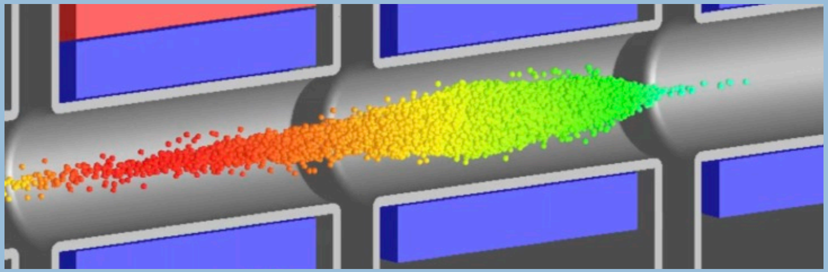
LLNL-PRES-627422

Heavy Ion Beams and Interactions with Plasmas and Targets (HEDLP and IFE)



Alex Friedman

LLNL Fusion Energy Sciences Program

and

Heavy Ion Fusion Science
Virtual National Laboratory

Workshop on Large Scale Production Computing and Storage Requirements for Fusion Energy Sciences
Rockville, MD, March 19-20, 2013

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… and in general:
the worldwide ion-driven HEDP community, with other centers in Germany, Russia, Japan, and China.

Outline

- Introduction to heavy ion fusion science research
- 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

The front page of DOE/FES's website lists four strategic goals; the 2nd of them concerns HED Plasma Science

"Pursue scientific opportunities and grand challenges in high energy density plasma science

to explore the feasibility of the inertial confinement approach as a fusion energy source,

to better understand our universe,

and to enhance national security and economic competitiveness"

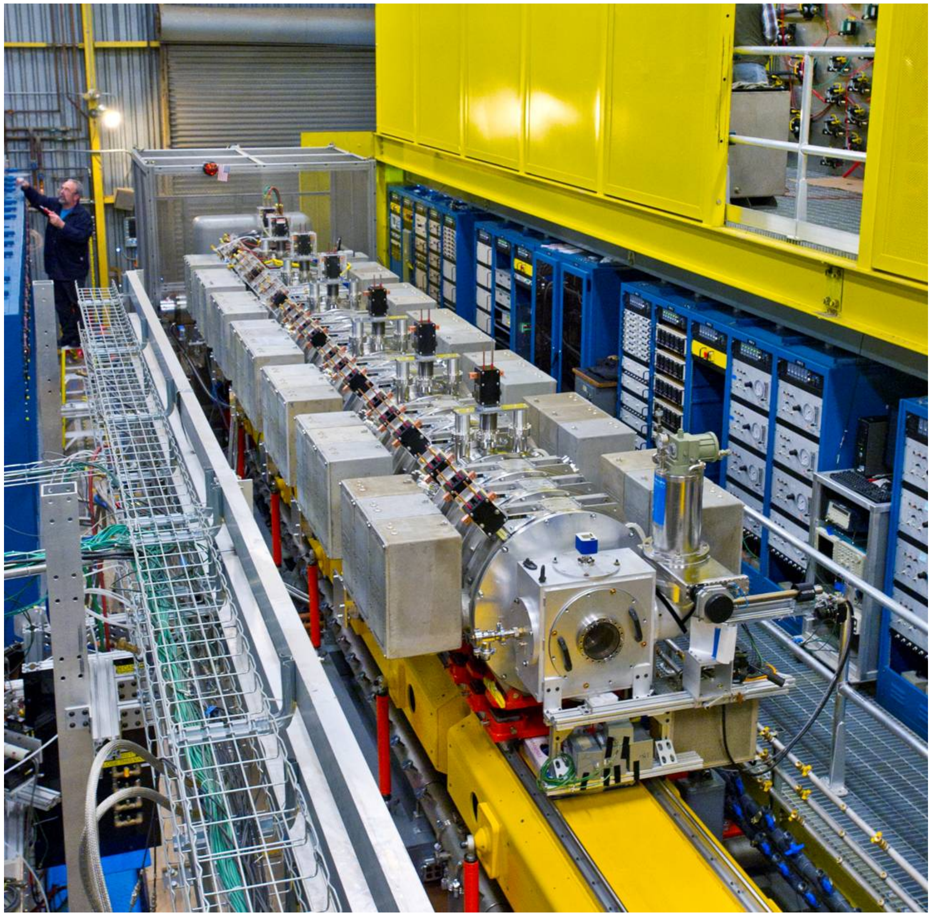
(from http://science.energy.gov/fes/ as of March 12, 2013; regrouped for readability by this author)

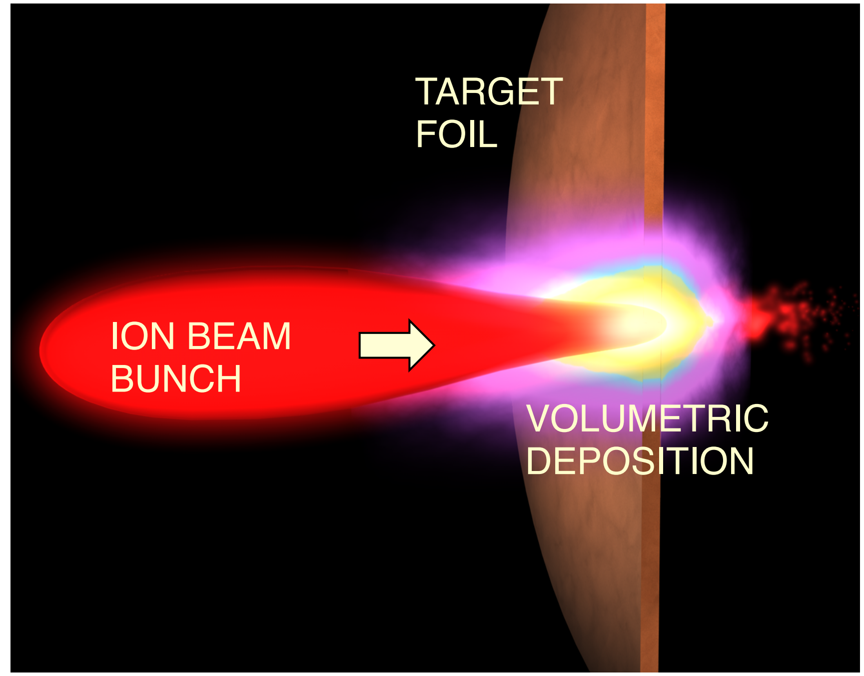
The HIFS-VNL employs intense ion beams for High Energy Density Physics and Inertial Fusion Energy (IFE) target physics

- Heavy Ion Fusion has long been considered an attractive approach to Inertial Fusion Energy.
- In the early 200's, the VNL's mission was shifted to emphasize HEDP, especially Warm Dense Matter (WDM) physics.
- Heavy-ion IFE target physics has re-emerged as a goal.
- Space-charge-dominated beam physics and enabling technology are essential elements of the program.
- We're commissioning a new facility, NDCX-II, to support this program.

The recent NRC report on Inertial Fusion Energy affirms that research on the HIF approach to IFE, as on other approaches, should go forward.

Neutralized Drift Compression Experiment-II (NDCX-II)





A new user facility for studies of:

- warm dense matter physics
- heavy-ion-driven target physics
- space-charge-dominated beams

