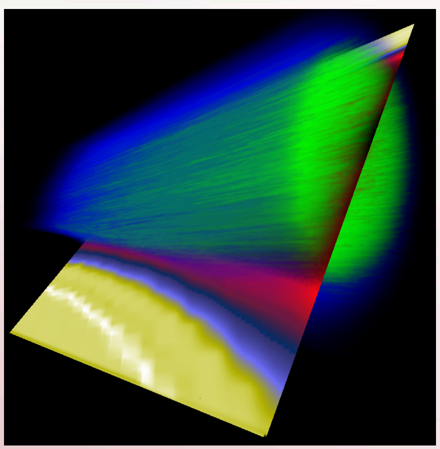
This research used resources of the Argonne Leadership Computing Facility at Argonne National Laboratory,
which is supported by the Office of Science of the U.S. Department of Energy under contract DE-AC02-06CH11357.

NIC

Computational Challenges in Hot, Dense Plasmas



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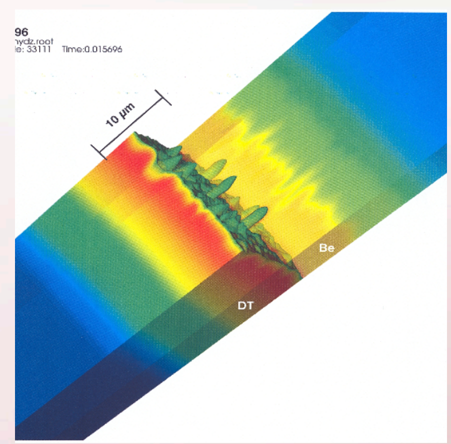
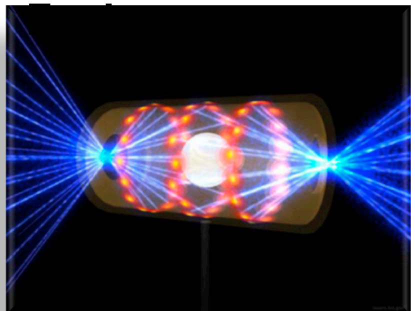
March 26, 2012



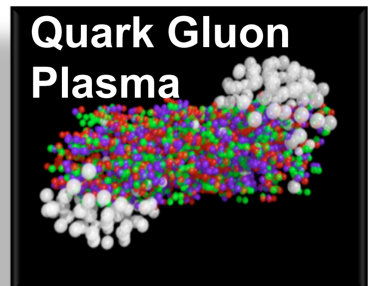
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

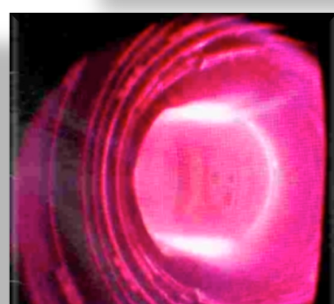
The NAS report: “frontiers in High Energy Density Physics are the X-Games of contemporary science”

