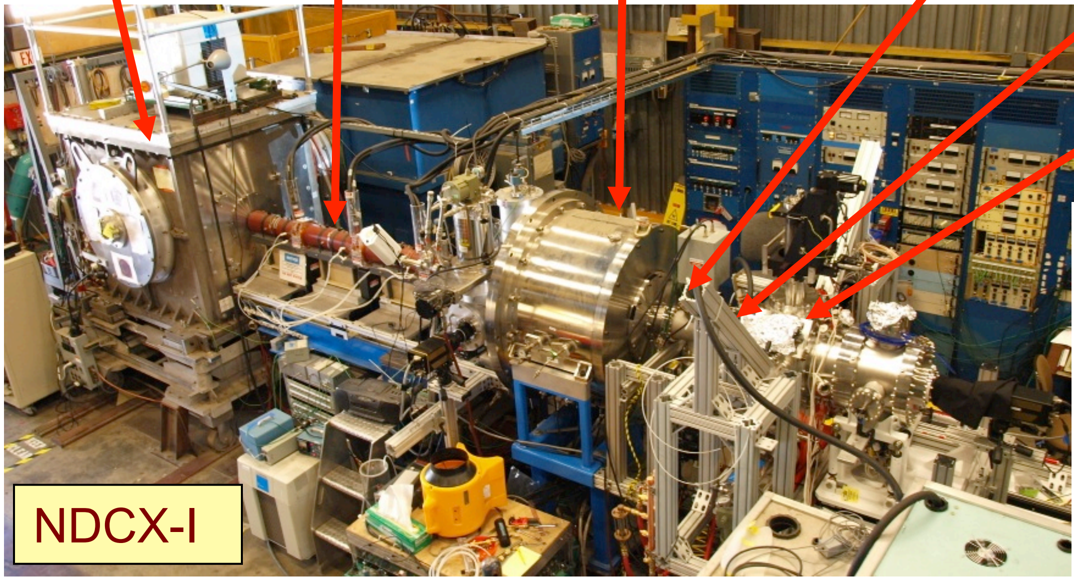
Ablation front

Fuel

Beam with ramped kinetic energy

Blow-off plasma

Neutralized Drift Compression Exp't (NDCX-I) at LBNL routinely achieves current and power amplifications exceeding 50x



injector

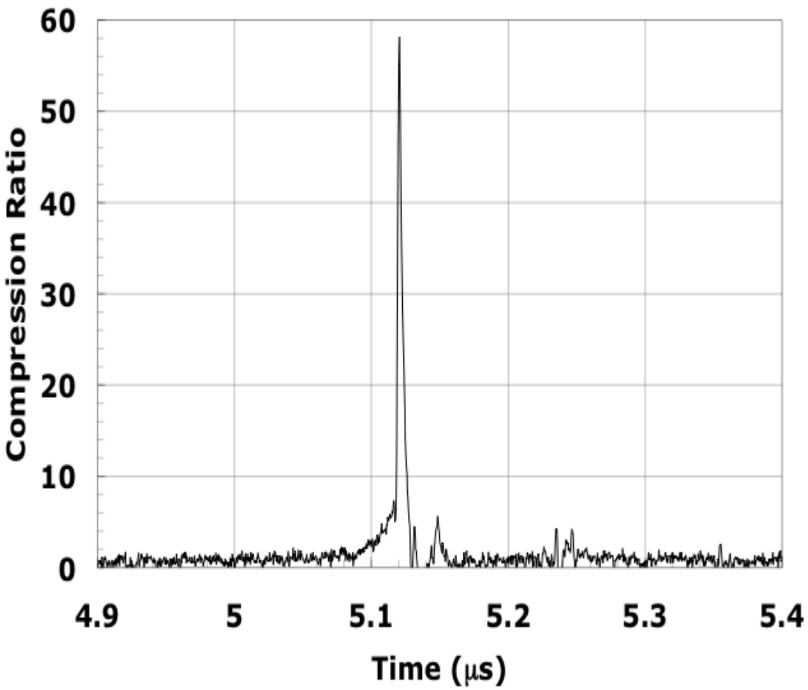
beam transport solenoids

induction bunching module

drift compression line

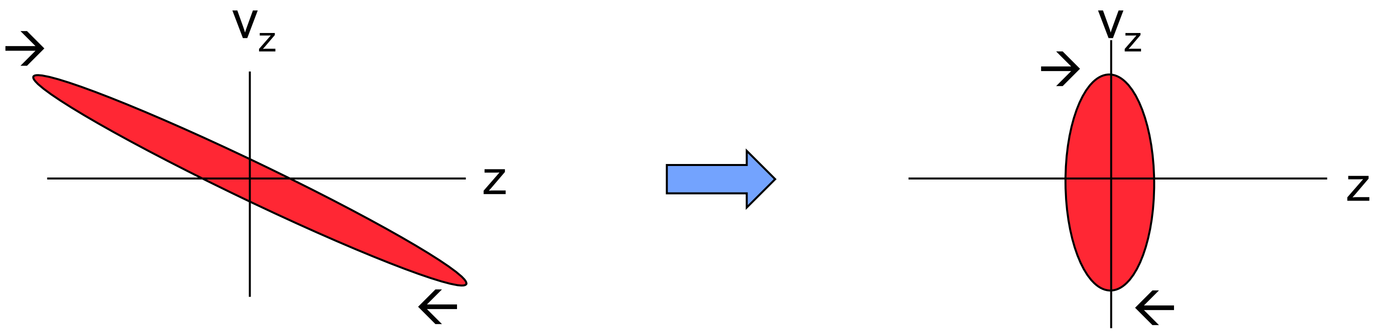
final focus solenoid

target chamber with plasma sources



The “drift compression” process is used to shorten an ion bunch

- Induction cells impart a head-to-tail velocity gradient (“tilt”) to the beam
- The beam shortens as it moves down the beam line (pictures in beam frame):



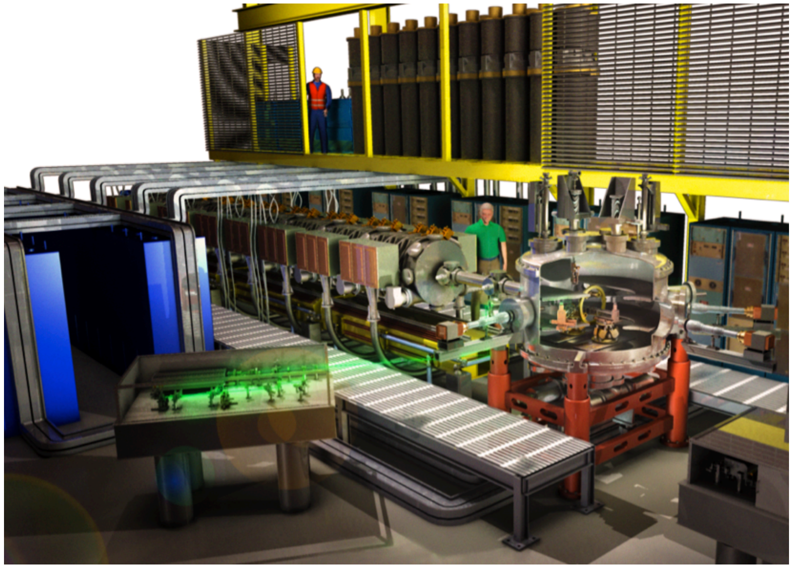
Initial beam,
with velocity tilt

compressed beam

- Space charge, if present, limits this inward motion
- To obtain a short pulse on target, we introduce neutralizing plasma; this is neutralized drift compression.

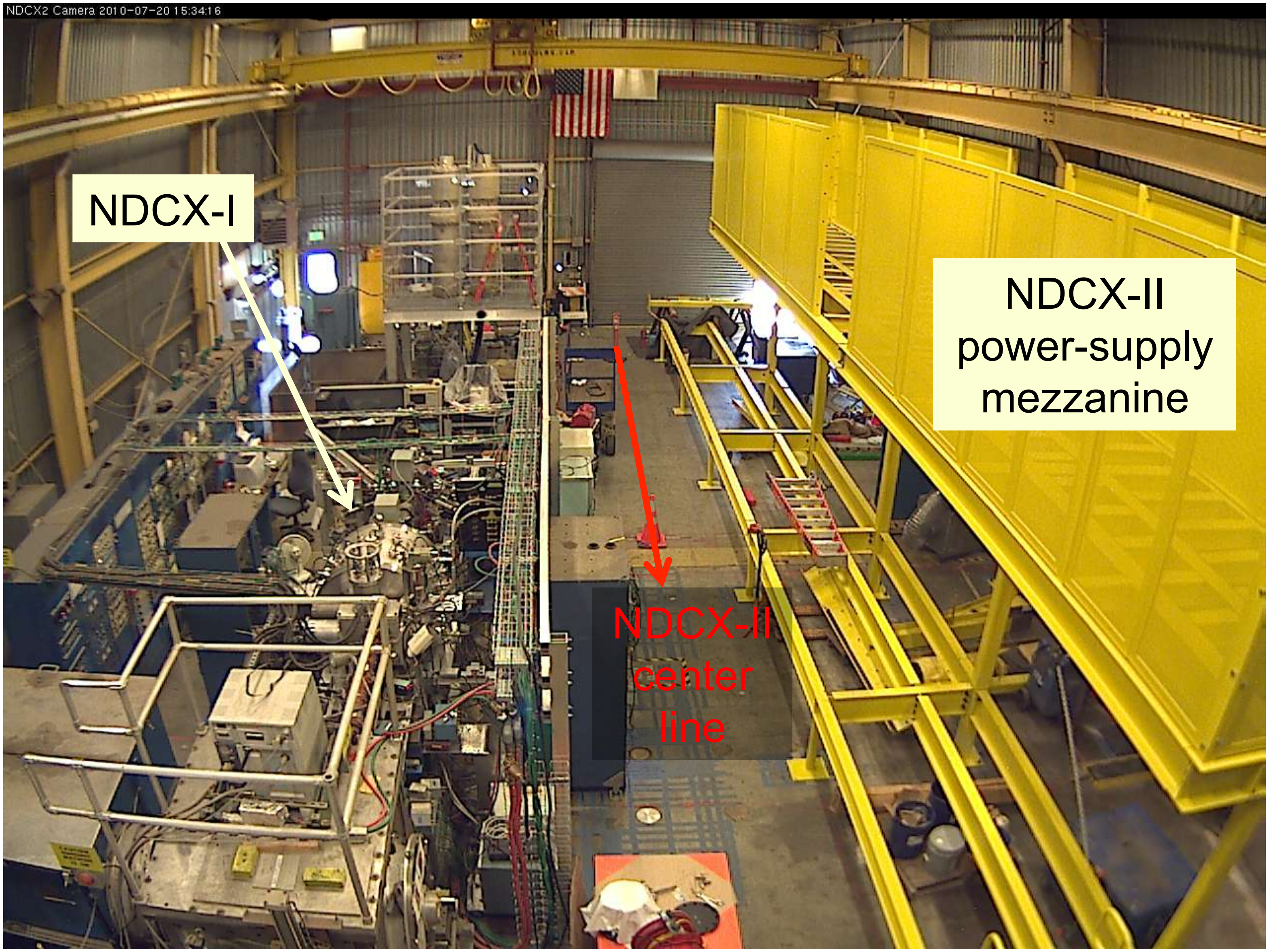
Our next-step facility, NDCX-II, is under construction at LBNL

- The Office of Fusion Energy Sciences approved the project early in 2009.