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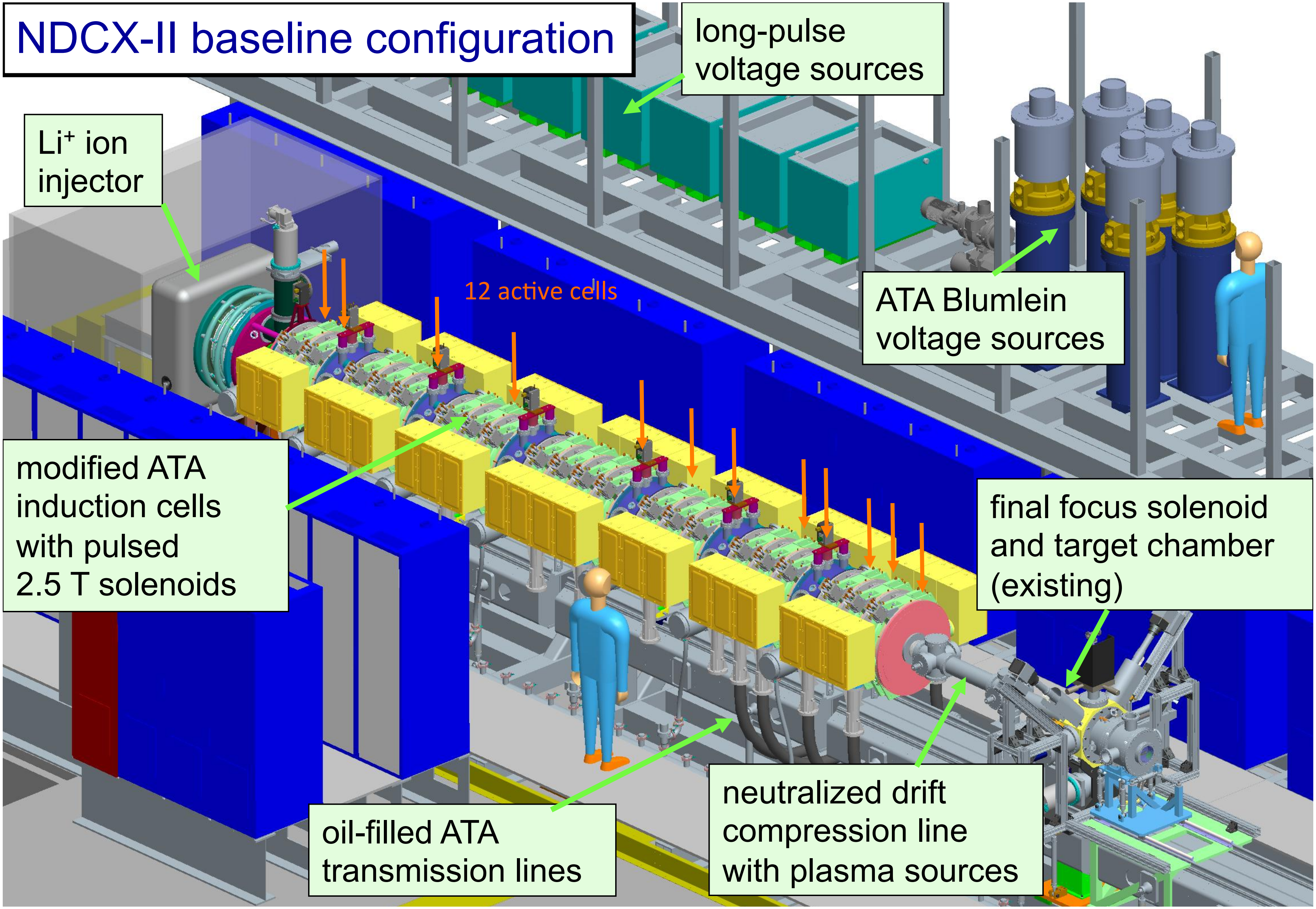
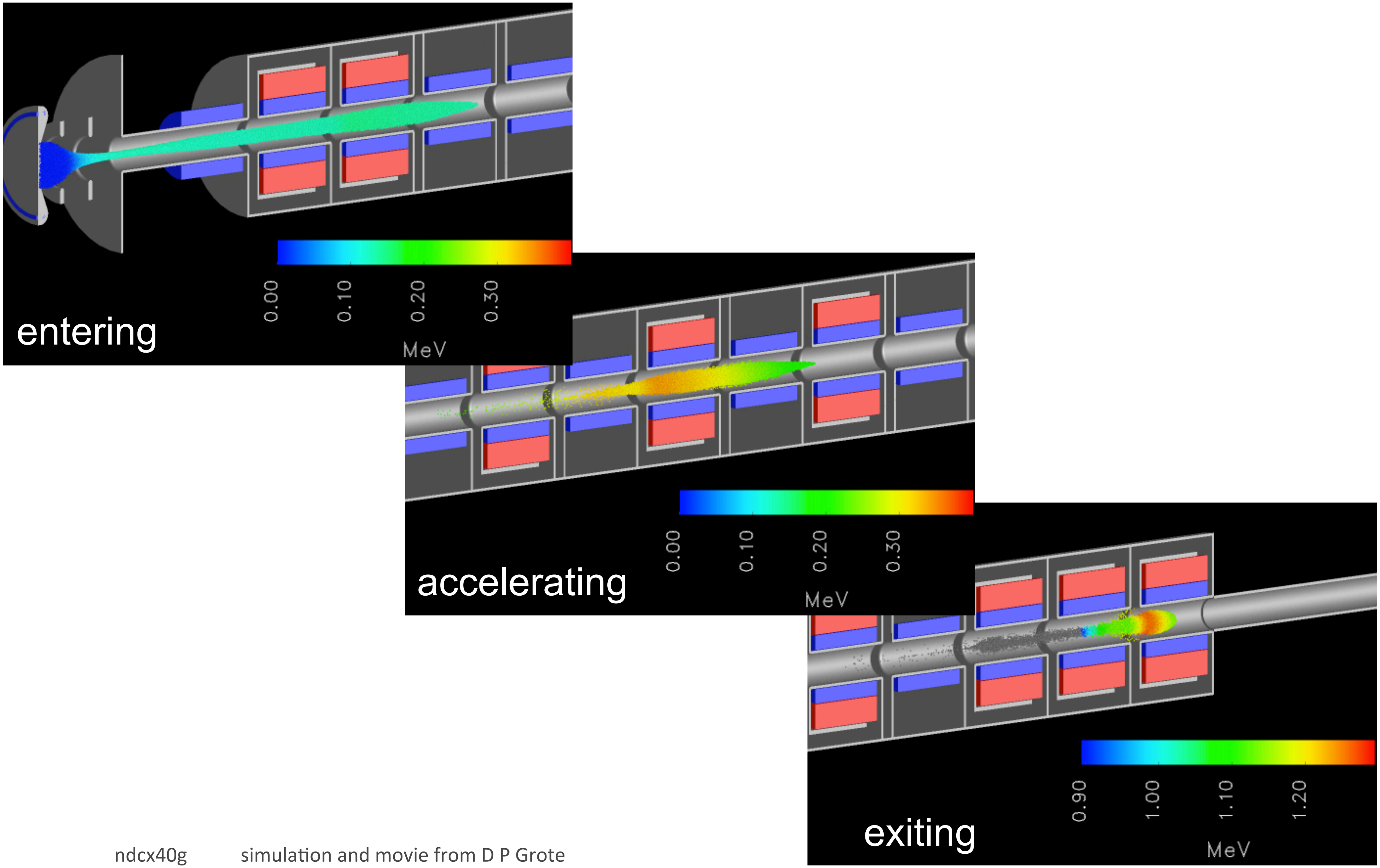
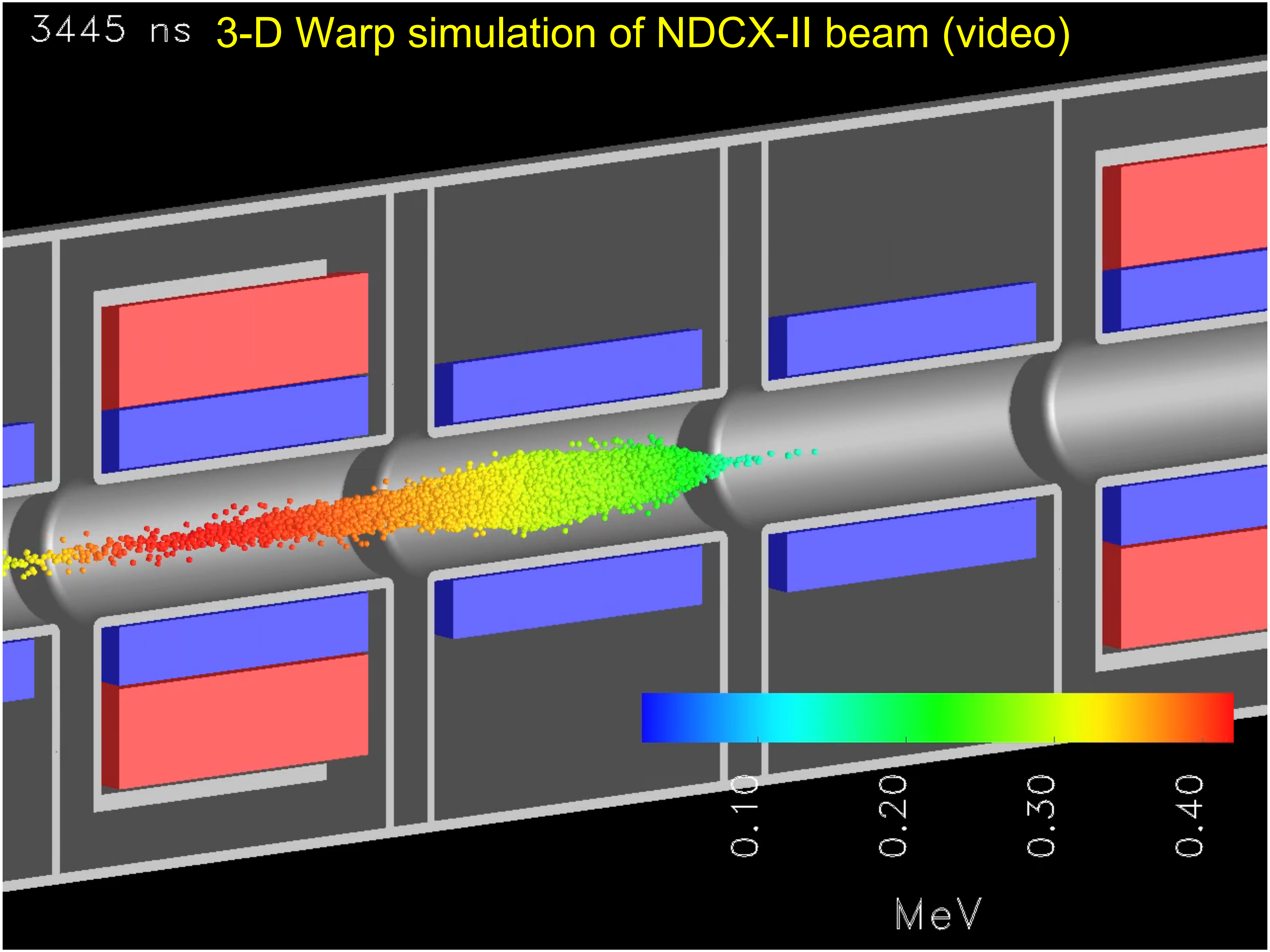
NDCX-II baseline configuration