Inertial Confinement

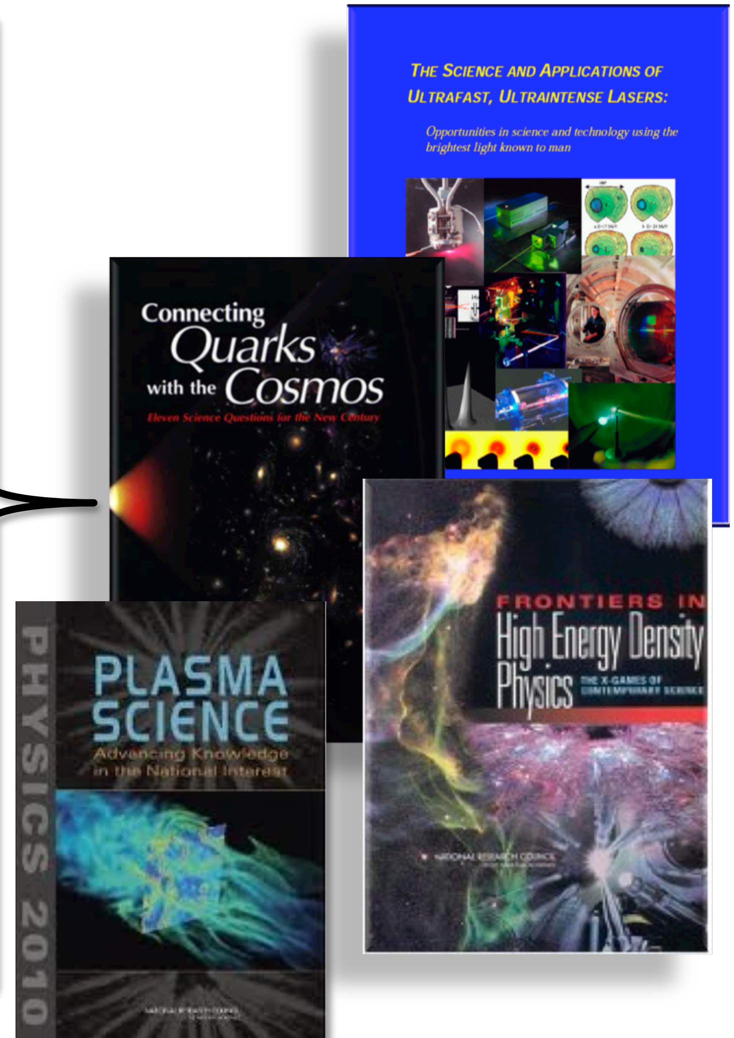


Astrophysics

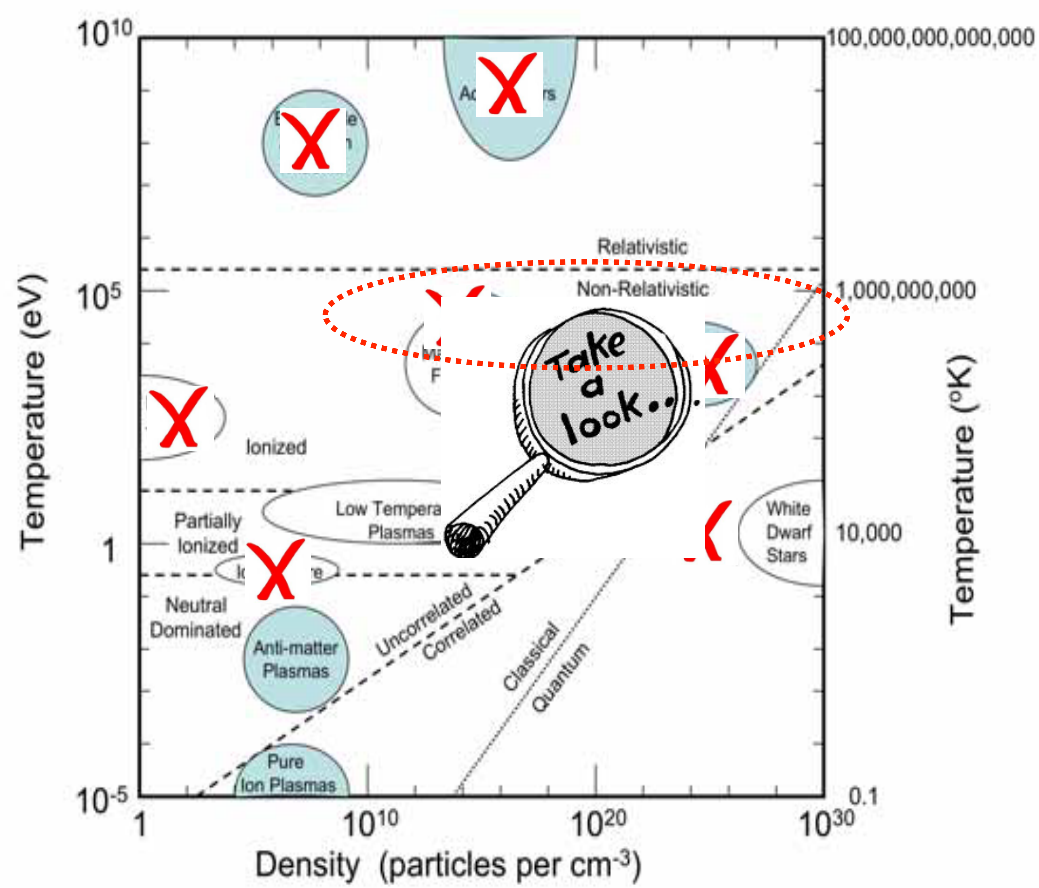




Magnetic Fusion

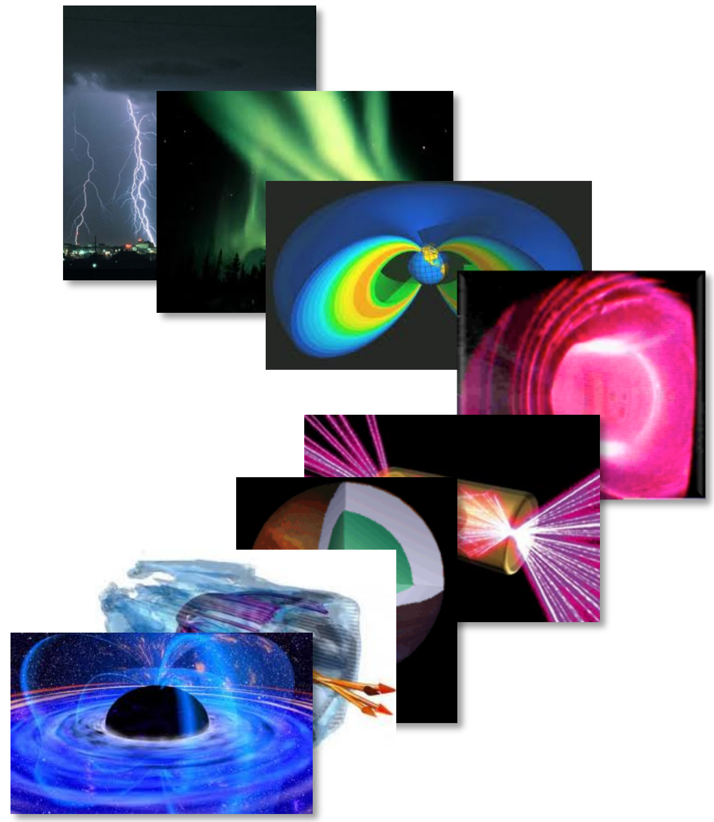


Plasmas consist of mobile charged particles interacting by long-range electromagnetic N-body forces



Our understanding of plasma behavior in each of these regimes differs widely

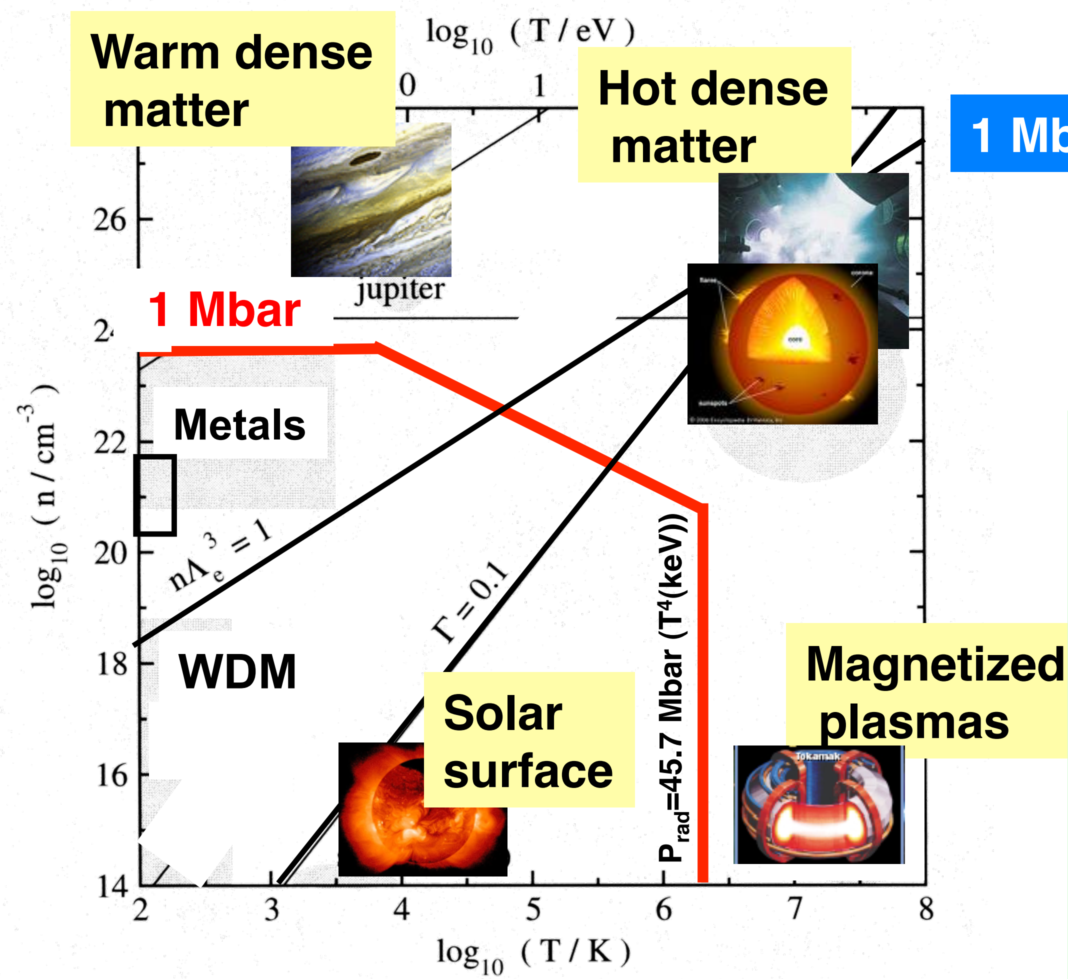
Matter in the plasma state exists in an unimaginable variety



$$1\,\text{eV} = 1.16 \times 10^4\ \text{K}$$

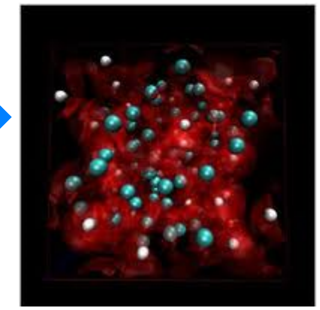
National Academy of Sciences: Plasma Science
Advancing Knowledge in the National Interest