- Construction of the initial configuration began in July 2009.
- Completion planned for March 2012.
- Target experiments start ~ October 2012.

LBNL Building 58, as viewed from webcam on July 20, 2010



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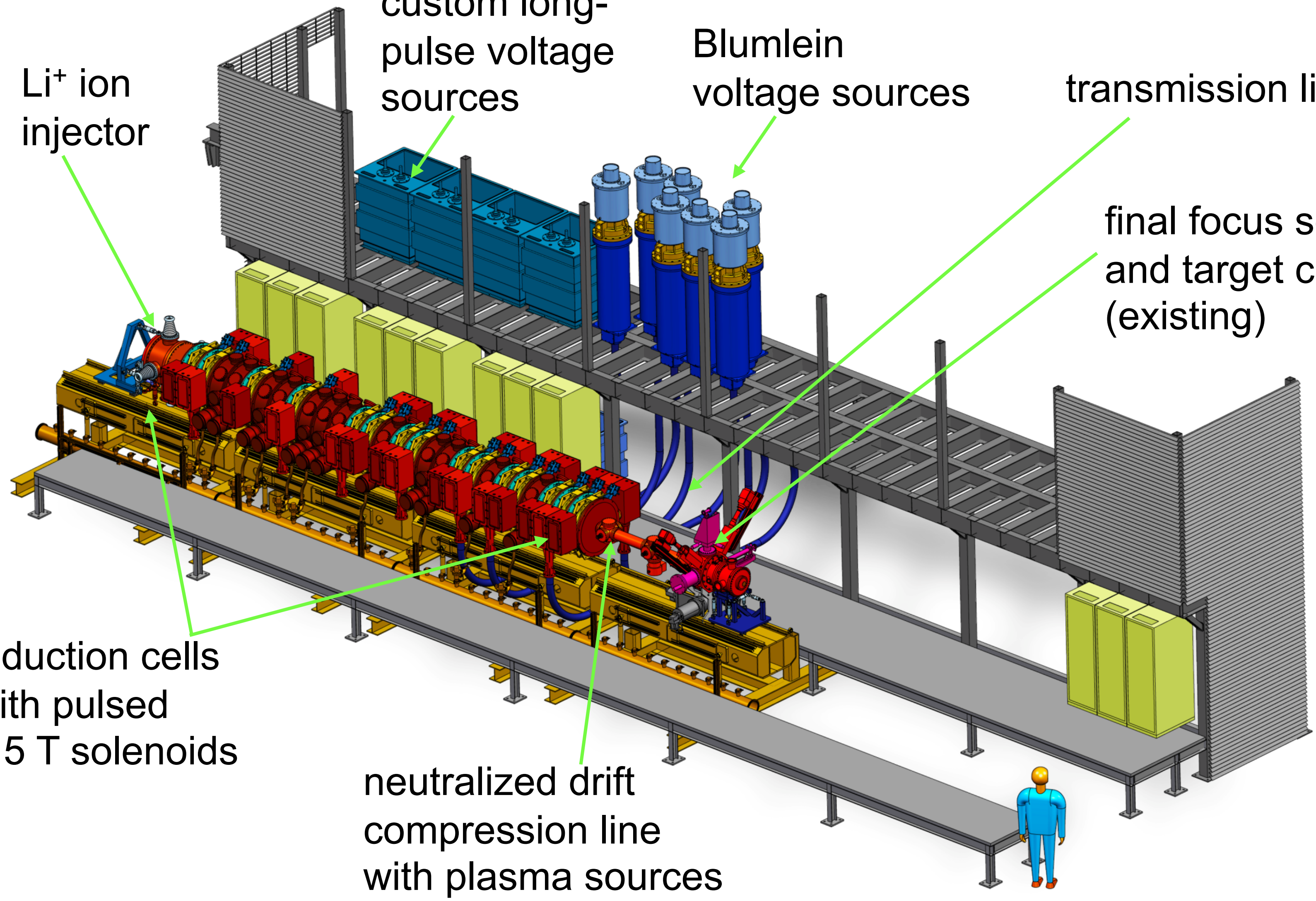
NDCX-II principal systems



Li$^+$ ion injector

custom long-pulse voltage sources

Blumlein voltage sources

transmission lines

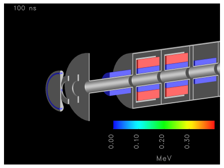
final focus solenoid and target chamber (existing)

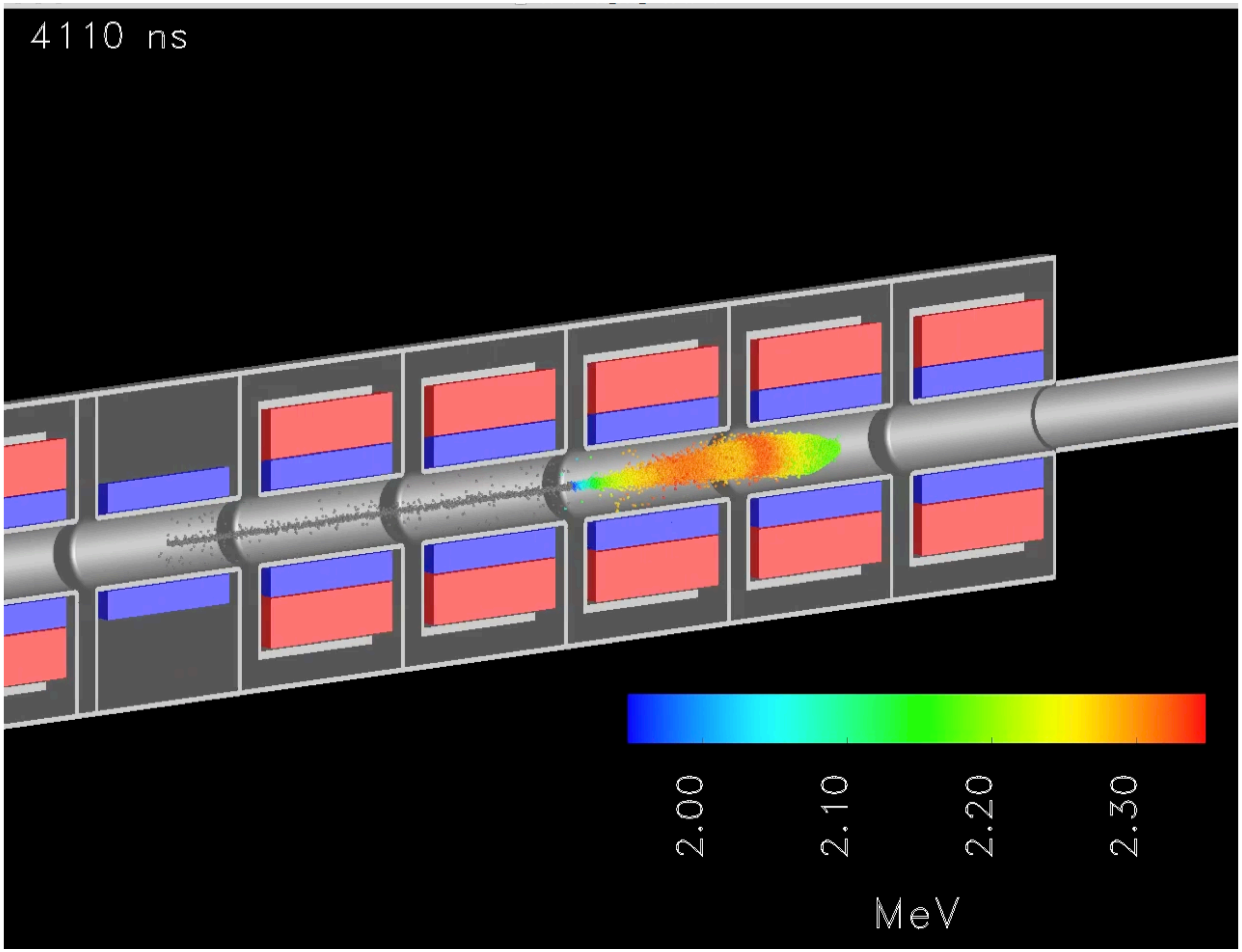
induction cells with pulsed 2.5 T solenoids

neutralized drift compression line with plasma sources

Video: Warp 3D simulation of 18-cell NDCX-II, including random offsets of solenoid ends by up to 2 mm (0.5 mm is nominal)