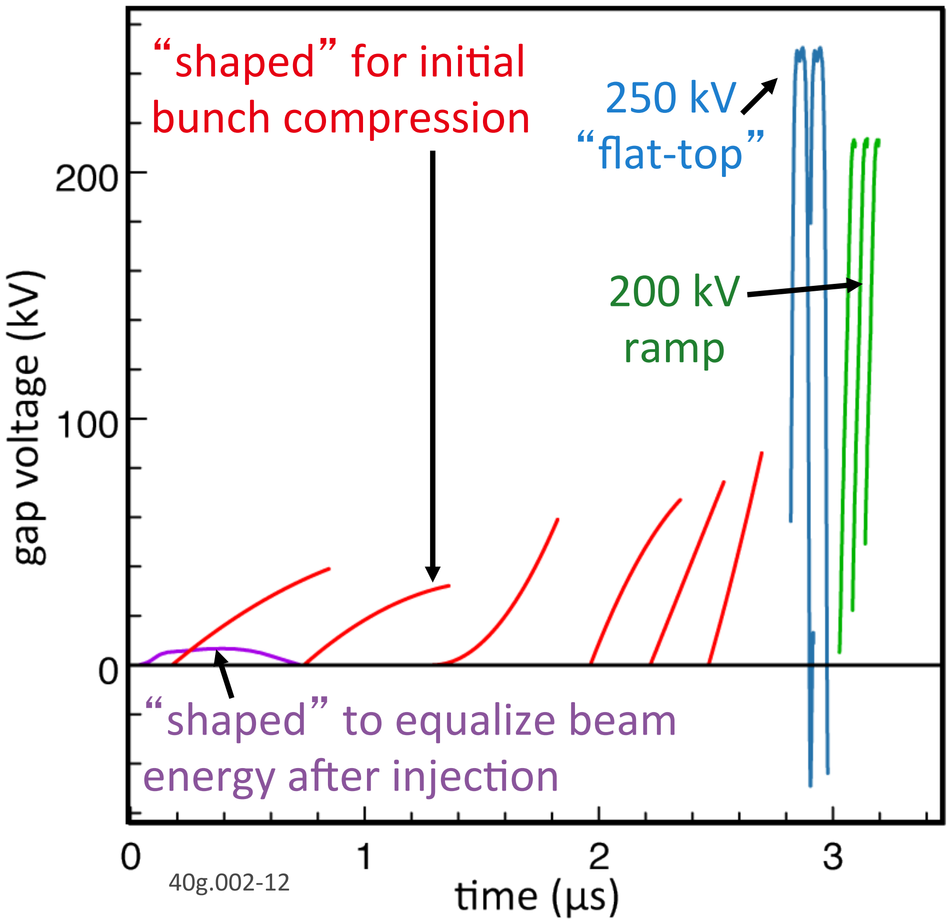
3-D Warp simulation of beam in the NDCX-II linac



ndcx40g   simulation and movie from D P Grote


3445 ns
3-D Warp simulation of NDCX-II beam (video)
0.10
0.20
0.30
0.40
MeV

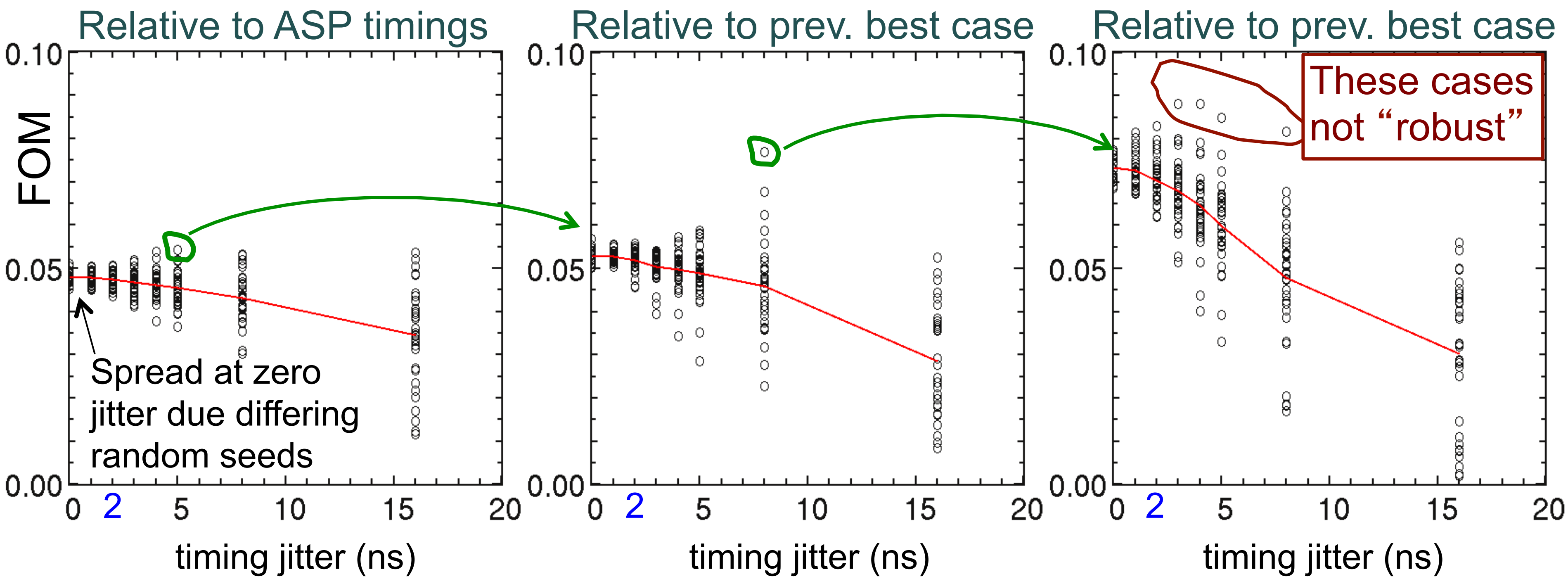
The shapes and timings of the accelerating waveforms are critical



- Waveforms are originally derived using 1-D ASP simulations
- They are then imported into Warp
- Iteration with engineering team yields achievable ones, used here
- Optimized timings for all 12 acceleration cells are sought by "large-scale trial and error"

“Ensemble” Warp PIC runs led to an optimized 12-cell design

- Multiple (typically 256) cases were run in each NERSC batch job
- Random shifts were imposed on the start times of the acceleration pulses
  - This established a 2-ns tolerance on the timing jitter
  - It also enabled identification of an improved “base case”



- Figure-of-merit (FOM) is related to pressure generated in a nominal target
- Spread in results increases because optimized cases are more sensitive

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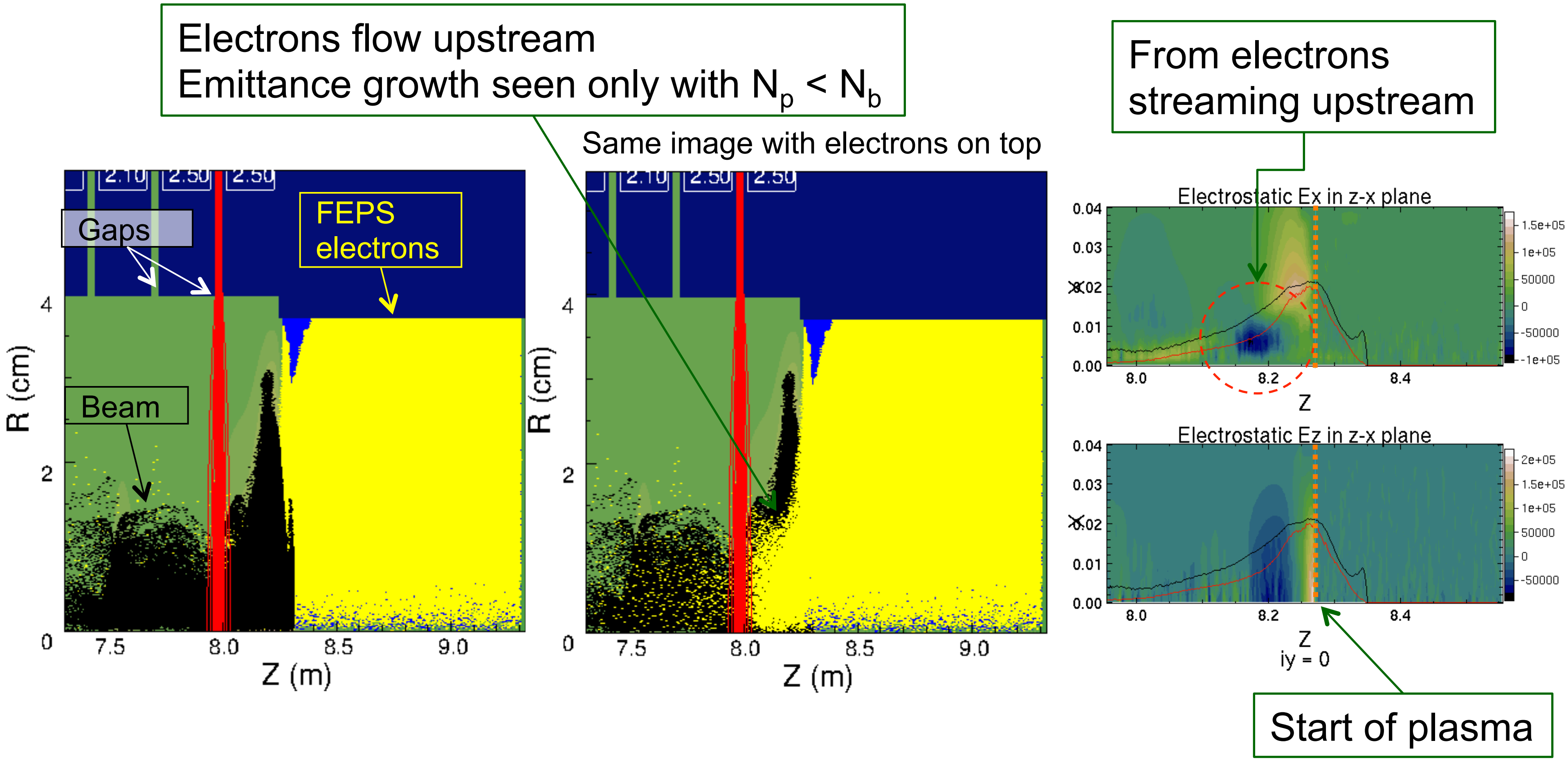
NDCX-II neutralized drift – Beam-plasma interaction