HED matter exhibits complex behavior not typically associated with classical plasmas



Kremp et al., *"Quantum Statistics of Non-ideal Plasmas"*, Springer-Verlag (2005)

1 Mbar = 10^{12} erg/cm^3



Bulk modulus ~ 1 Mbar

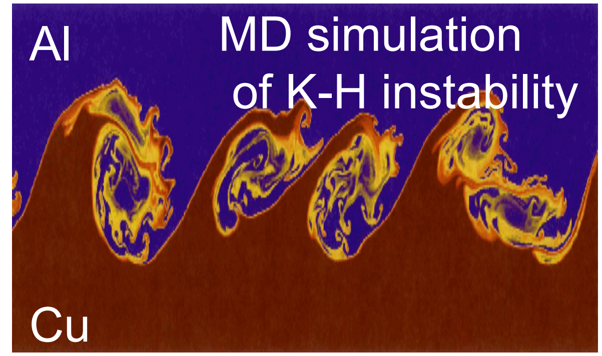
- **Radiation dominated**
- **Strong correlations**
- **Multiple species**
- **Fermi degeneracy**
- **Hybrid quantum and classical behavior**
- **Bound states**
- **ionization**

NIC

What are the computational challenges confronting HED physics?

Multi-scale modeling

- *Micro- and meso- scale physics impacts meso- and macro-scale*
- *A significant and fascinating challenge!*
- *On-going efforts in materials science, ICF, MFE, astrophysics, …*



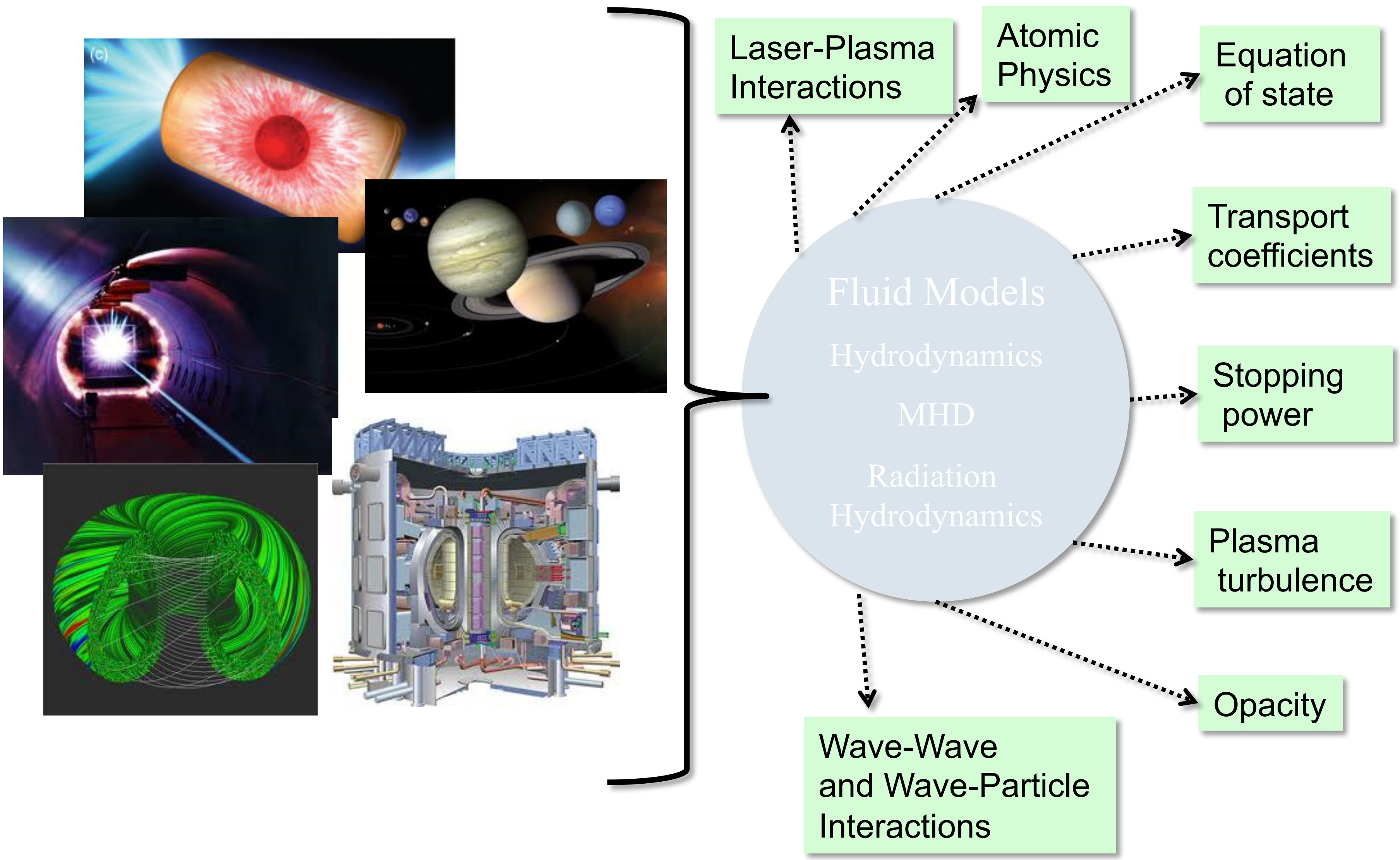
Computer hardware and architecture

- *Algorithmic R&D on efficient uses of new GPU machines*
- *Visualization and data analysis*
- *A national user facility for HEDP simulations (MD, QMD, PIMC, PIC, electronic structure, direct numerical simulation of multi-scale phenomena)*