play video

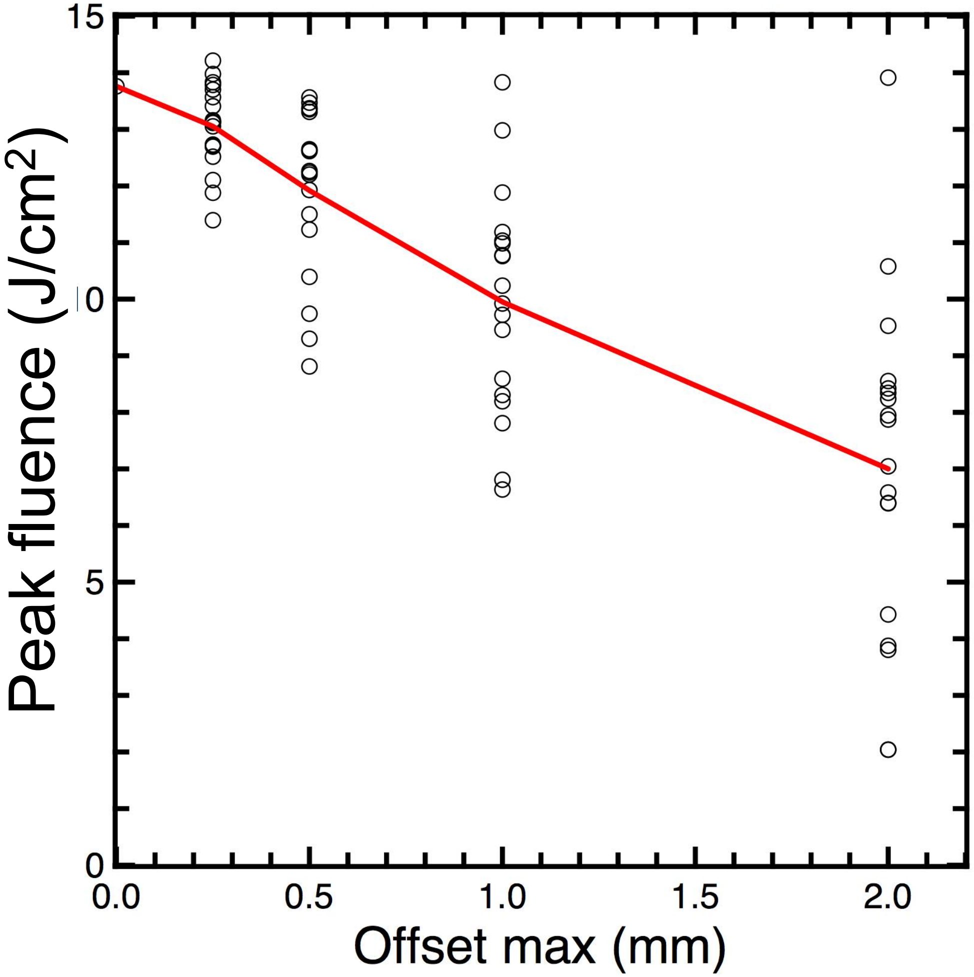




NDCX-II design physics: A. Friedman, *et al.*, *Phys. Plasmas* **17**, 056704 (2010).

Warp 3D simulations indicate slow degradation of the focus as misalignment of the solenoids increases (without steering)

- Random offsets in x and y were imposed on the solenoid ends.
- The offsets were chosen from a uniform distribution with a set maximum.



(This series used an older 15-cell design based on a 2 mA/cm^2 source)

35g-15

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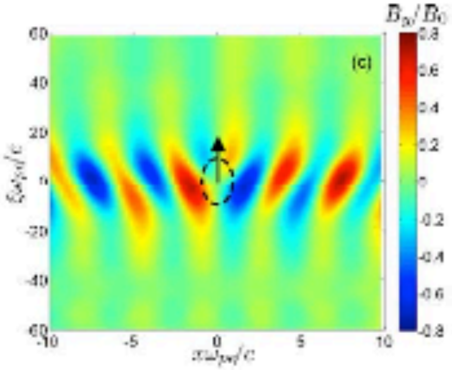
NDCX-II will enable greater understanding of beams in plasmas

Electromagnetic fields are excited by a moving beam in a magnetized plasma:

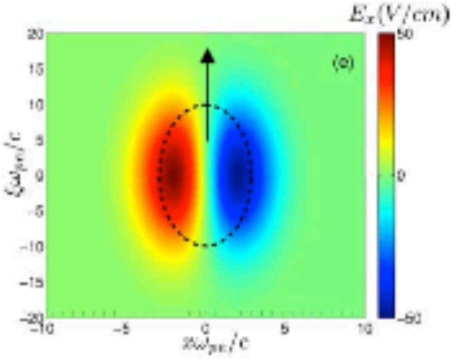
Wave field (can extend far outside the bunch)



Can be used for diagnostics

M. Dorf, I. Kaganovich, E. Startsev, and R. C. Davidson, Phys. Plasmas **17**, 023103 (2010).

Local field (falls off rapidly outside the bunch)



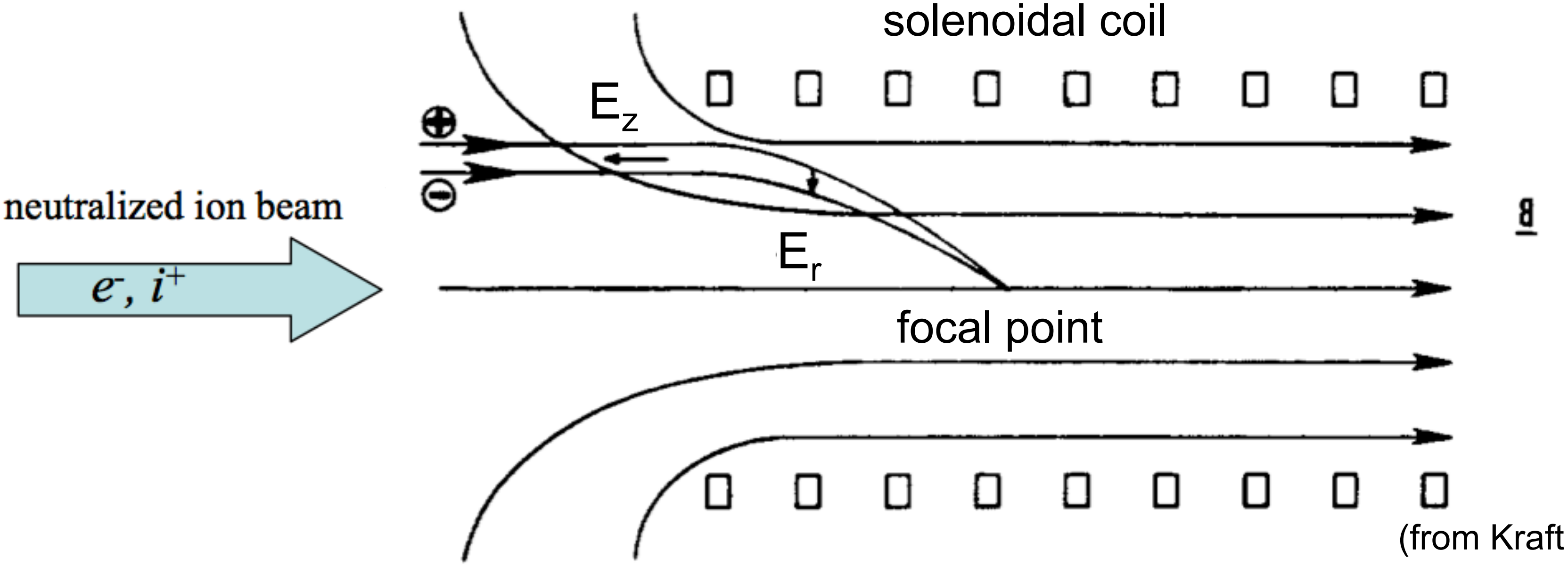
Can provide bunch focusing

M. Dorf, I. Kaganovich, E. Startsev, and R. C. Davidson, PRL **103**, 075003 (2009)

Review paper: I. D. Kaganovich, *et al.*, Phys. Plasmas **17**, 056703 (2010)

The “Robertson lens” is an example of a multi-species system that we need to simulate in full kinetic detail

- An ambipolar electrostatic field brings both species to a common focus
- For a given focal length, the required B_0 is smaller by a factor of $(m_e/m_i)^{1/2}$



(from Kraft paper)

Focusing force on beam: $F_r = -\frac{r}{4} m_i \Omega_e \Omega_i \quad (\Omega_i = Z_b e B_0 / m_i c)$

References: S. Robertson, *Phys. Rev. Lett.* **48**, 149 (1982).
R. Kraft, B. Kusse, & J. Moschella, *Phys. Fluids* **30**, 245 (1987).

requires:
$r_b << c/\omega_{pe}$
$\omega_{pe} >> \omega_{ce}$

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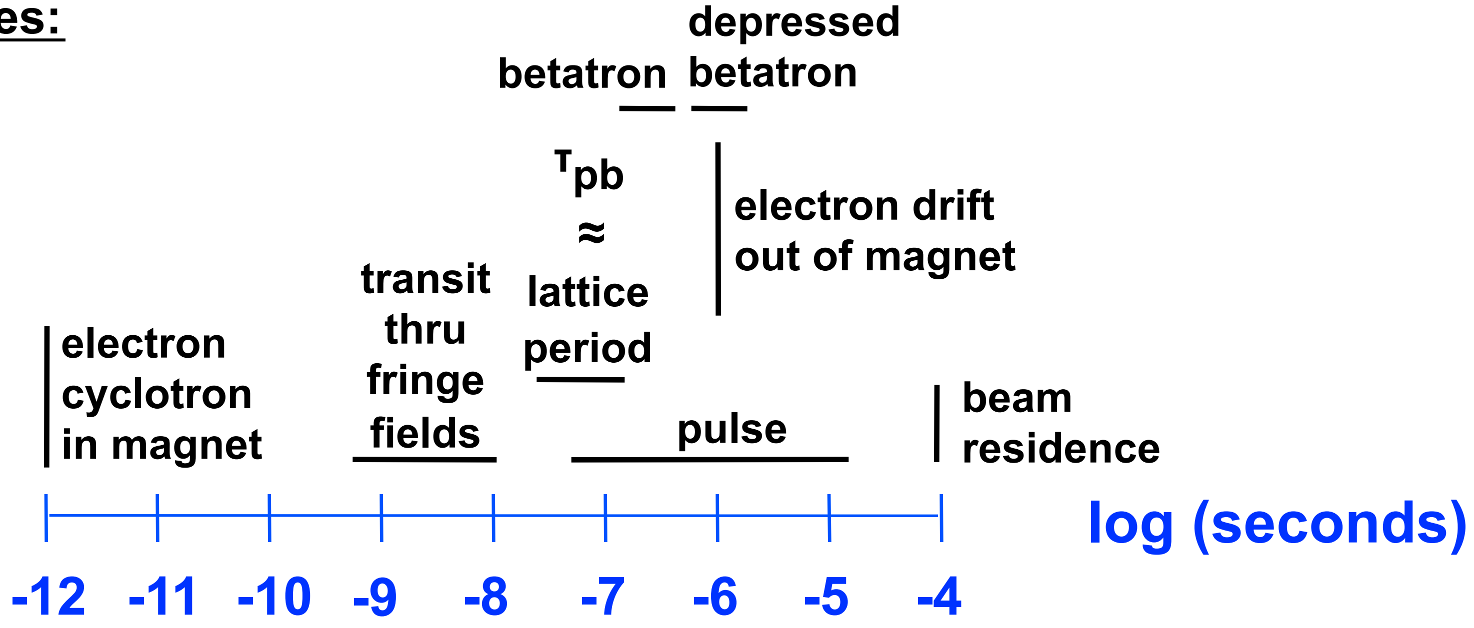
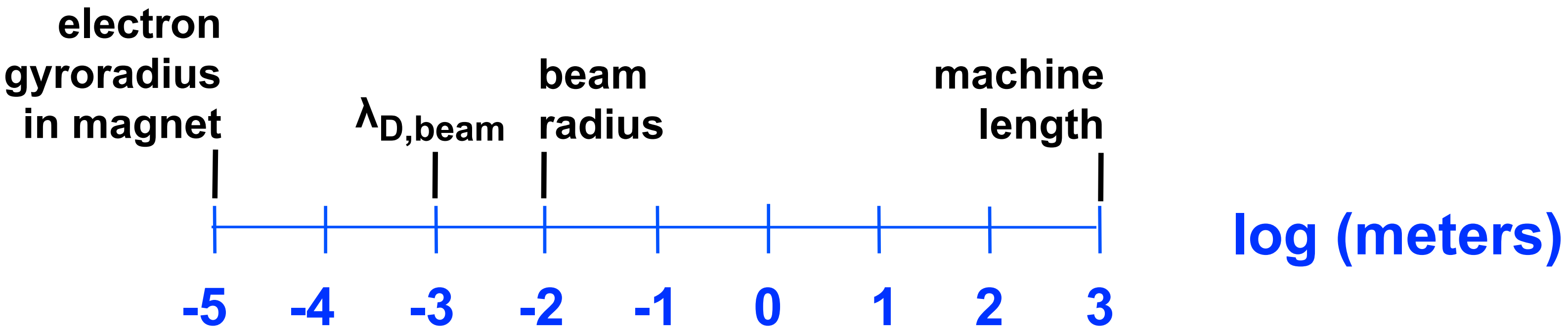
For HIF driver, time and length scales span a wide range