- Expect rich behavior, but challenging to simulate at NDCX-II parameters
- Beam is slow, with $\beta \sim 0.02$
  - Wavelengths are short:
    for plasma oscillation and two-stream $\lambda \sim v_b/\omega_{pe} \sim$ few mm or smaller
  - Propagation time is long
- Want $N_p >> N_b$ to maintain good neutralization
  - N_p set by peak compression and focus
  - For typical values, $r_b \sim c/\omega_p$, the skin depth
  - Makes step size, $dt < 1/\omega_p$, small
  - Requires many simulation particles to reduce noise
- Electrostatic simulations require ~3000 CPU hours
- Electromagnetic simulations longer – smaller step size needed because of the Courant condition, $dt \sim dz/c_{light}$

Beam pulls electrons upstream at plasma entrance

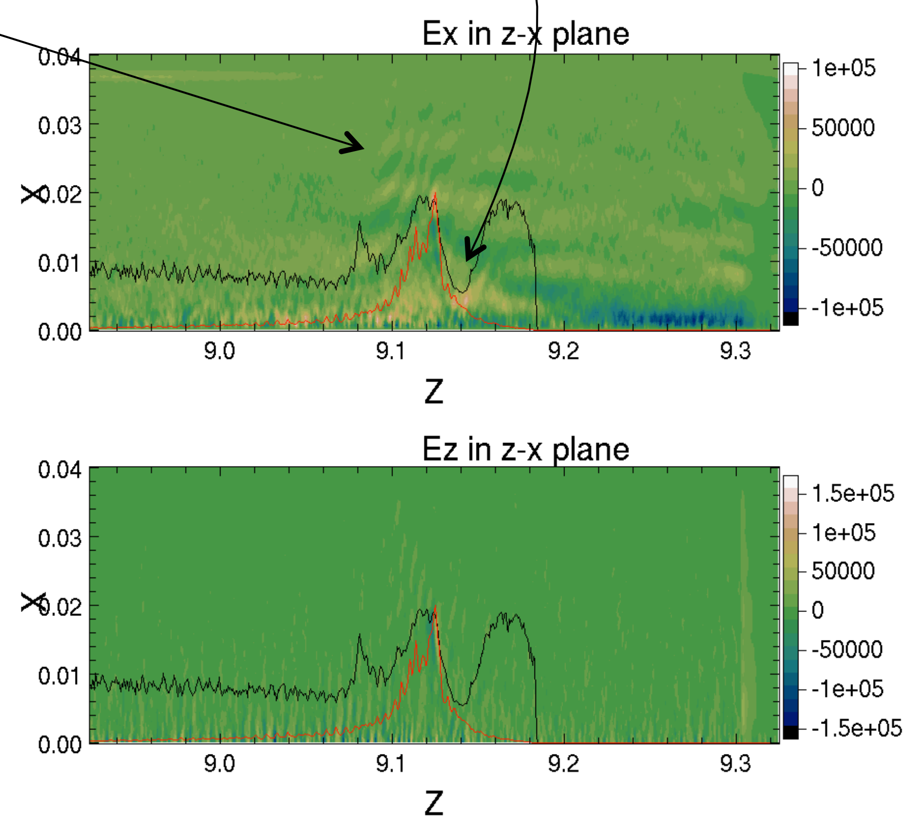
Example with Ferro-Electric Plasma source (FEPS) $N_p = 10^{15}\ /m^3 \leq N_b$



Electrons become magnetized at the entrance to the final-focus solenoid (warp run in electromagnetic mode)

- Bz ramps up from ~100 Gauss to ~2000 Gauss from z=9.0 to 9.2 m
- Nonlinear radial fields form
- And wave structures

t = 4.05 μs

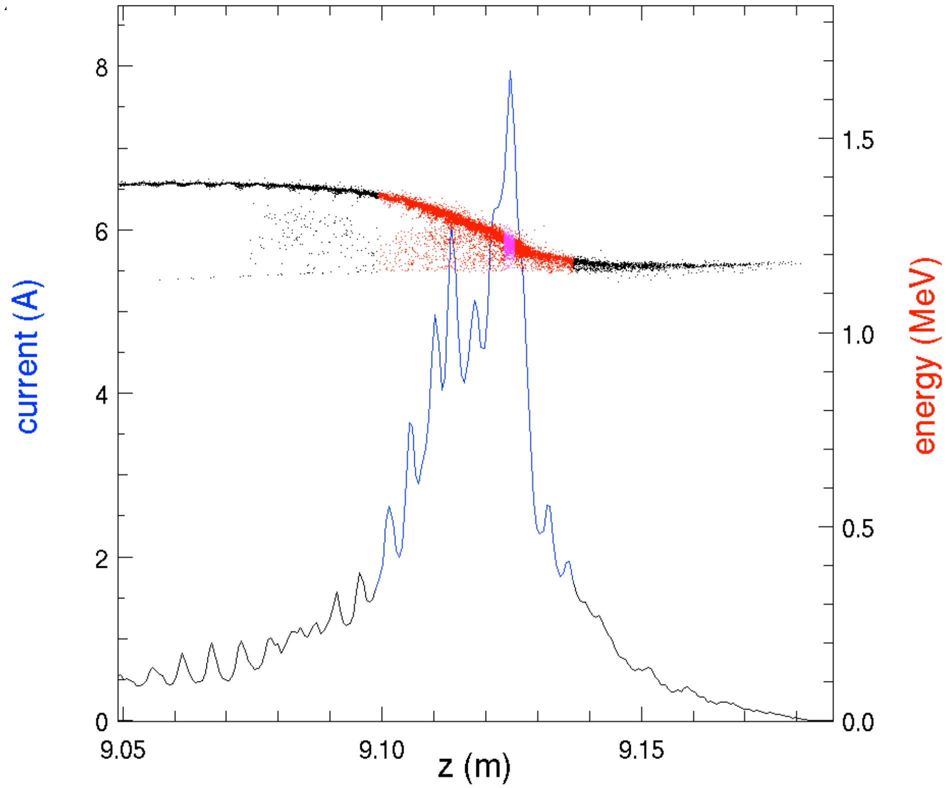


Electron-ion two stream instability in FEPS plasma

- Longitudinal structure forms on the beam
- Wavelengths comparable to most unstable mode
- Does not disrupt beam compression (thanks to detuning by velocity "tilt")

$$\lambda_{\max} \approx \frac{2\pi v_b}{\omega_{pe}}$$

FEPS $N_p = 10^{16}$ /m^3



N_p/m^3	λ_{max}	Simulation λ
1×10^{16}	6.4 mm	4.4 – 5.7 mm
4×10^{16}	3.2 mm	2.8 – 3.3 mm
8×10^{16}	2.3 mm	2.2 – 2.7 mm
1×10^{17}	2.0 mm	2.5 – 2.7 mm

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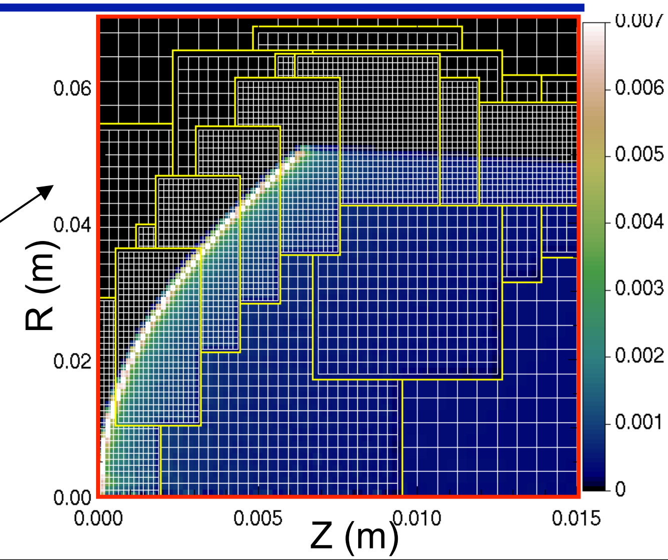
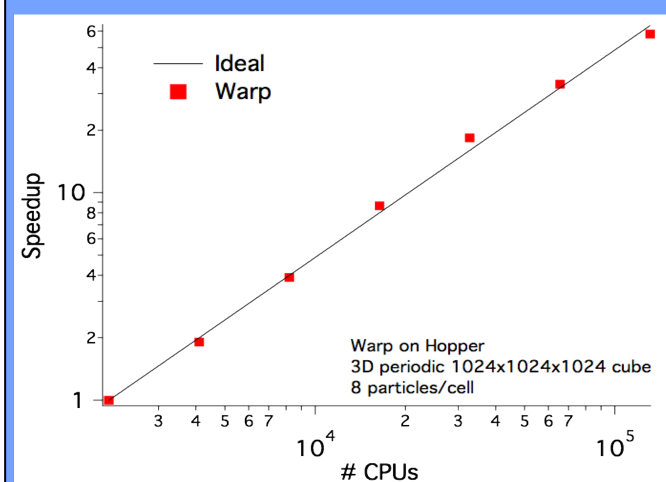
Warp: a parallel framework combining features of plasma (Particle-In-Cell) and accelerator codes

- **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)