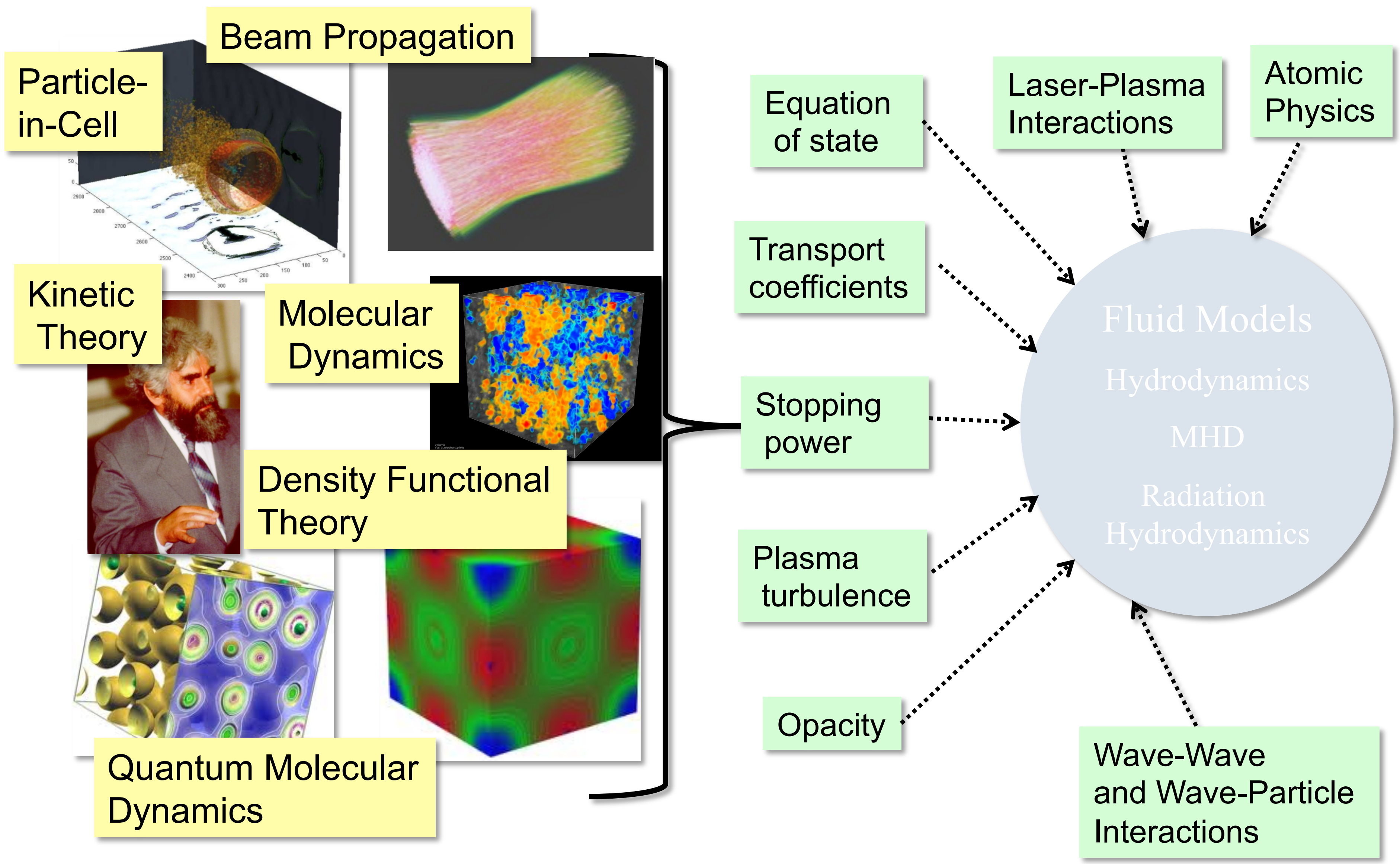
Verification and validation

- *Robust V&V program for computational tools*
- *Validation of sub-scale physics simulations*

Multiscale Physics: macroscale simulations require fundamental physics information from the meso-/micro-scale



Multiscale Physics: meso-/micro-scale simulations provide input to the macroscale



The advent of exascale computing provides opportunities for paradigm shifts

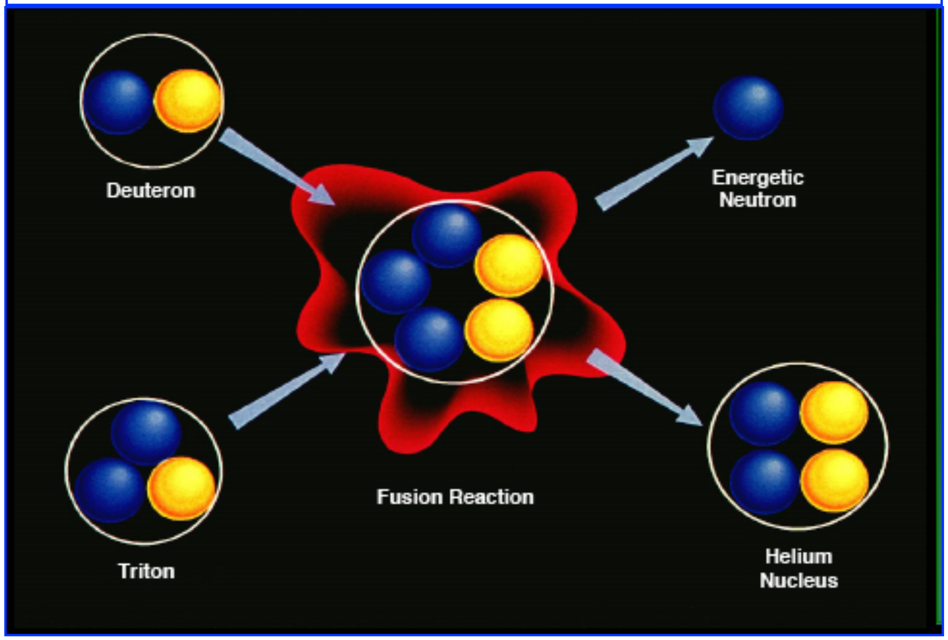
- How do we most advantageously utilize increased computational resources?

Current Scenario	Future Scenario #1	Future Scenario #2
• Continue to simulate as we do currently (but perform more simulations): -- macroscale simulations with mesoscale/microscale physics crudely approximated and/or informing macroscale simulations through databases approximating actual physics	• Perform macroscale simulations with higher spatio-temporal resolution and include more detailed meso-/micro-scale physics reduced model descriptions and begin integration of meso-scale physics into the macroscale	• Perform macroscale simulations with direct numerical simulation of mesoscale physics and perform mesoscale simulations with direct numerical simulation of microscale physics

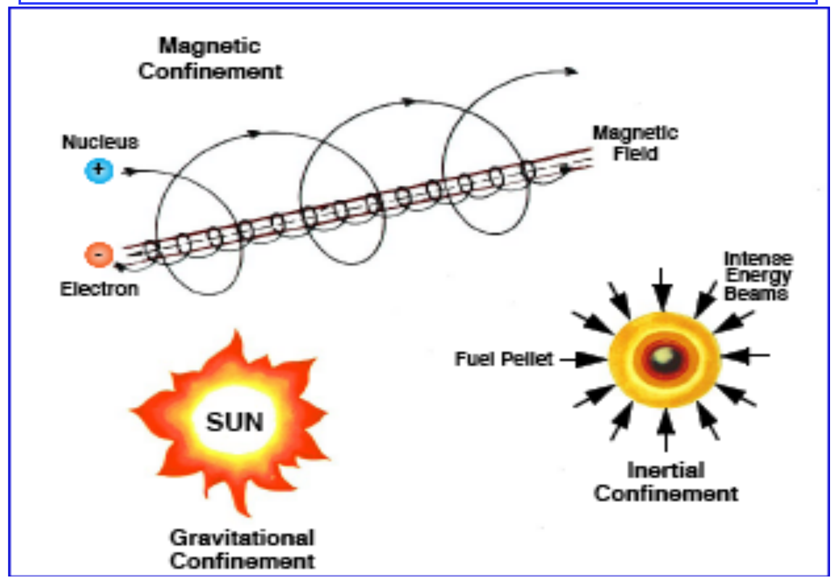
Direct numerical simulation from the micro-to-macro-scale is computationally unfeasible even at exascale!