Time scales:

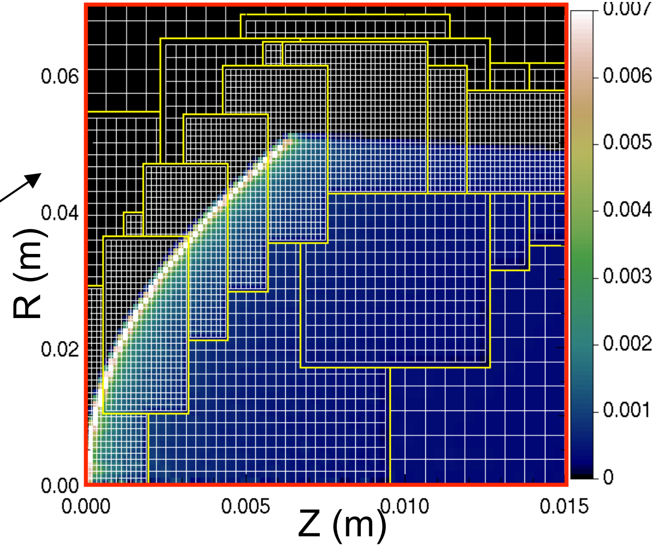


Length scales:

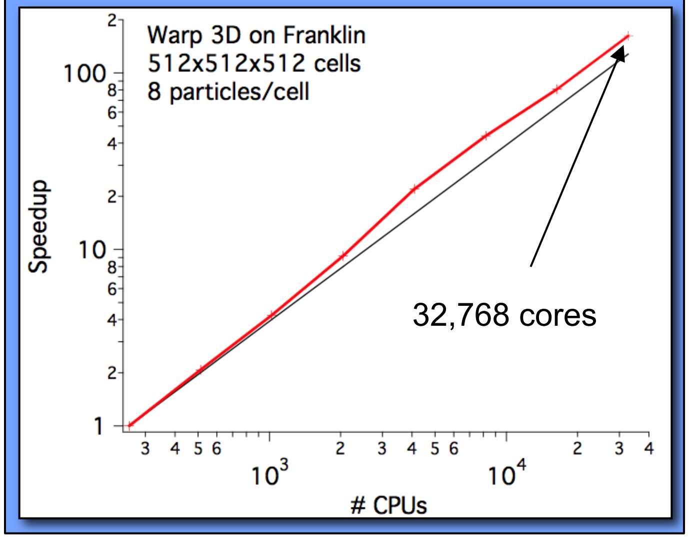


Warp: a parallel framework combining features of plasma (Particle-In-Cell) and accelerator codes

- **Geometry:** 3D (x,y,z), 2-1/2D (x,y), (x,z) or axisym. (r,z)
- **Python and Fortran:** "steerable," input decks are programs
- **Field solvers:** Electrostatic - FFT, multigrid; implicit; AMR
  Electromagnetic - Yee, Cole-Kark.; PML; AMR
- **Boundaries:** "cut-cell" --- no restriction to "Legos"
- **Applied fields:** magnets, electrodes, acceleration, user-set
- **Bends:** "warped" coordinates; no "reference orbit"
- **Particle movers:** Energy- or momentum-conserving; Boris, large time step "drift-Lorentz", novel relativistic Leapfrog
- **Surface/volume physics:** secondary e^- & photo-e^- emission, gas emission/tracking/ionization, time-dependent space-charge-limited emission
- **Parallel:** MPI (1, 2 and 3D domain decomposition)



Warp 3D EM/PIC on Franklin

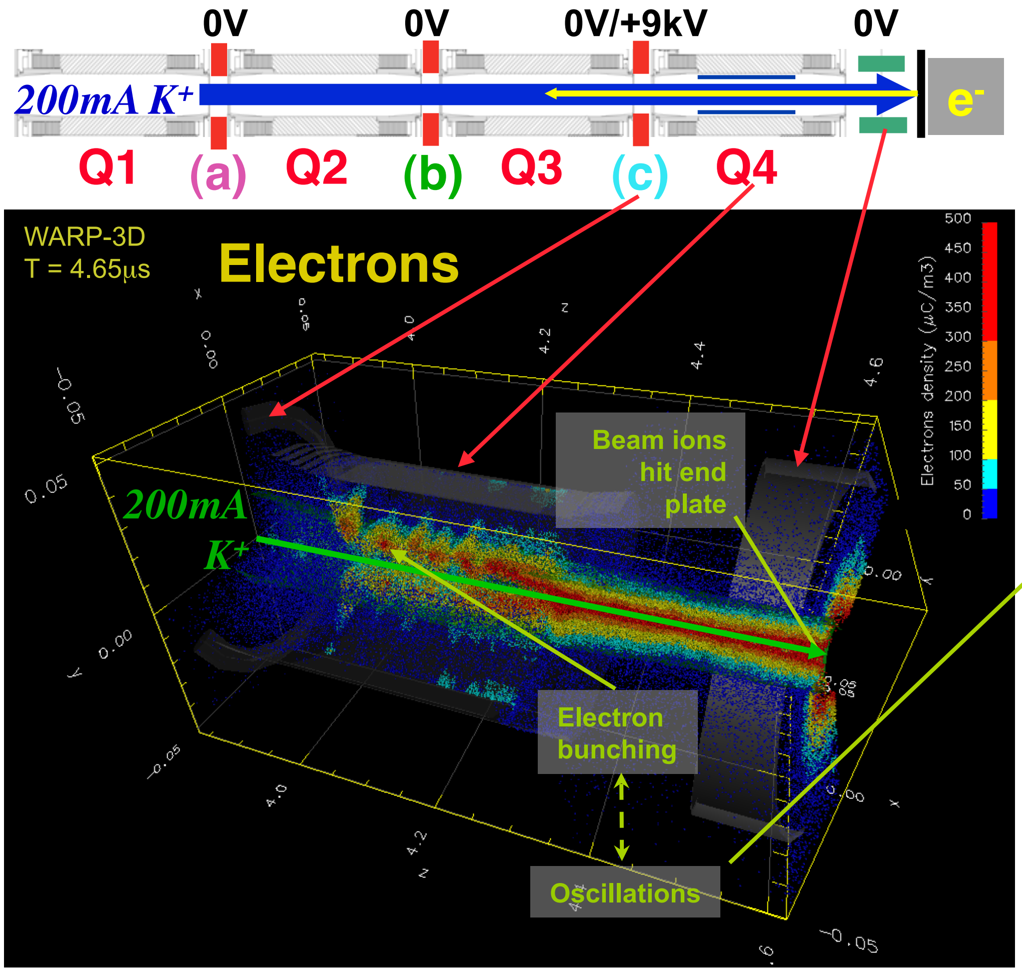


Warp 3D on Franklin
512x512x512 cells
8 particles/cell

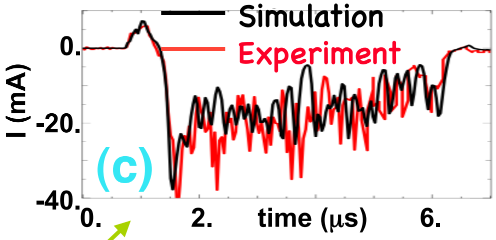
32,768 cores

Warp has been compared extensively vs. experiment

Deliberate e-cloud generation on HCX:



~6 MHz signal at (c) in simulation AND experiment:



run time ~3 cpu-days; would be ~1-2 months without new electron mover and MR.