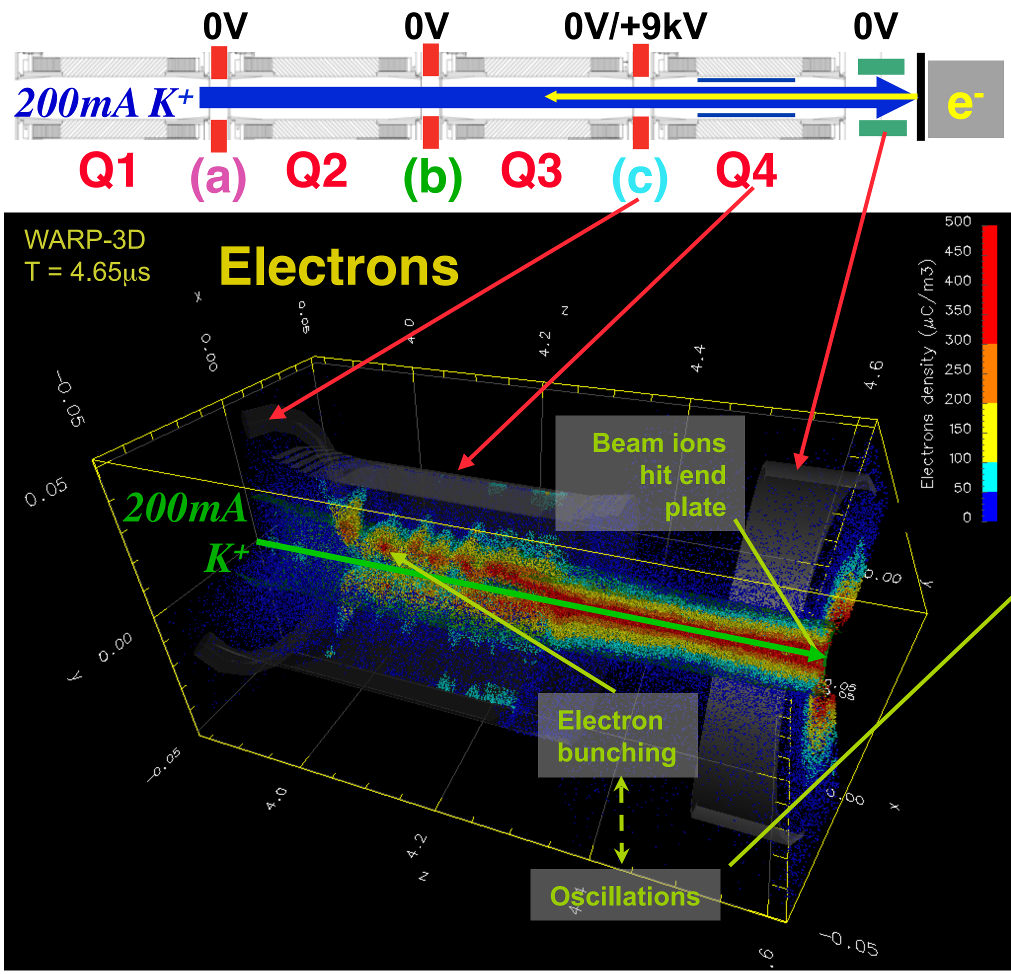


Warp 3D EM/PIC on Hopper

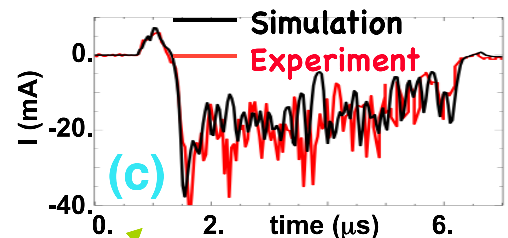


Warp has been compared extensively vs. experiment

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.

Most Warp runs modeled the non-neutral beam in the NDCX-II accelerator; we now are seeking to routinely include plasma

- Iterative design and assessment (on NERSC and LBNL clusters) --- *ensembles* of runs with random errors:
  - Typically run 256 cases in a single batch job
  - 24 cores/case x 256 cases, < 1 GB/core, 2 TB total, ~5 hours
  - 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* plasma problems:
  - 100's x 100's x 1000's of cells, millions of particles (13 or more variables per particle)
  - Most beam-in-plasma work for NDCX-II has been in (r,z) geometry
  - Uses 512, 1024, and sometimes 4096 processors

Our need for NERSC time is growing; plasma problems are more demanding, and we hope to do iterative optimization including plasma

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
   – 3-D (offsets, possible non-axisymmetric instabilities)
4. Detailed simulations resolving short scales for, *e.g.*, two-stream instability

HPC requirements for 5-year timescale based on Warp runs

	Used in 2012	Need in 2017
Computational Hours (Hopper core-hour equivalent)	0.6 M	40 M
Scratch storage (bandwidth not critical)	0.3 TB	3 TB
Shared global storage (/project)	0.1 TB	1TB
Archival storage (HPSS)	1 TB	40 TB
Number of conventional cores used for production runs	3000	100,000
Memory per node	1 GB	1 GB
Aggregate memory	3 TB	100 TB

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 $\Delta x \gg \lambda_D$)
- require a small computer program

Special considerations

- Warp uses Python at its highest level, for flexibility.
  - Fortran and 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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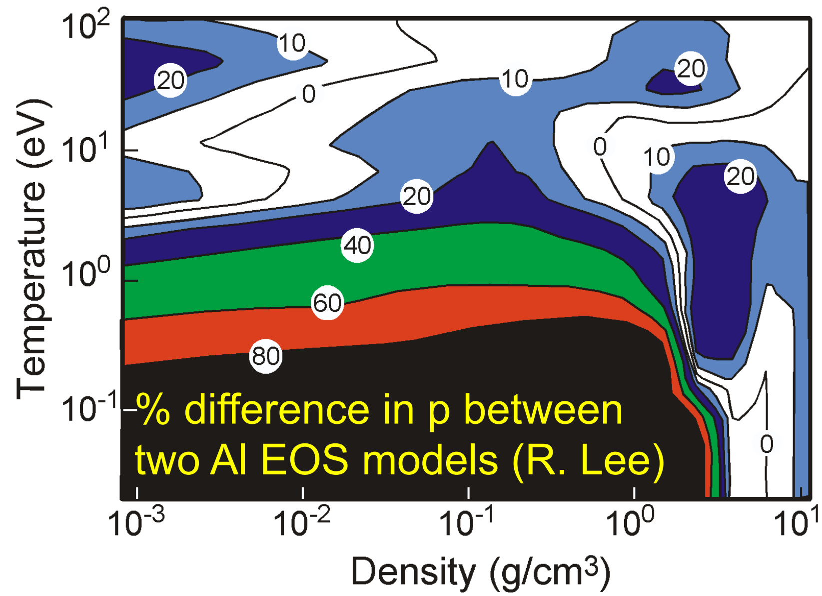
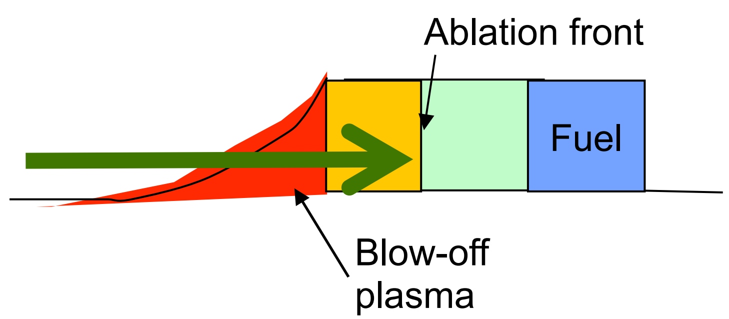
Studies of WDM science & IFE target science are complementary

- 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.