A current multi-scale challenge: simulating fusion experiments for the National Ignition Facility

Fusing deuterium and tritium into a helium nucleus releases an energetic neutron



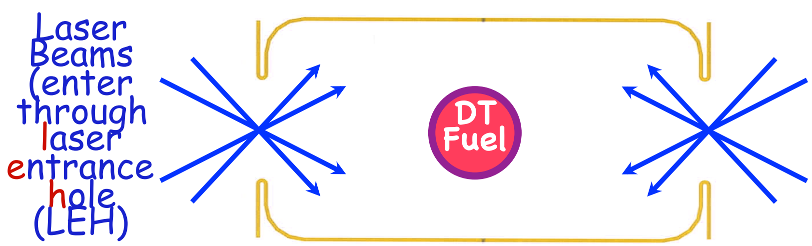
Fusion is accomplished via gravitational, magnetic and inertial confinement



The goal of upcoming experiments on the National Ignition Facility (NIF) is to achieve fusion in a laboratory setting

Inertial confinement fusion (ICF) relies on the inertia of the fuel to provide confinement

- <u>INDIRECT DRIVE:</u> laser energy is converted to x-ray energy by target

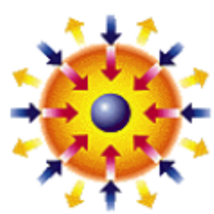


Hohlraum (laser target)

- x-rays bathe ICF capsule, heating it up -- it expands

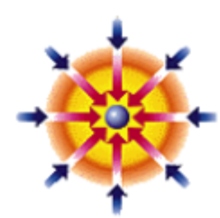
Ablator heats up

- conservation of momentum: ablated shell expands outward, rest of shell (frozen DT) is forced inward



Rocket effect

- fusion initiates in a central hot spot containing ~ 5% of the fuel, and a thermo-nuclear burn front propagates outward



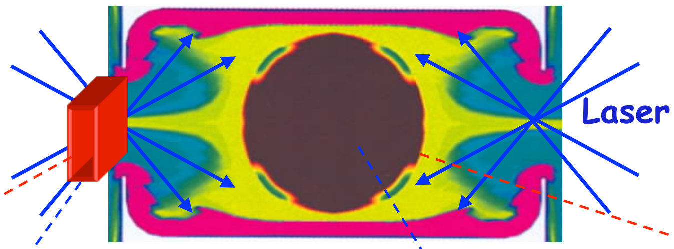
Ignition

Burn wave

Ignition targets span a wide range of length and time scales

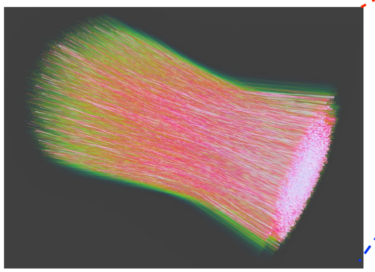
macroscale

- Hydrodynamic length and time scales are set by target size [O(mm)] and laser pulse length [O(ns)]



⇒ *environment -- plasma parameters and scale lengths*

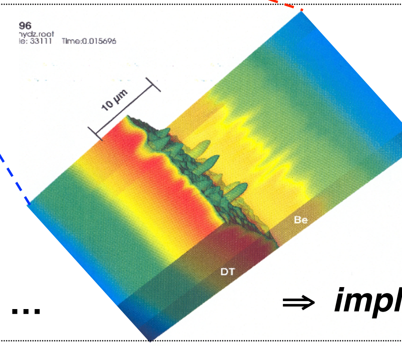
mesoscale



⇒ *beam propagation*

- evolves on:
  μm length scales
  ps time scales

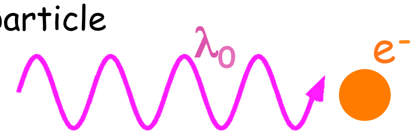
- Other examples:
  atomic physic, eos, opacity, non-local electron transport, …



⇒ *implosion stability*

microscale

wave-particle



wave-wave

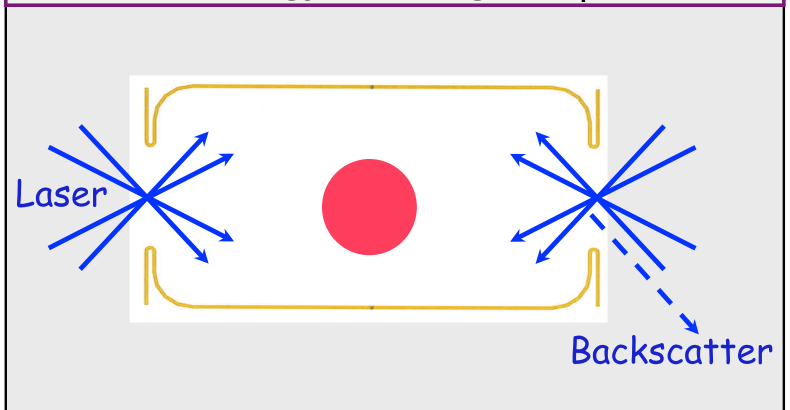
- Detailed processes of beam propagation occur on "light" spatial and temporal scales

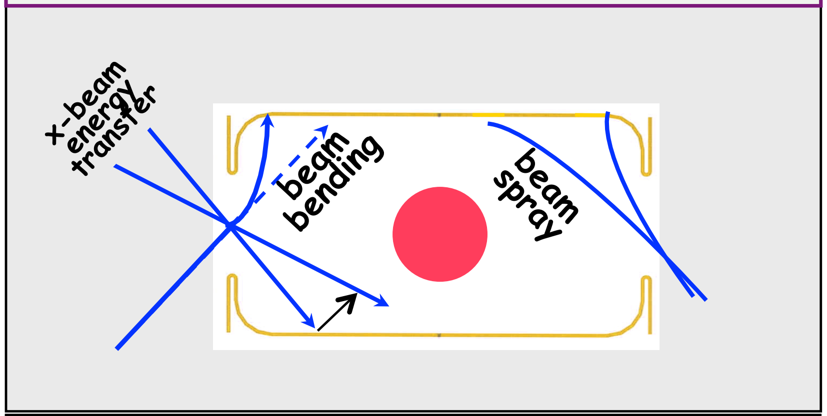
The multi-scale challenge: incorporate all necessary physics at all relevant length and time scales

We use laser energy coupling to the ignition target as a detailed example of multi-scale modeling