Warp work has focused on NDCX-II physics design; now, scope is expanding

- Iterative design and assessment (on NERSC and LBNL clusters) --- *ensembles* of runs with random errors:
  - Typically run 256 cases in a single batch job, 8 at a time
  - 128 cores, < 1 GB/core, 60 GB total memory, 35 hours wall-clock time
  - Much data processing is in-line; I/O is only about 100 GB / job
  - Very light traffic in and out of NERSC (results stored at center)

- On *current* beam-in-plasma problems, and others:
  - Warp uses 100's x 100's x 1000's of cells, and millions of particles (13 or more variables per particle)
  - On Franklin, uses 512, 1024, and sometimes 4096 processors
  - EM tests show good scaling at 512^3 cells, to nearly 35,000 processors

Our need for NERSC time is rapidly growing; we used 200k core hours in the first half of 2010 (vs. just 74k in all of 2009)

We project the need for four classes of Warp runs during the next five years

1. Ensemble runs to optimize output beam from *accelerator,* for each class of target being shot on NDCX-II
   - So far, we haven't been able to use gradient methods for optimization because of particle noise; hope to overcome this with larger runs
2. Simulations of plasma injection from sources into the drift-compression line and final-focus solenoid
   - These are quite costly because the plasma flow is relatively slow (~10 μs), and we need to operate on an electron timescale
   - So far ES; but EM would be comparable since run is near the Courant limit (and EM scales better)
3. Integrated simulations of beam & plasma (from above runs, or measured)
   - Each, faster than above, because beam is in system for < 1 μs
   - However, ensembles of runs are needed
4. Detailed simulations resolving short scales for, *e.g.*, two-stream instability

HPC requirements for 5-year timescale based on Warp runs

- Franklin core hours / year: 60,000,000
- Cores: 10,000 / simultaneous case (5 or more simultaneous cases)
- Wall-clock time: 1 – 10 hours / case
- Memory: 600 GB / simultaneous case
- Minimum memory per core: 1 GB
- Total data read & written / run: 100 GB / case
- Checkpoint files: < 100 GB / case
- Online storage for running job: 10 TB and 1000 files
- Data moved in and out of NERSC: 100 GB / month
- Off-line archival storage: 100 TB and 10,000 files

A proper estimate of the computer resources required for an integrated, end-to-end kinetic simulation of beam(s) and plasma would:

- assess the several regions of the system separately
- assume AMR, variable Δt, perhaps high-order differencing (for $\Delta x >> \lambda_D$)
- require a small computer program

Special considerations

- Warp uses Python at its highest level, for flexibility.
  - Fortran and C / C++ are underneath, for number-crunching.
  - It requires dynamic loading of shared objects on the compute nodes.
  - It also requires that Python on the nodes can rapidly read in start-up scripts and dynamic objects.
- Warp produces many of its diagnostics on-line
  (so it offloads mostly processed data and avoids massive transfers).
- At present, we “optimize” by running ensembles --- we can’t use enough particles for gradient-based optimizers. We hope that more NERSC resources will fix this.
- Interactivity is useful for debugging and for diagnostics development.
  - At NERSC, the batch-queue wait times and the limitations on interactive use have been impeding factors.
  - The Lawrencium and Fusion clusters at LBNL are convenient, even for multi-week runs, but are limited in capacity, capability, and availability.

Some detailed studies will require long runs, fine grids

- Two-stream instability driven by beam ion motion through background electrons heats the beam longitudinally *(in 1D infinite-space simulations)*.
- Detuning mechanisms include rapid beam bunching & transverse convergence; also, the initial beam temperature > 10 eV is ~ that needed for stabilization.
- Consider $n_p = 10^{11}$ cm^{-3}, $n_b = 10^{10}$ cm^{-3}, $v_b/c = 0.03$, $L_{drift} = 200$ cm, $t_{pulse} = 50$ ns
- Resolving the plasma wavelength $\lambda_p = v_b / \omega_{pe} = 0.05$ cm with 5 cells requires $\Delta x = 0.01$ cm; $N_z = 2 \times 10^4$ cells
- With explicit EM (for best scaling), Courant requires $\Delta t = 3.2 \times 10^{-4}$ ns
- Total number of time steps $N_t = L_{drift} / (v_b \Delta t) = 7 \times 10^5$
- Assume axisymmetry; AMR, resolve just beam region; for $r_b = 2$ cm, $N_r = 400$
- Then, 8 million grid points, 0.5 million steps
- Rough estimate 80 hours x 6,400 processors for 100 particles / cell
- 3-D would be 4 x 400 larger, *e.g,* 320 hours x 3 million processors (upper bound)

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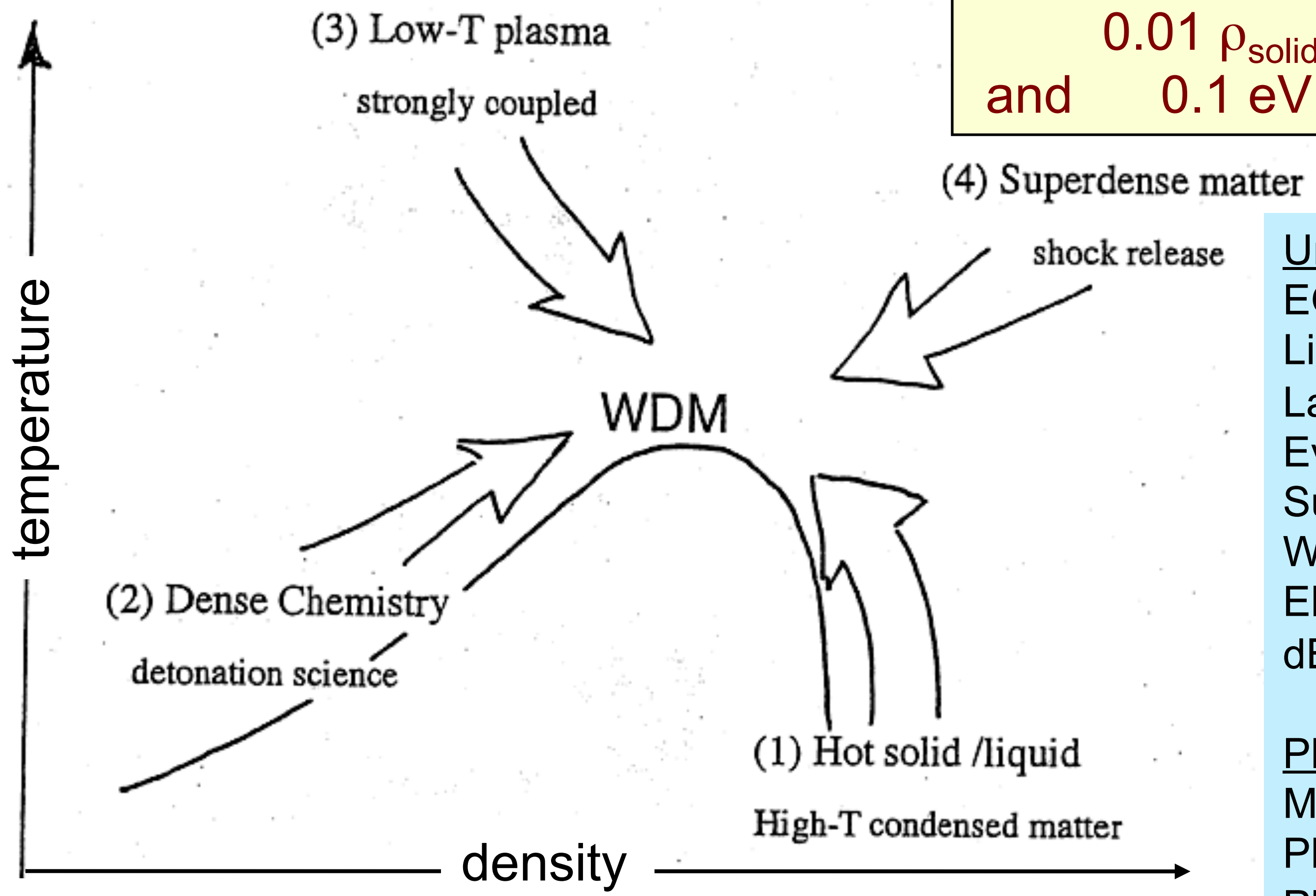
The WDM regime is at the meeting point of several distinct physical regimes -- a scientifically rich area of HEDP

Interesting phenomena at:

$0.01\ \rho_{solid} < \rho < 1.0\ \rho_{solid}$

and $0.1\ \text{eV} < T < 10\ \text{eV}$



Unknown properties:

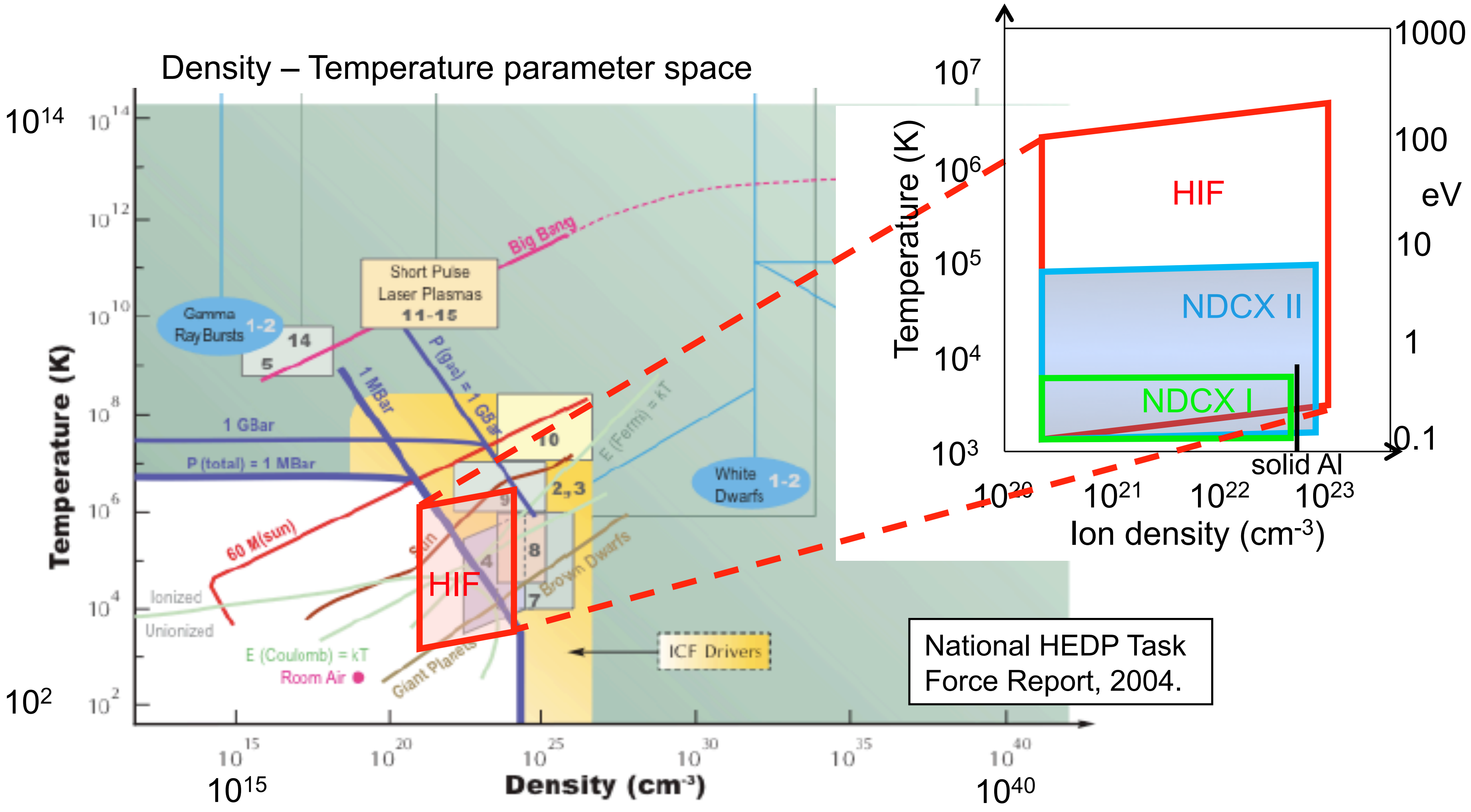
EOS ($p(\rho,T)$, $E(\rho,T)$)
Liquid-vapor boundary
Latent heat of evap.
Evaporation rate
Surface tension
Work function
Electrical conductivity
dE/dX for hot targets

Phenomena:

Metal-insulator transition
Phase transitions?
Plasma composition?