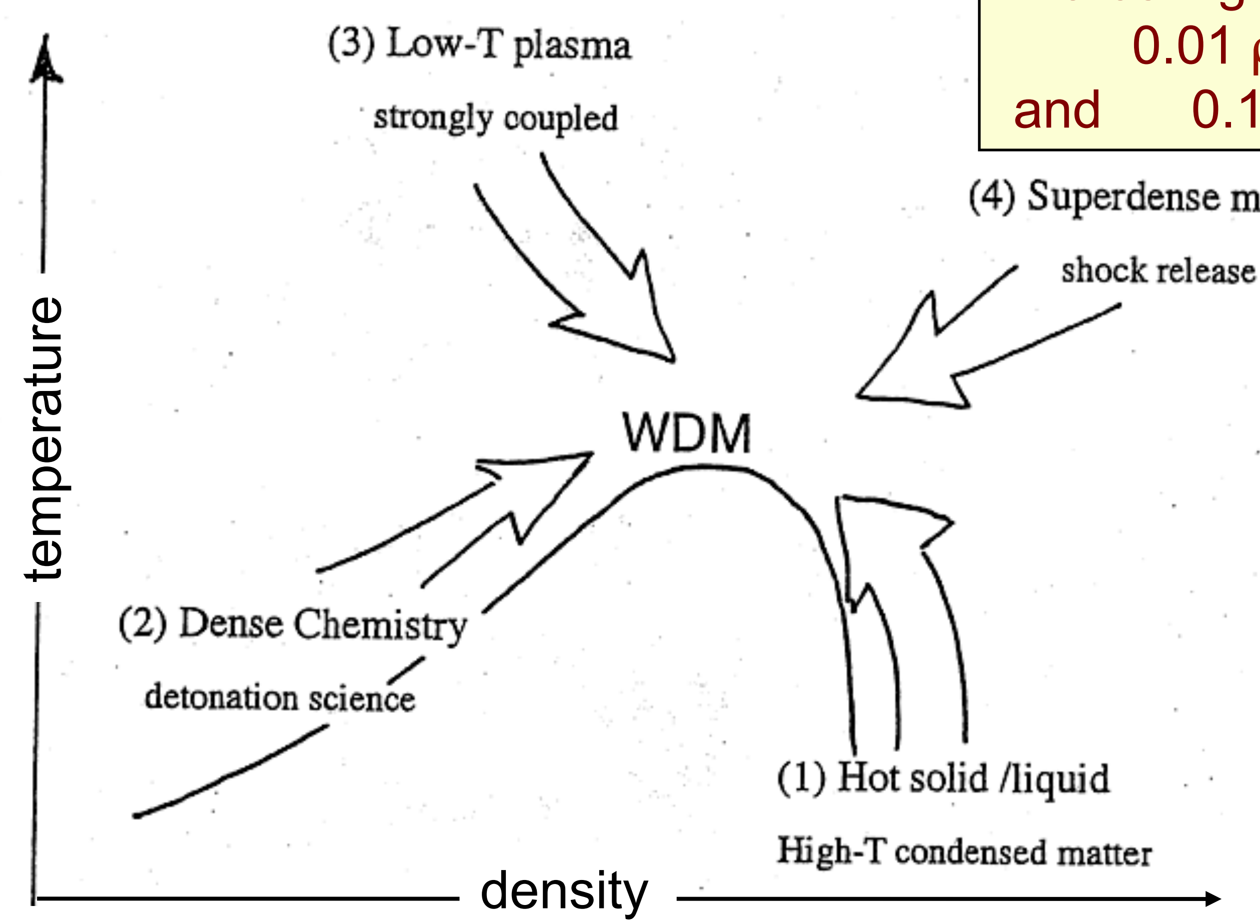


- Heavy-ion-driven IFE is attractive due to driver efficiency, compatibility with liquid walls, robust final optics, and more.
  - Advanced target concepts may lead to simpler / cheaper drivers
  - NDCX-II experiments will explore ion energy coupling that drives target ablation



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

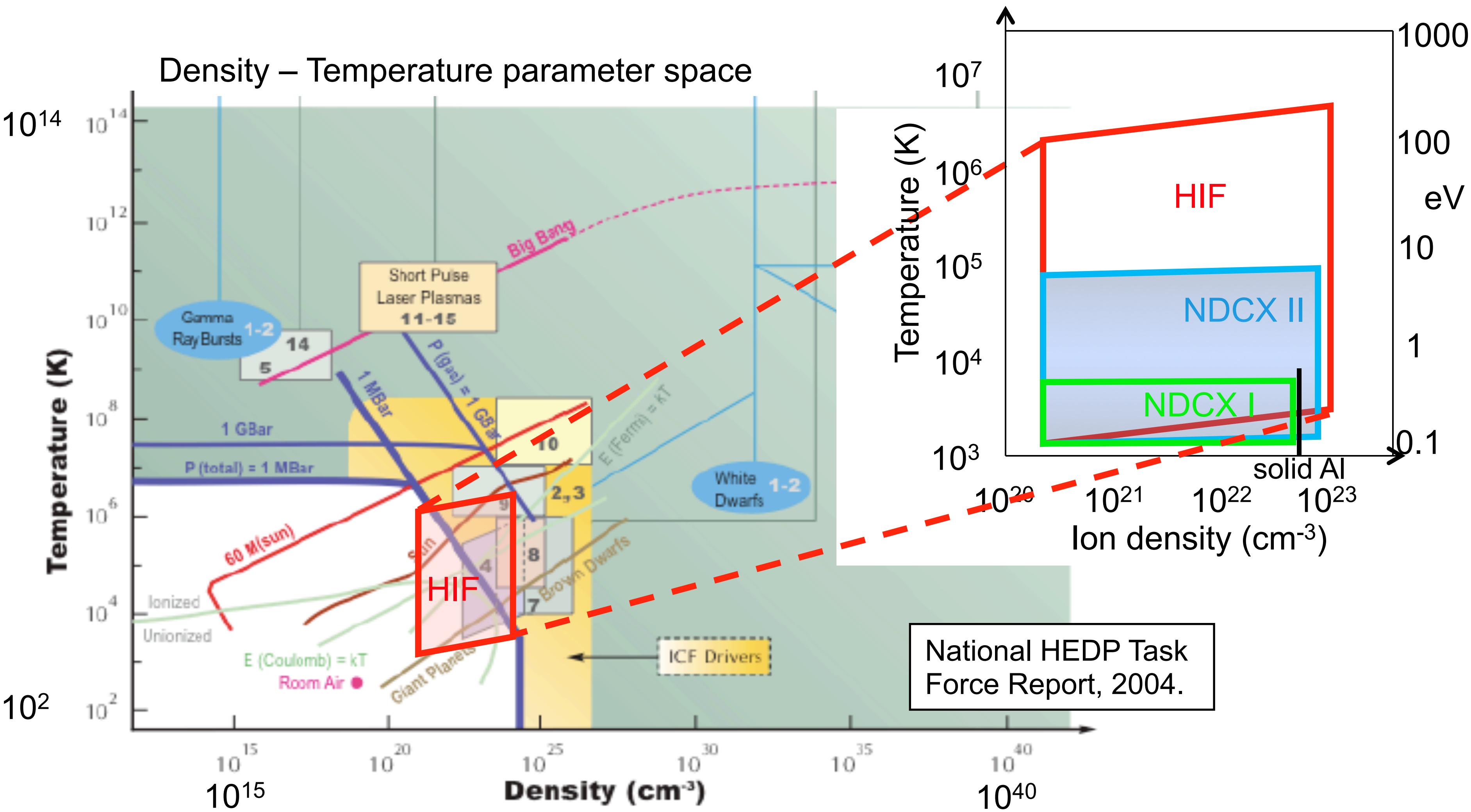


<u>Unknown properties:</u>
EOS ($p(\rho,T)$, $E(\rho,T)$)
Liquid-vapor boundary
Latent heat of evap.
Evaporation rate
Surface tension
Work function
Electrical conductivity
dE/dX for hot targets

<u>Phenomena:</u>
Metal-insulator transition
Phase transitions?
Plasma composition?

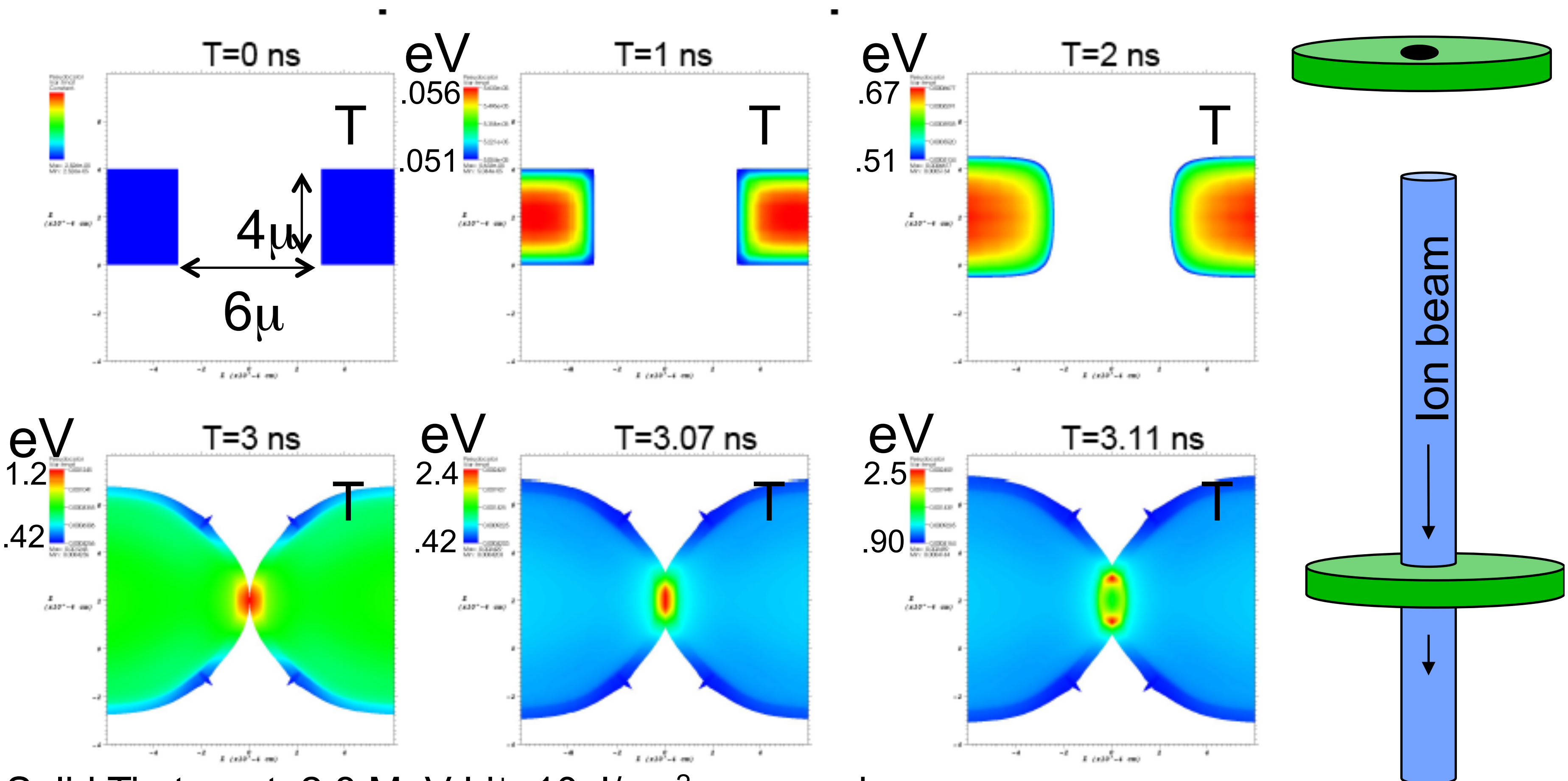
(From: R. More, Warm Dense Matter School, LBNL, January 2008)