- *Laser-plasma interactions modify the laser energy coupling to the hohlraum target*

Energy Coupling ➔ T_r	Energy Re-direction ➔ symmetry change





SBS: laser scatters off self-generated ion acoustic waves (iaws)

SRS: laser scatters off self-generated electron plasma waves (epws)

Beam spray: intensifies & scatters light

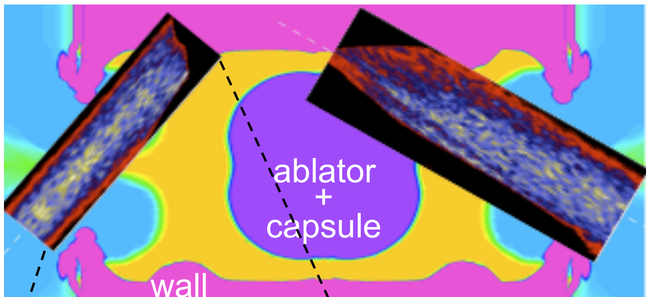
Beam bending: moves light pattern on wall

Cross-beam transfer: moves laser power among beams

Re-absorption of scattered light: alters symmetry

LPI processes span a wide range of length and time scales

macroscale

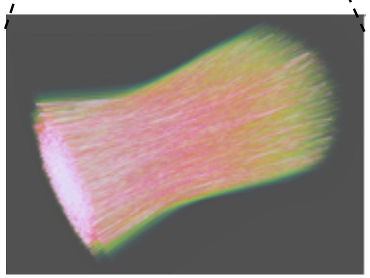


- Hydrodynamic length and time scales are set by target size **[O(mm)]** and laser pulse length **[O(ns)]**

  environment -- plasma parameters and scale lengths

need accurate plasma conditions

mesoscale

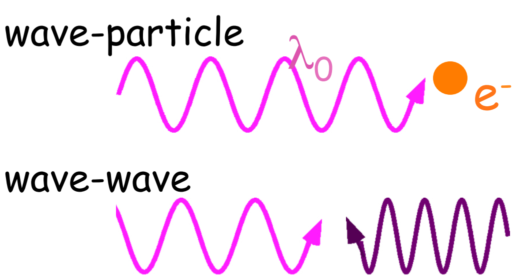


- LPI evolves on: **μm length** and **ps time** scales

  beam propagation

need accurate beam model (including effects of cross-beam energy transfer, pump depletion, competition)

microscale



- Detailed processes of LPI occur on **"light" spatial and temporal scales**

  kinetic effects

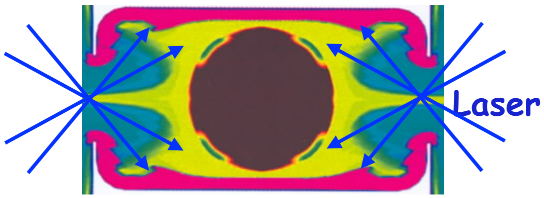
need accurate interactions – when do kinetic effects matter?

Our approach to multi-scale modeling uses a suite of tools

NIC

macroscale

Lasnex/Hydra

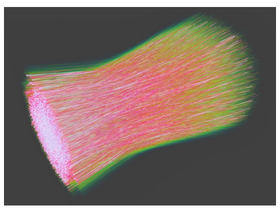


Radiation/Hydrodynamics simulations

laser energy → heat e⁻'s → make x-rays; transport; hydro motion → implosion & burn

mesoscale

pF3D

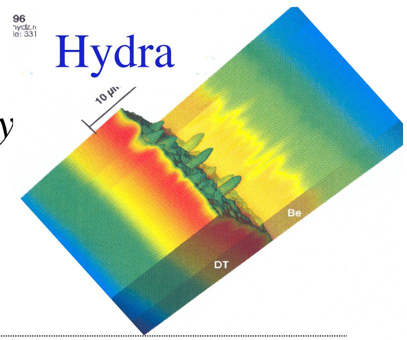


Wave propagation simulations

incident laser propagation ↔ fluid plasma model ↔ scattered light propagation ↔ incident laser propagation

High resolution implosion stability simulations

Hydra

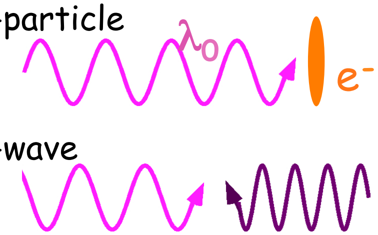


microscale

Z3/BZohar

wave-particle

wave-wave



Particle in cell (PIC) simulations

particle phase space → Maxwell Equations (ρ,**j**) → EM fields → Lorentz Force → particle phase space

Coupling these scales allows us to develop a predictive capability, validated by experiment

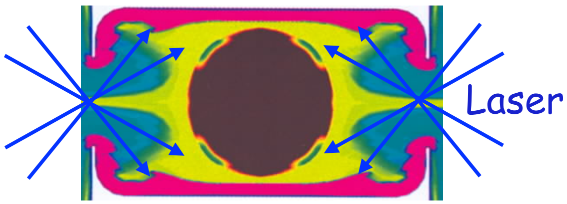
Here is how we model LPI for the National Ignition Campaign (NIC):

feedback

feedback not yet a reality

macroscale

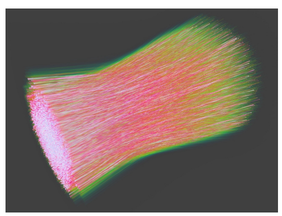
Lasnex/Hydra



- *Use plasma conditions + nominal laser intensity to:*
  - -- calculate spectrum of reflected light
  - -- define spatio-temporo-wavelength region over which to perform more detailed simulations
  - -- track "gain" of reflected light as a metric to compare amongst designs/experiments

mesoscale

pF3D



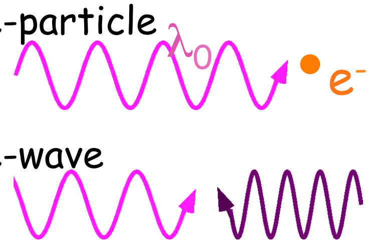
- *Perform detailed beam propagation simulations to:*
  - -- calculate reflectivity of one quad of beams
    - - at a particular time in the laser pulse
    - - over the volume specified at the macroscale
  - -- compute changes in energy deposition
  - -- synthesize backscatter diagnostics

microscale

PIC/Vlasov Codes

wave-particle

wave-wave

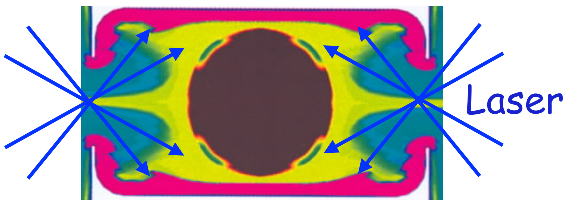


- *Perform microscale simulations to:*
  - -- assess impact of kinetic effects
  - -- determine changes in reflectivity
- The microscale component of LPI for NIC has not been as extensively analyzed because of the "flowdown" effect