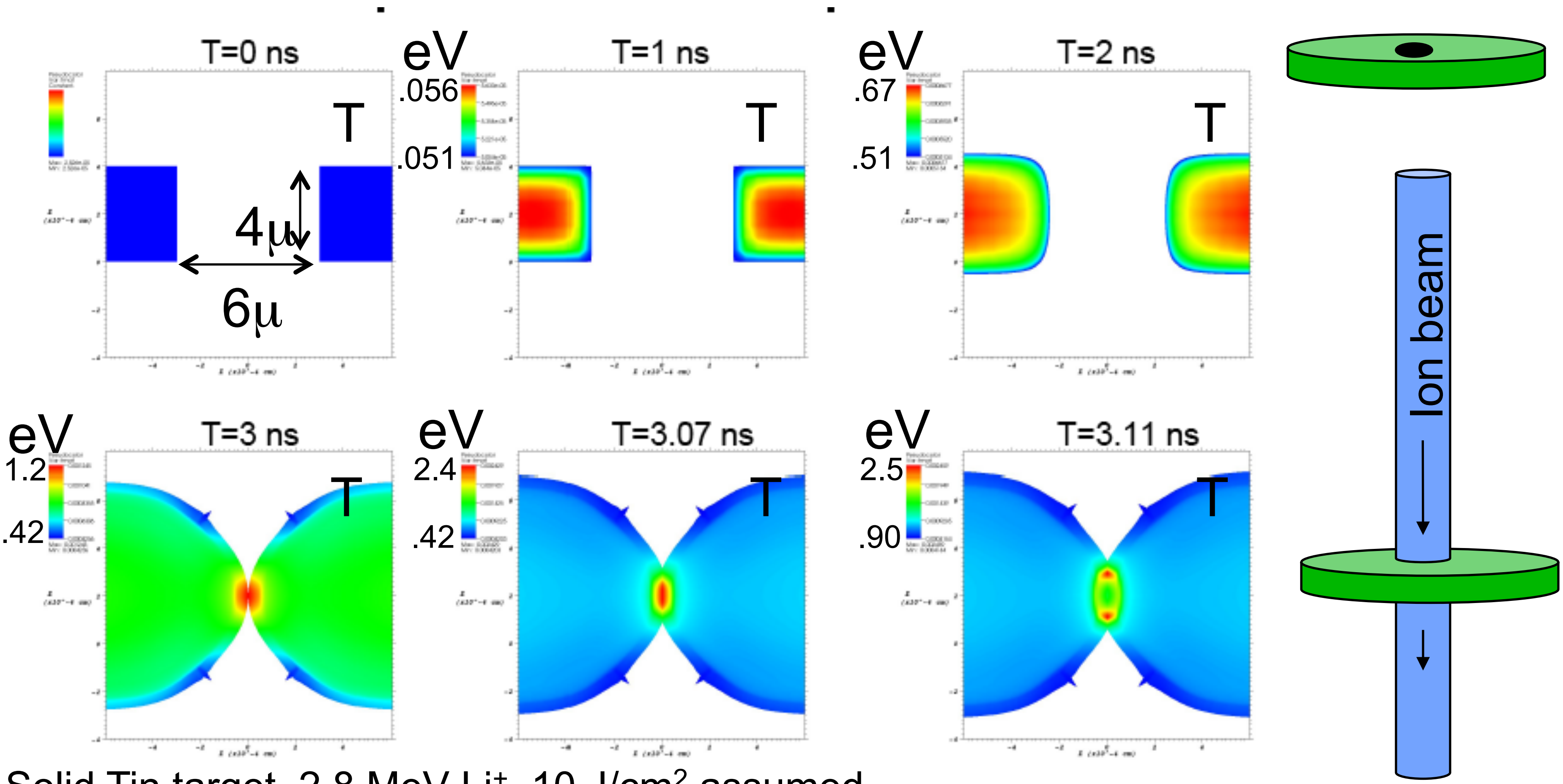
(From: R. More, Warm Dense Matter School, LBNL, January 2008)

NDCX-II experiments can explore much of the WDM regime



National HEDP Task Force Report, 2004.

WDM studies use detailed simulations (here, a foil with a hole)



Solid Tin target. 2.8 MeV Li$^+$, 10 J/cm^2 assumed.

Above used Hydra; we'll use the new ALE-AMR code for many WDM studies

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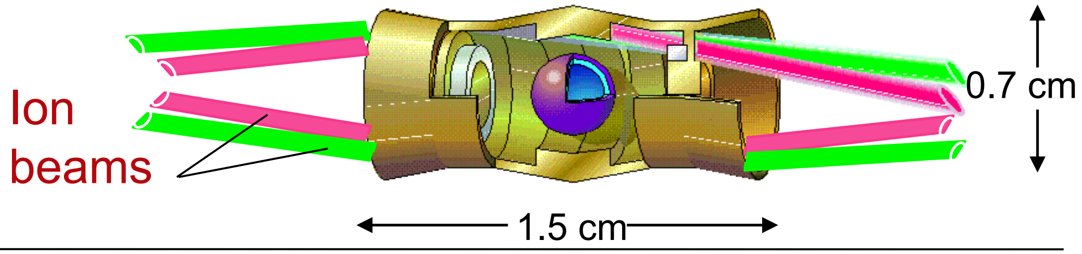
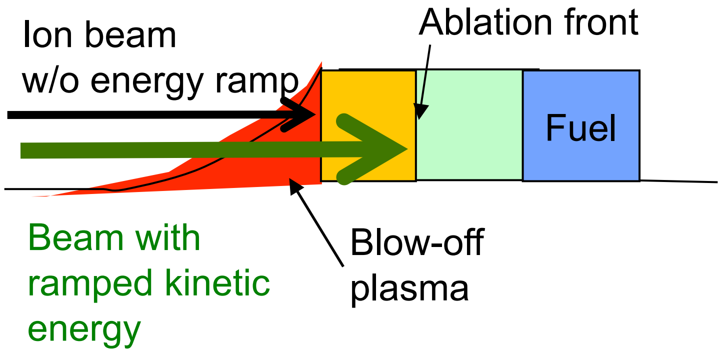
HYDRA is being used (on LLNL computers) to explore new heavy-ion IFE target concepts

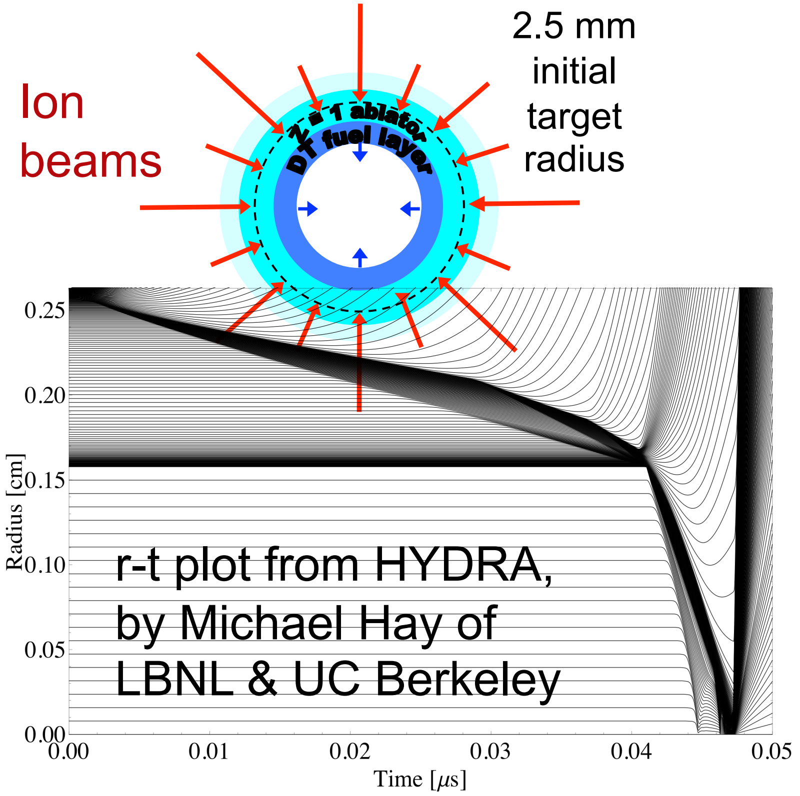
In indirect drive (similar to NIF), ion energy heats converter material, which then produces x-rays.



In direct drive, ions heat the ablator directly, so the coupling of the beams’ energy into motion of the fuel layer can be more efficient.



Ramping the beam energy keeps the deposition close to the ablation front.



r-t plot from HYDRA, by Michael Hay of LBNL & UC Berkeley

Other new concepts include ion fast ignition, and a single-sided variant thereof.