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 ALE-AMR code for many WDM studies

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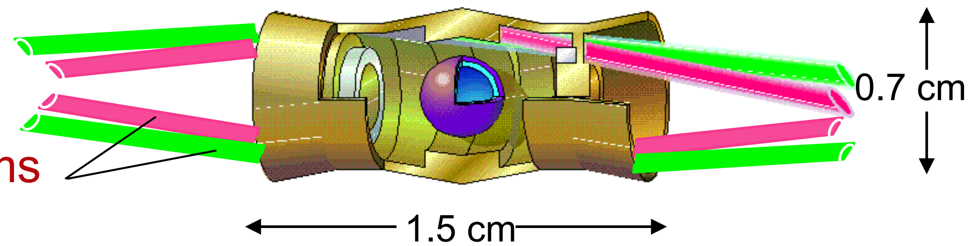
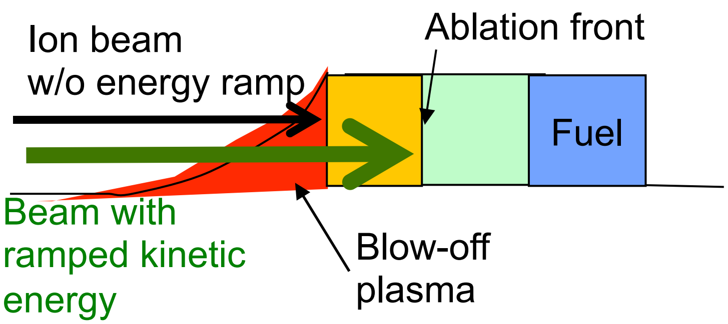
HYDRA is being used (on LLNL computers) to explore new heavy-ion IFE target concepts

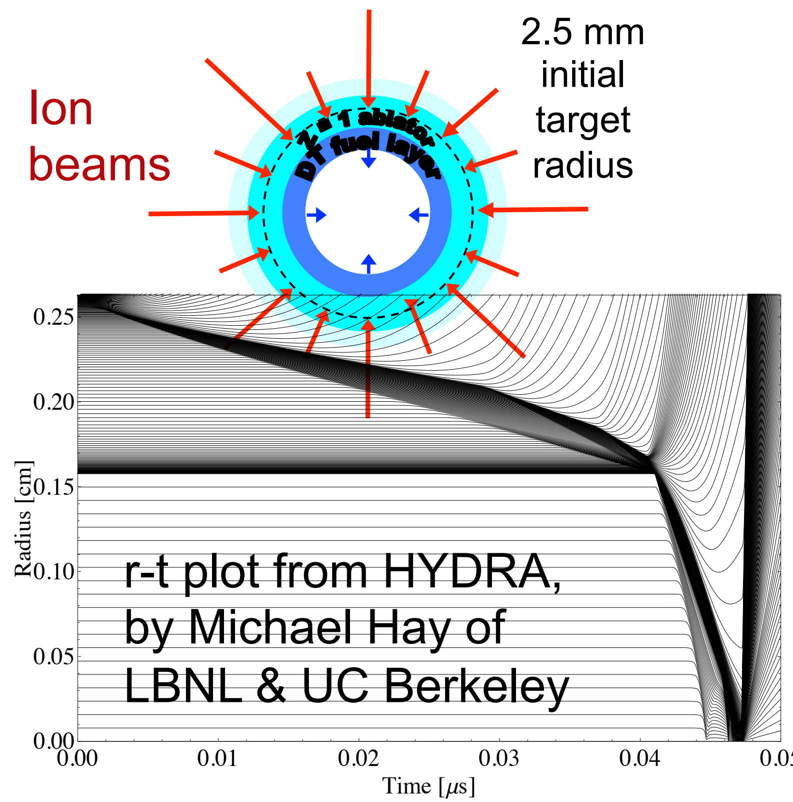
In indirect drive, ion energy heats converter material, which then produces x-rays.



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.



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

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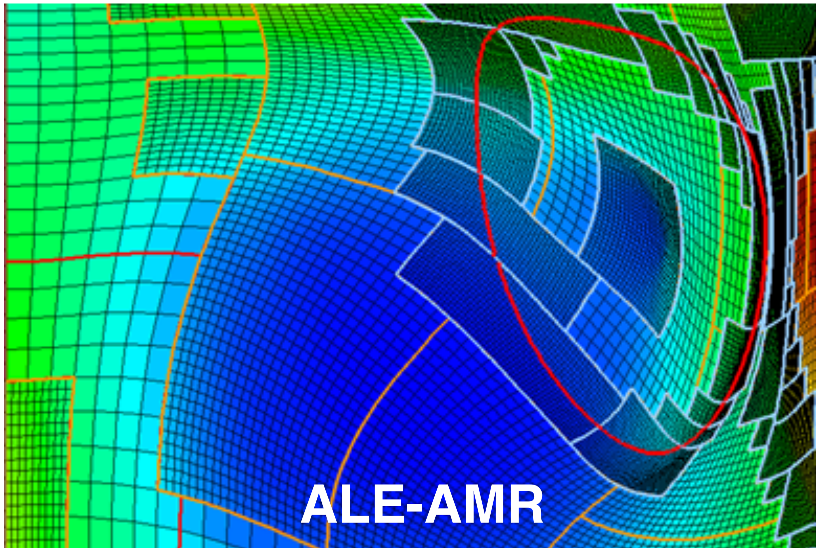
ALE-AMR was developed by DOE labs (LLNL & LBNL) and UC campuses (UCSD & UCLA)



ALE - Arbitrary Lagrangian Eulerian
AMR - Adaptive Mesh Refinement

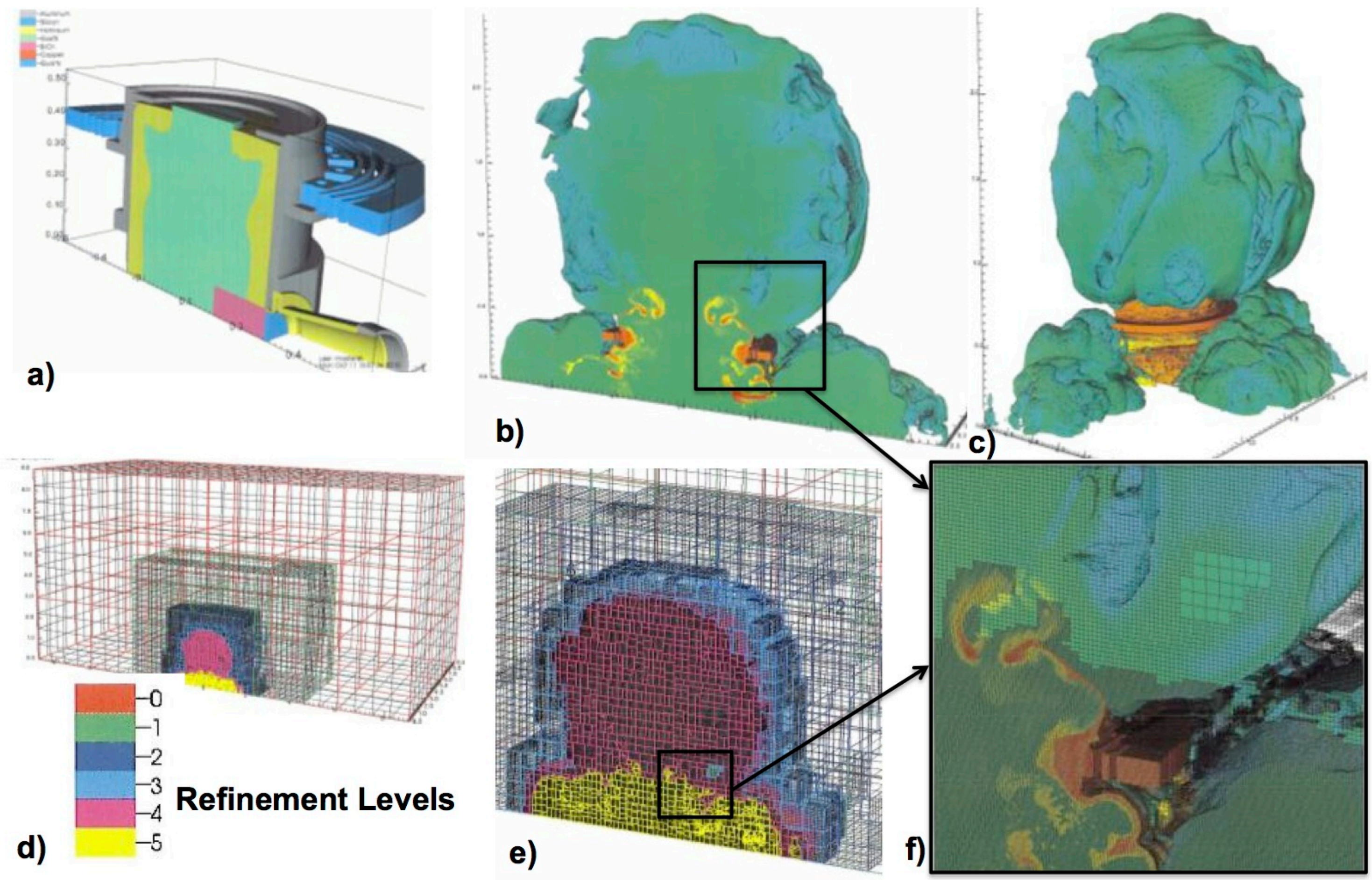
ALE-AMR is an open code that runs at various centers including NERSC, and has no export control restrictions