What kind of computational resources do we use at each scale?

macroscale

Lasnex/Hydra

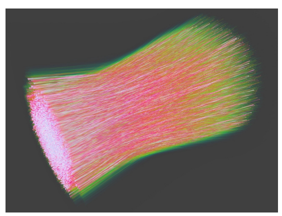


- 2D rad-hydro simulations: ~ 100 cpus for ~ 2 days (workhorse)
- 3D rad-hydro simulations: ~ 1000 cpus for ~ 10 days
- Integration of "mesoscale hydrodynamics":
  -- requires >> 1000 cpus for >> 1 week

feedback

mesoscale

pF3D

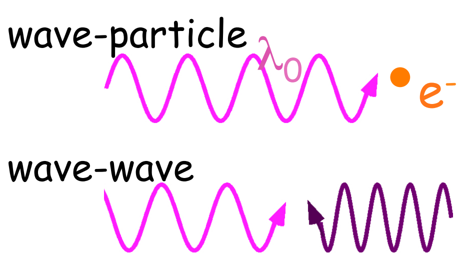


- Beam propagation simulations:
  -- full machine runs for > 1 week (have run on up to ~ 196,000 cpus)
- Will test on LLNL's Sequoia machine later this year

feedback not yet a reality

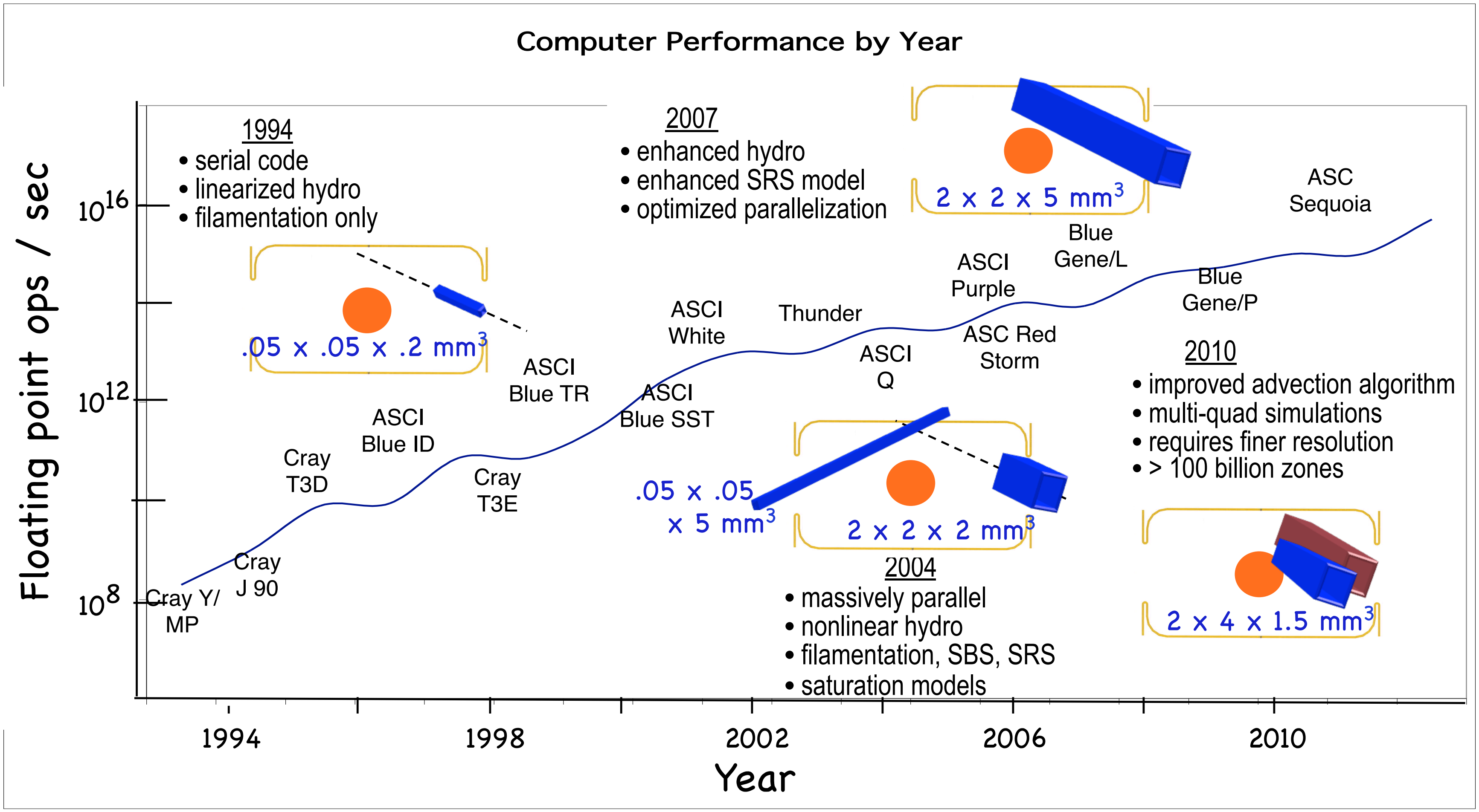
microscale

PIC/Vlasov Codes



- Microscale simulations:
  -- some groups run on > 10,000 cpus

Rapidly increasing computer performance enables LPI calculations unimaginable just twelve years ago



Both laser and plasma modeling improvements have impacted large-scale LPI simulations

- Modified plasma conditions from hohlraum modeling
  (improved atomic physics, electron transport)
  -- results in a cooler plasma – SRS region moves closer to LEH
  -- experimental and synthetic SRS spectra show SRS at similar wavelengths

- Realistic laser beams that include the effects of cross-beam energy transfer (XBT)
  -- increased power on inner beams (symmetry)
  -- spatial non-uniformity in cross section

- Laser quad overlap: simulate beam propagation (pF3D) for two quads of beams
  (overlap contributes to the intensity; simulate 3-5 quads of beams?)

A promising start: simulated reflectivity approaches experimental levels when these models are used