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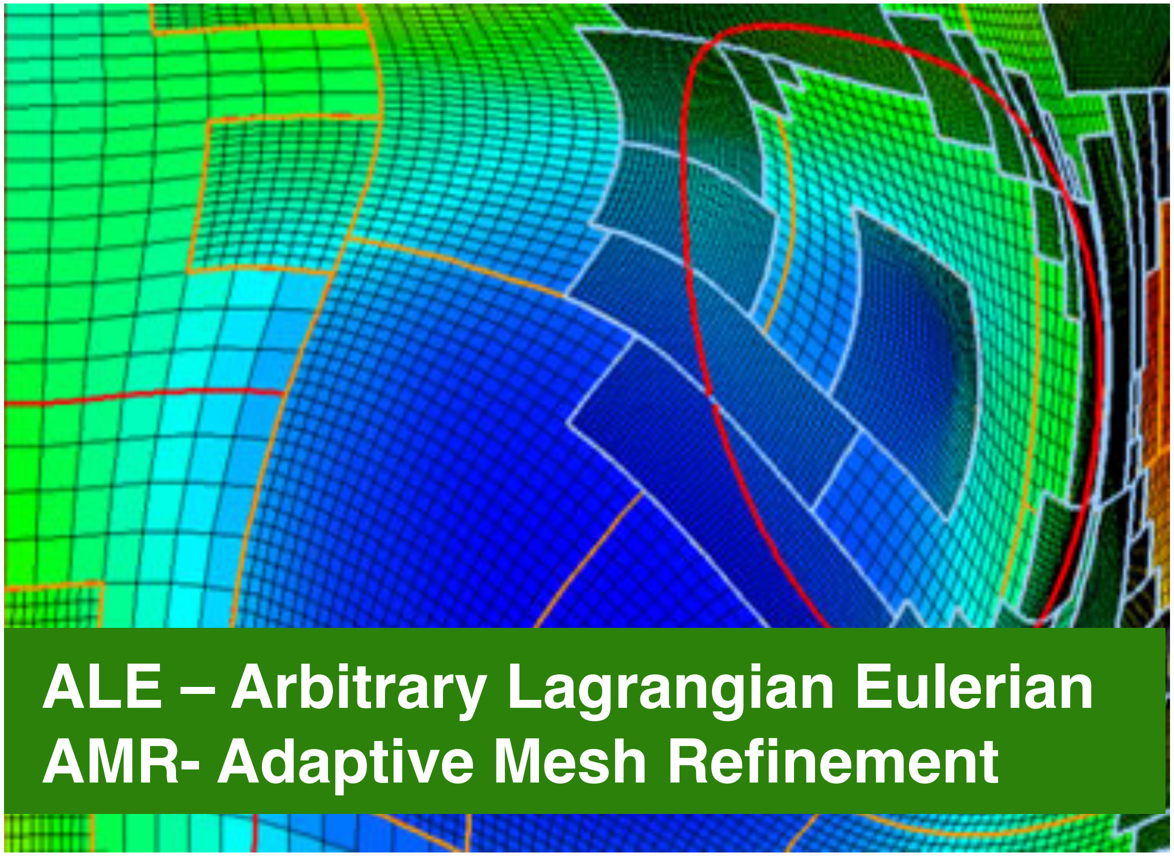
ALE-AMR is a new 3D multi-physics code for open science

- 3D runs can take a week or so if run on a thousand processors (often don't get more than 1000 processors)



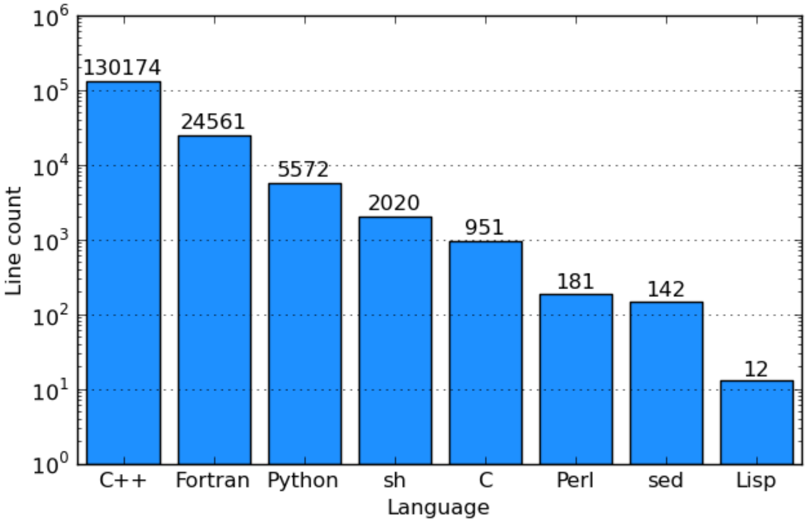
ALE – Arbitrary Lagrangian Eulerian
AMR- Adaptive Mesh Refinement

- Fluids + radiation diffusion
- Fully anisotropic material strength and failure
- 2 or 3 Dimensions
- Moving AMR grid—different from usual Eulerian AMR
- Built on AMR library with scalability to 10's of thousands of processors
- Ion-Beam Sources for NDCX-II and IFE

ALE-AMR is Portable and Open Source

- C++, Fortran, Python, and some other languages

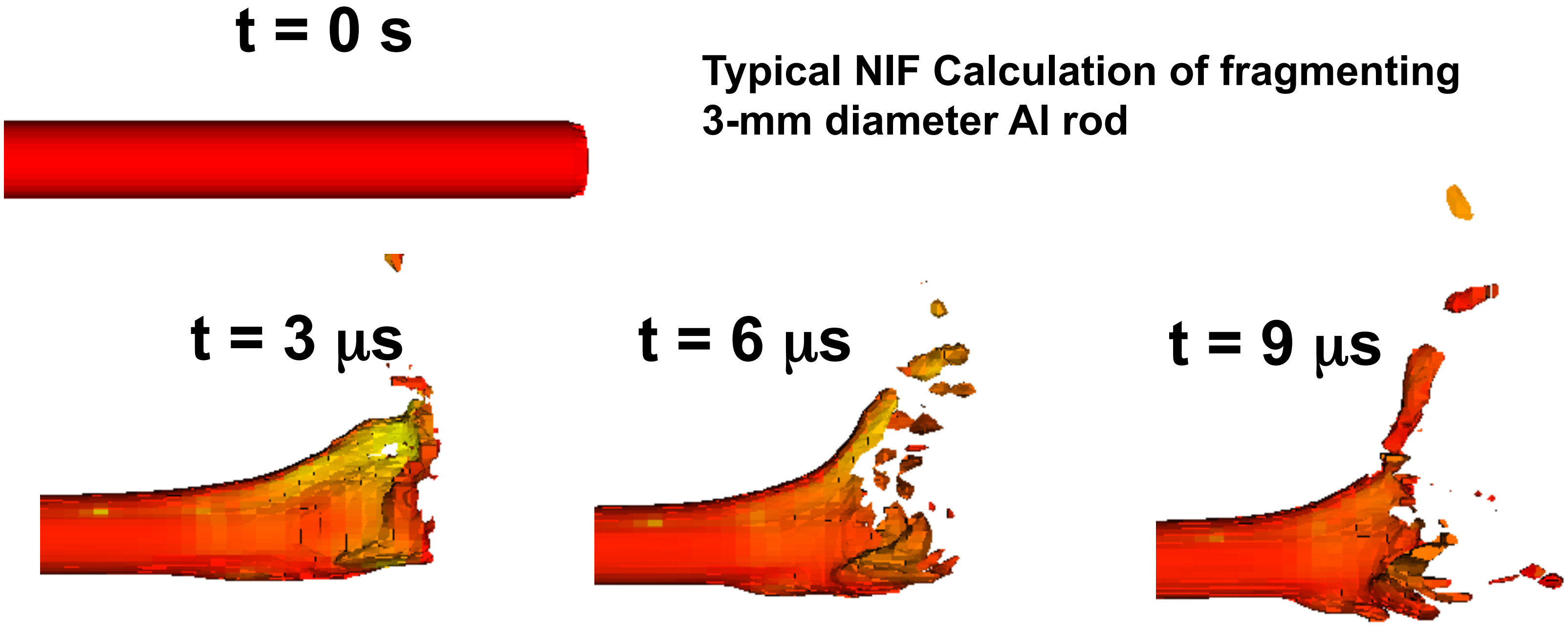
- Built with freely available libraries
  - Boost, Tvmet, GSL, CppUnit
  - SAMRAI, VisIt
  - MPICH
  - Emacs, Subversion
  - Python, SWIG, Wild Magic



- Runs on Linux
  - CHAOS at Livermore Computing
  - Cray Linux Environment at NERSC
  - SUSE at UCLA
  - Ubuntu on PC

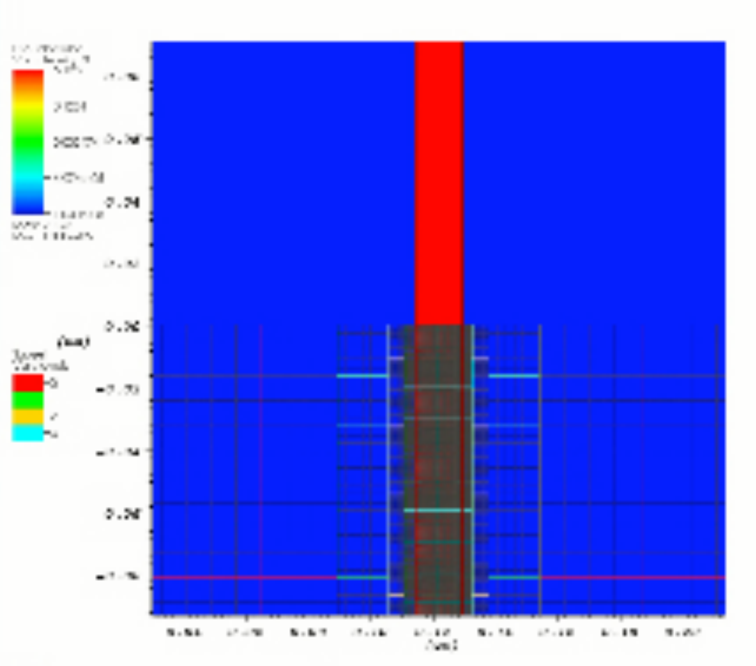
ALE-AMR models the break-up of targets and other structures such as used by NDCX-II and National Ignition Facility (NIF)

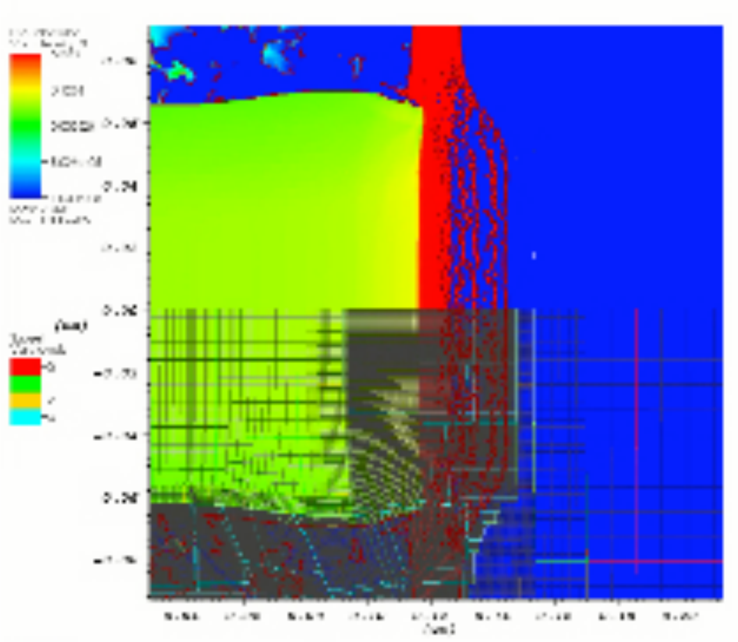
- Can model materials from hot radiating plasmas through phase changes using the Equation of State (EOS) and cold fragmenting solids
- Energy input to targets is through ion beam deposition (NDXC-II), laser deposition (NIF) or plasma surface interaction (magnetic fusion)