3-D runs take of order 1000 processor-weeks

- 3D ALE hydrodynamics
- Moving AMR grid (3X refinement)

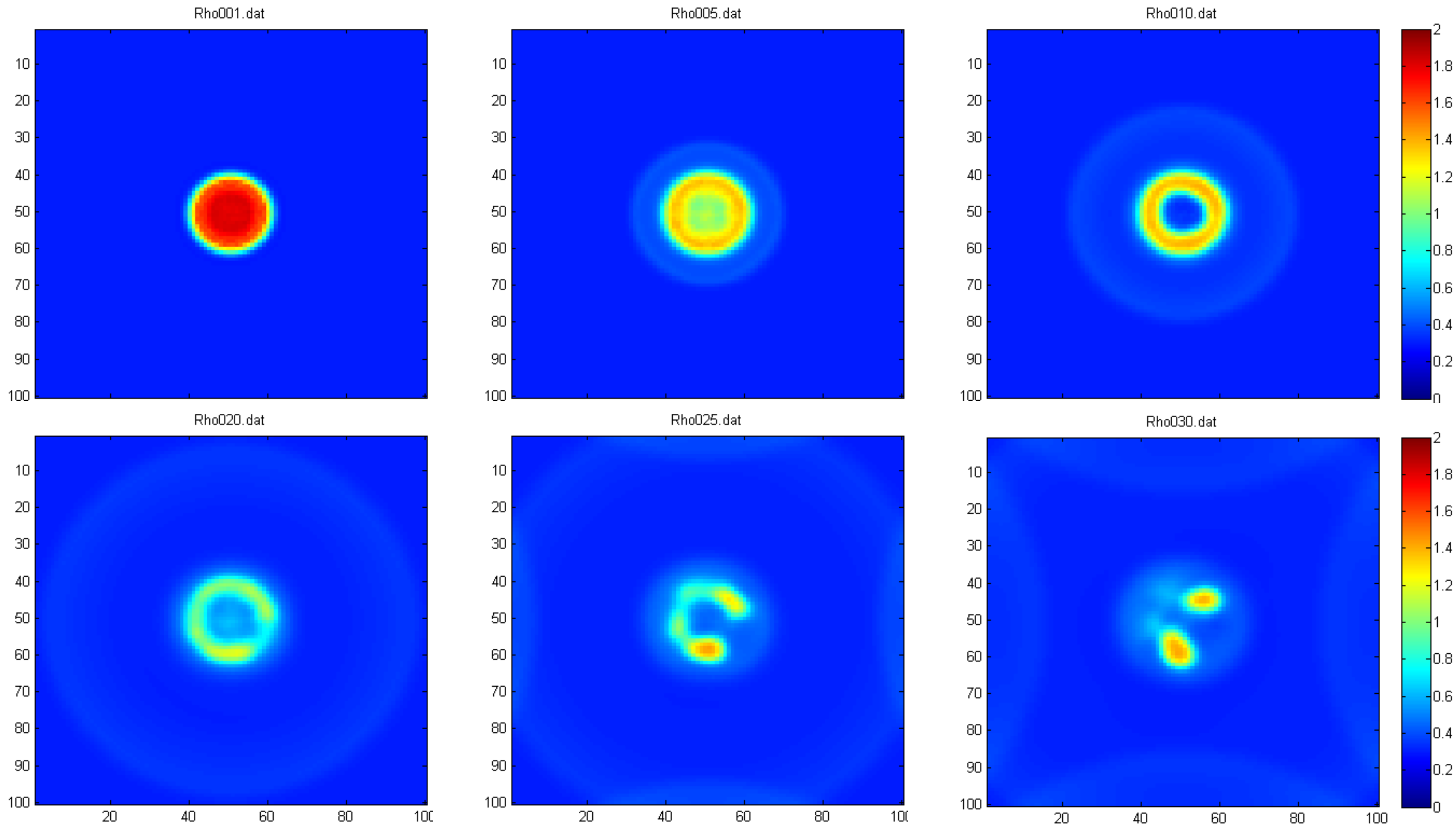
  with 6 levels, volume ratio = 10^7
- Material interface reconstruction
- Anisotropic stress tensor
- Material failure with history
- Laser & ion beams (for NDCX-II, HIF)
- Thermal conduction
- Radiation diffusion (new)
- 2D Axisymmetric capability (new)
- AMR with 3X in 1 direction (new)
- Surface tension (in progress)

ALE-AMR simulation showing mesh refinement levels



a) Initial material specification; b) Inside view showing plasma plume at 220 ns.; c) Outside view of plasma plume. d) Entire mesh, showing the 6 levels of refinement. e) Refinement levels and patch boundaries surrounding materials. f) Expanded view of the regions around the Si cooling rings.

We are developing surface tension models for ALE-AMR



A droplet in vapor, heated to a “threshold” temperature, with a localized perturbation.

Part of the droplet tends to expand and part tends to retract.

These two effects combined cause the droplet to break up.

ALE-AMR is becoming a key tool for our program

- We are planning to use ALE-AMR, on NERSC, to support both WDM and selected IFE studies.
  - It has been validated against analytic solutions, other codes, and experimental results
  - It scales well to thousands of CPU's at NERSC (addition of threads, e.g., OpenMP, could extend scaling)

- As an open code without export control restrictions, it is well positioned to support the full community of potential users of NDCX-II.

  However, it is not a complete inertial-fusion target design code.

- ALE-AMR runs 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

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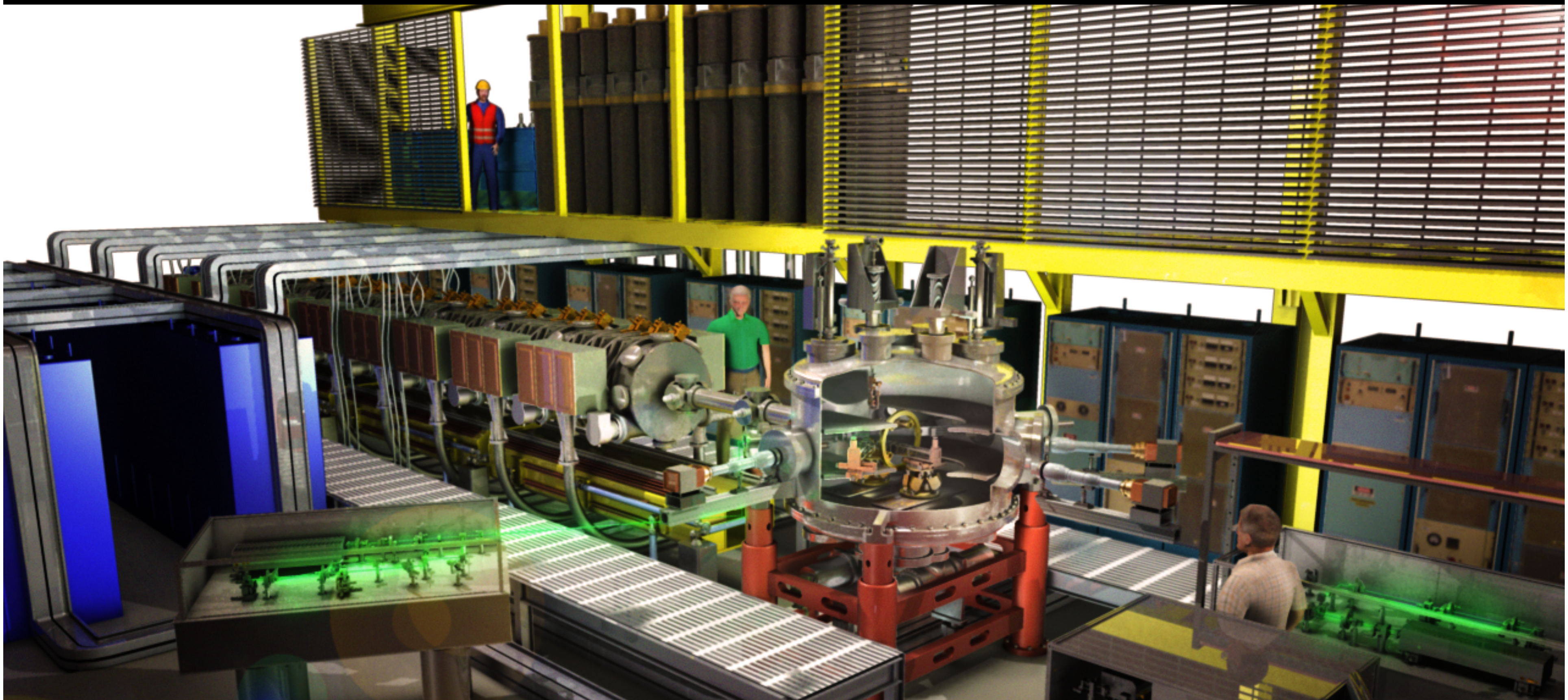
Our initial experience with Edison has been very favorable

- The start up of Python is significantly improved
  - 10-15x faster than Hopper
  - Special import code and static builds are no longer required

- We've found Edison to be faster overall
  - 30 to 50% faster for serial code
  - ~2x for parallel code (faster communication)

- We look forward to Phase 2

Large-scale simulations play an essential role in Heavy Ion Fusion Science research



- Support of the NDCX-II experimental program
- Simulations of targets for HEDP and IFE
- Development of future facilities