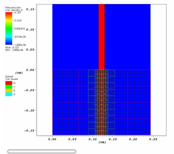
Typical NIF Calculation of fragmenting 3-mm diameter Al rod

Video of NDCX target simulation using ALE-AMR



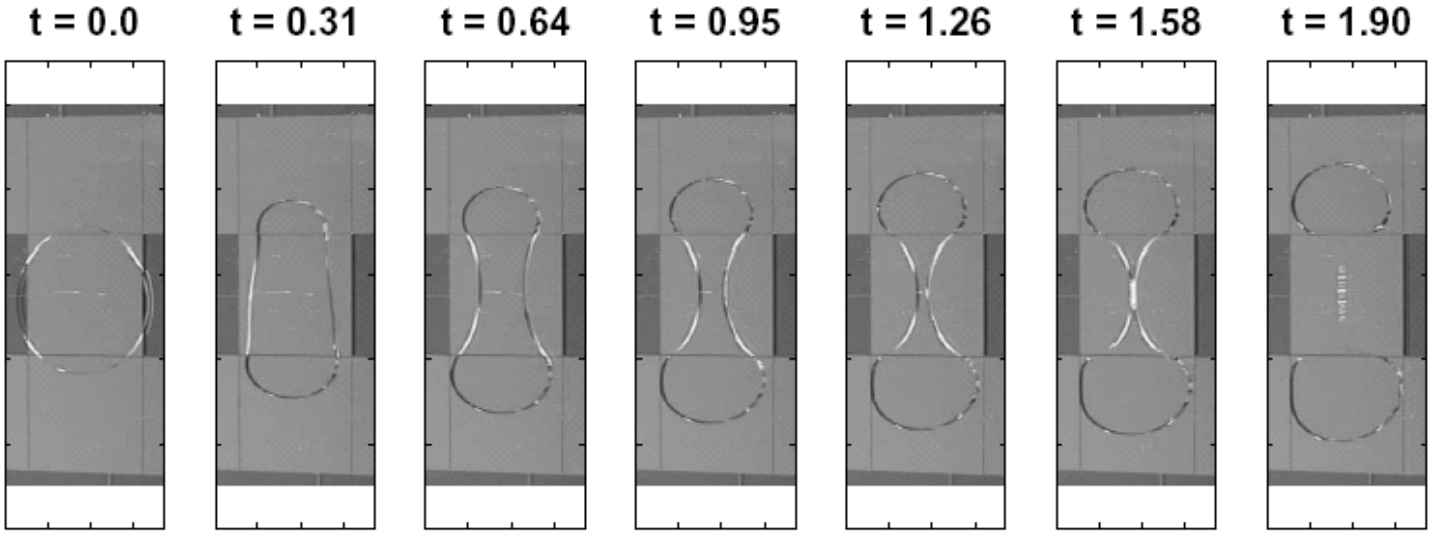


play video

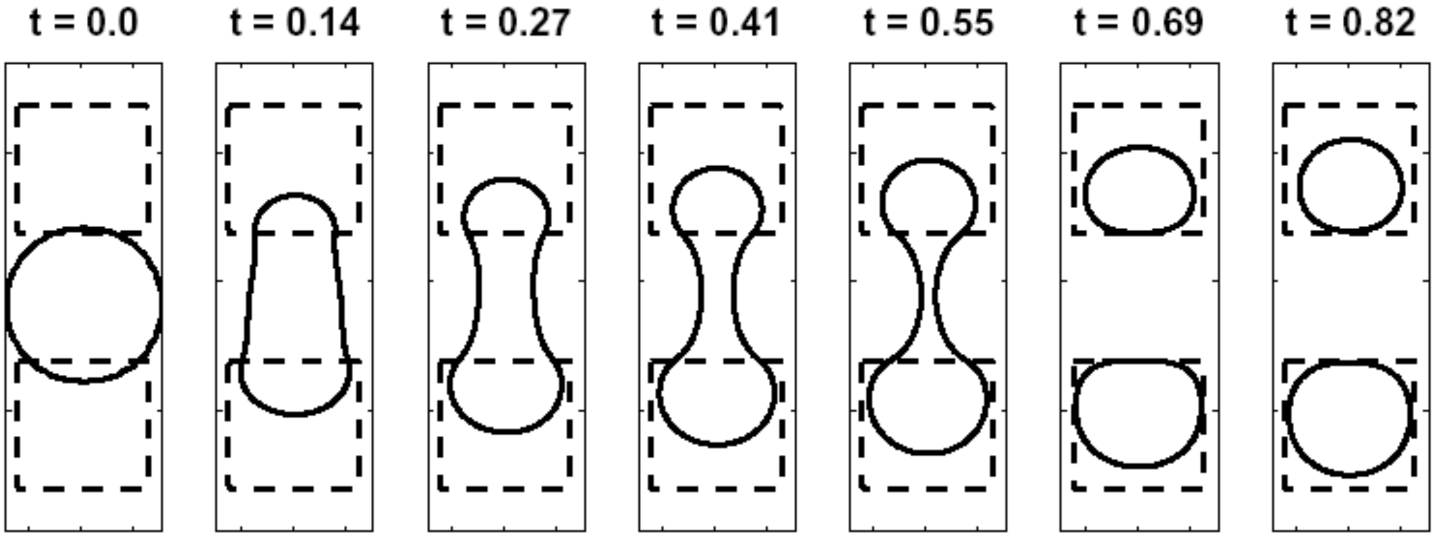


In collaboration with UCLA, we are adding surface tension effects to ALE-AMR for NDCX-II

V = 50.42 V



ω = 3.968



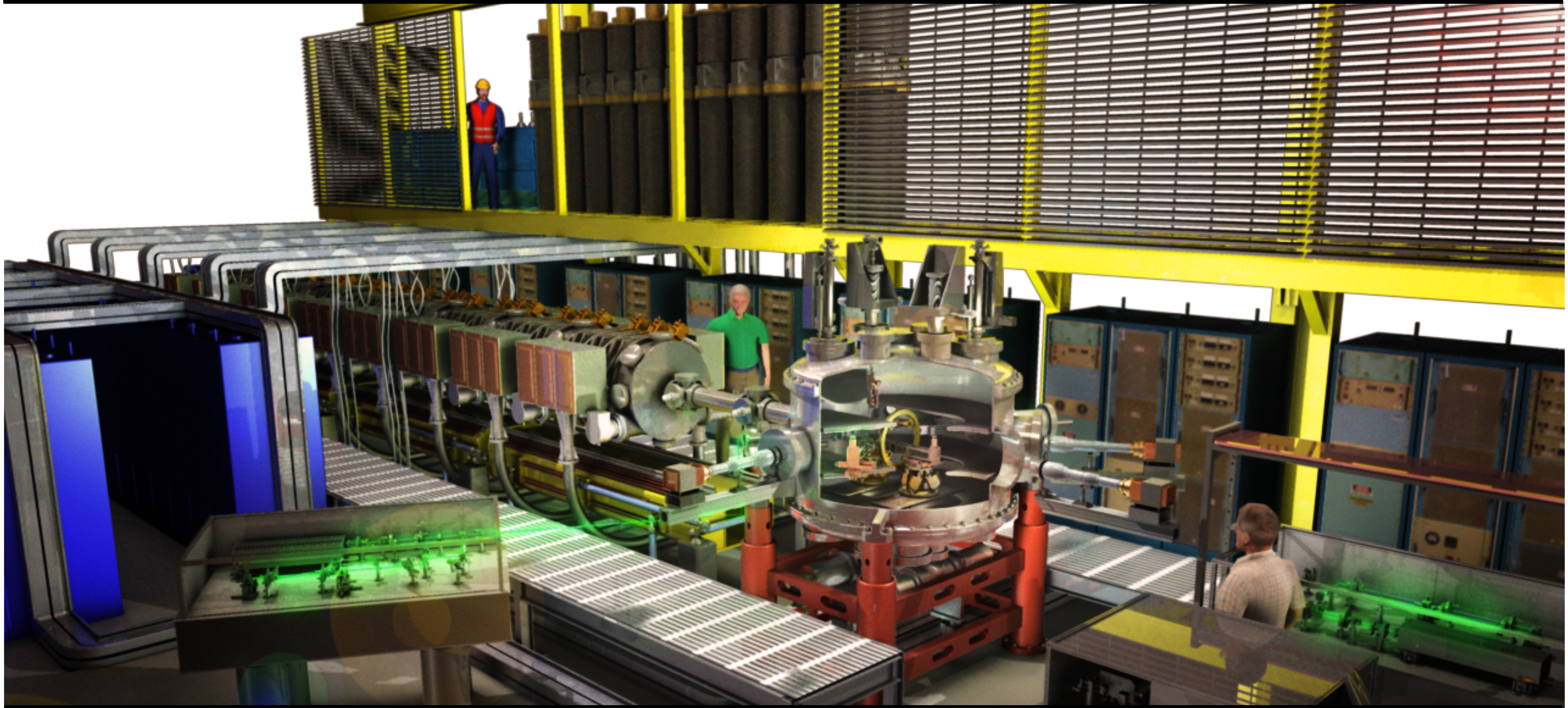
We expect ALE-AMR to become a key tool for our program

- We are planning to use ALE-AMR, on NERSC, for both WDM and selected IFE studies.
- Because of its novel use of AMR and ALE, it should be ideal for our applications (but it is not a complete IFE target design code)
- Nonetheless, it will require significant computing resources to resolve droplets and multi-phase regions while also capturing a macroscopic scale, e.g., spot size
- Large run in near future: 12 hrs, 4k nodes (16k cores): 200,000 hrs
- Typical run in 5 years: 24 hours, 32k nodes (128k cores): 3,200,000 hrs

Outline

- Introduction to the HIFS-VNL research program
- Intense ion beam physics
  - NDCX-II physics design
  - Beam-plasma interactions
  - Warp code plans and requirements
- Physics of ion-beam-heated targets
  - Warm Dense Matter
  - Inertial Fusion Energy
  - ALE-AMR code plans and requirements
- Final comments

We look forward to a much-enhanced simulation capability that will help the U.S. HIFS program achieve its goals



- Support of the NDCX-II experimental program
- Simulations of targets for HEDP and IFE
- Development of upgrades to NDCX-II