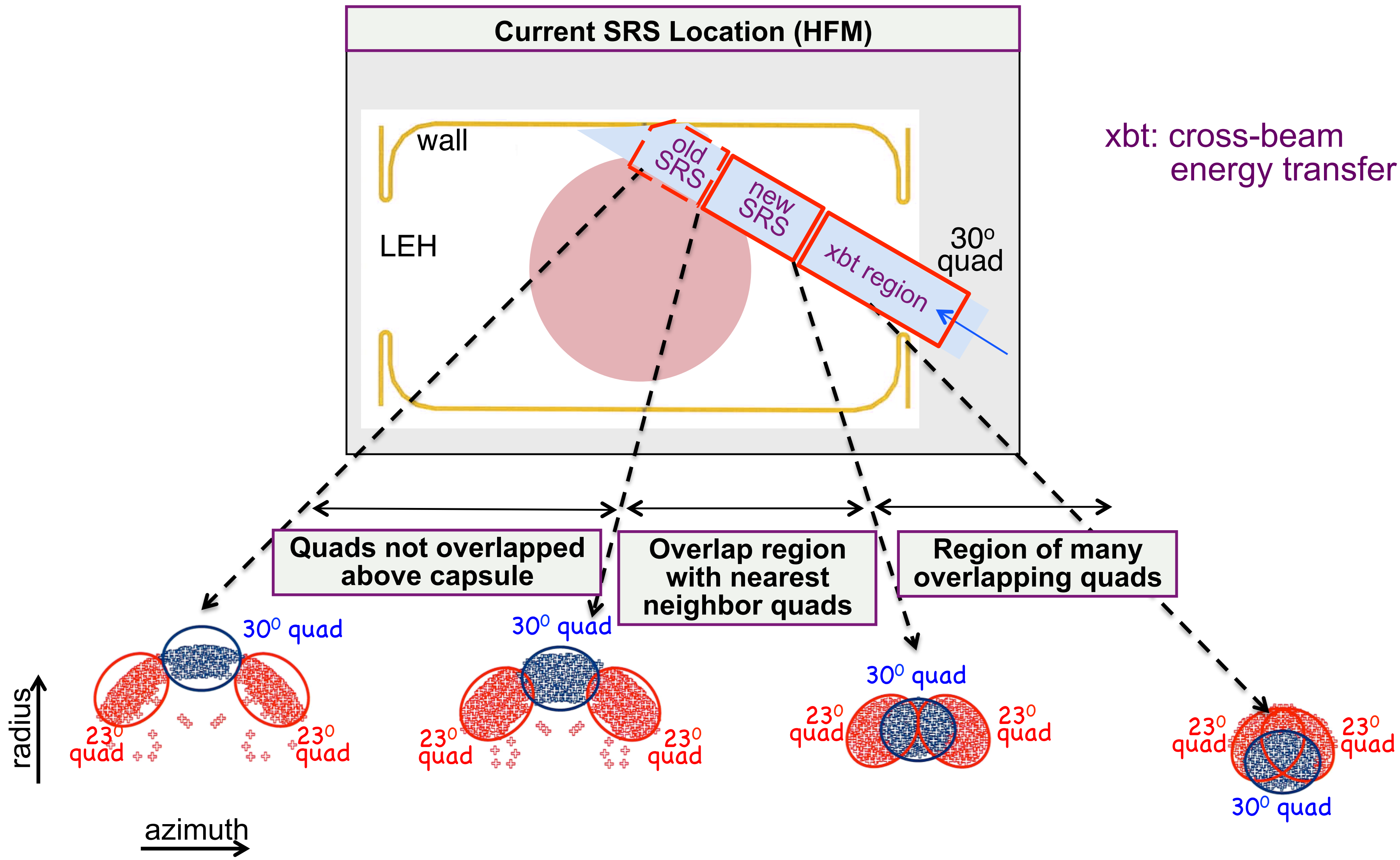
Experimental Result Vs Single Quad pF3D Simulations

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2009 pF3D: 1 Quad pre-2009 plasma spatially uniform beam			~ 0.1
2010 pF3D: 1 Quad high flux model plasma spatially uniform beam			0.18
2011 pF3D: 1 Quad high flux model plasma spatially non-uniform beam			0.43

Experimental Result Vs Double Quad pF3D Simulations

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2010 pF3D: 2 Quads high flux model plasma spatially uniform beams			0.62
2011 pF3D: 2 Quads high flux model plasma spatially non-uniform beams			0.67
2012 pF3D: 3 Quads high flux model plasma spatially non-uniform beams			~0.9-1.0

Different LPI regions are traversed by an inner cone quad of beams



LPI: Hohlraum modeling improvements have resulted in a change in backscatter location

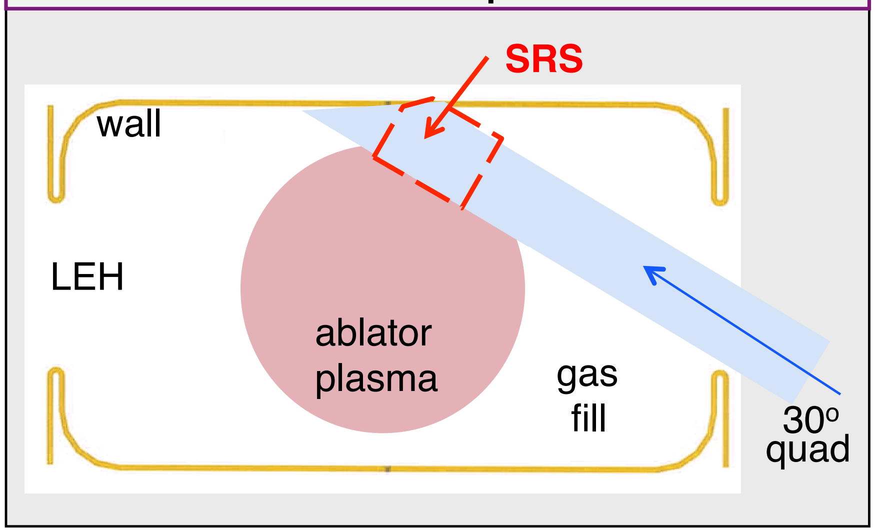
- SBS: laser backscatters off self-generated ion acoustic waves (iaws)
- SRS: laser backscatters off self-generated electron plasma waves (epws)

} results in direct energy loss

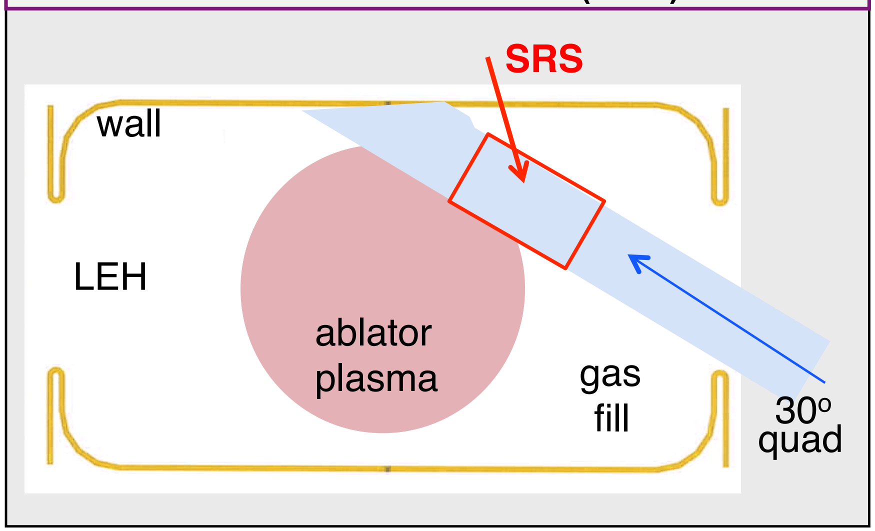
- High Flux Model (M. D. Rosen *et al.*, HEDP, 2011): improved atomic physics, non-local e- transport

  -- modifies n_e, T_e (and where SRS occurs)

SRS Location pre-2009

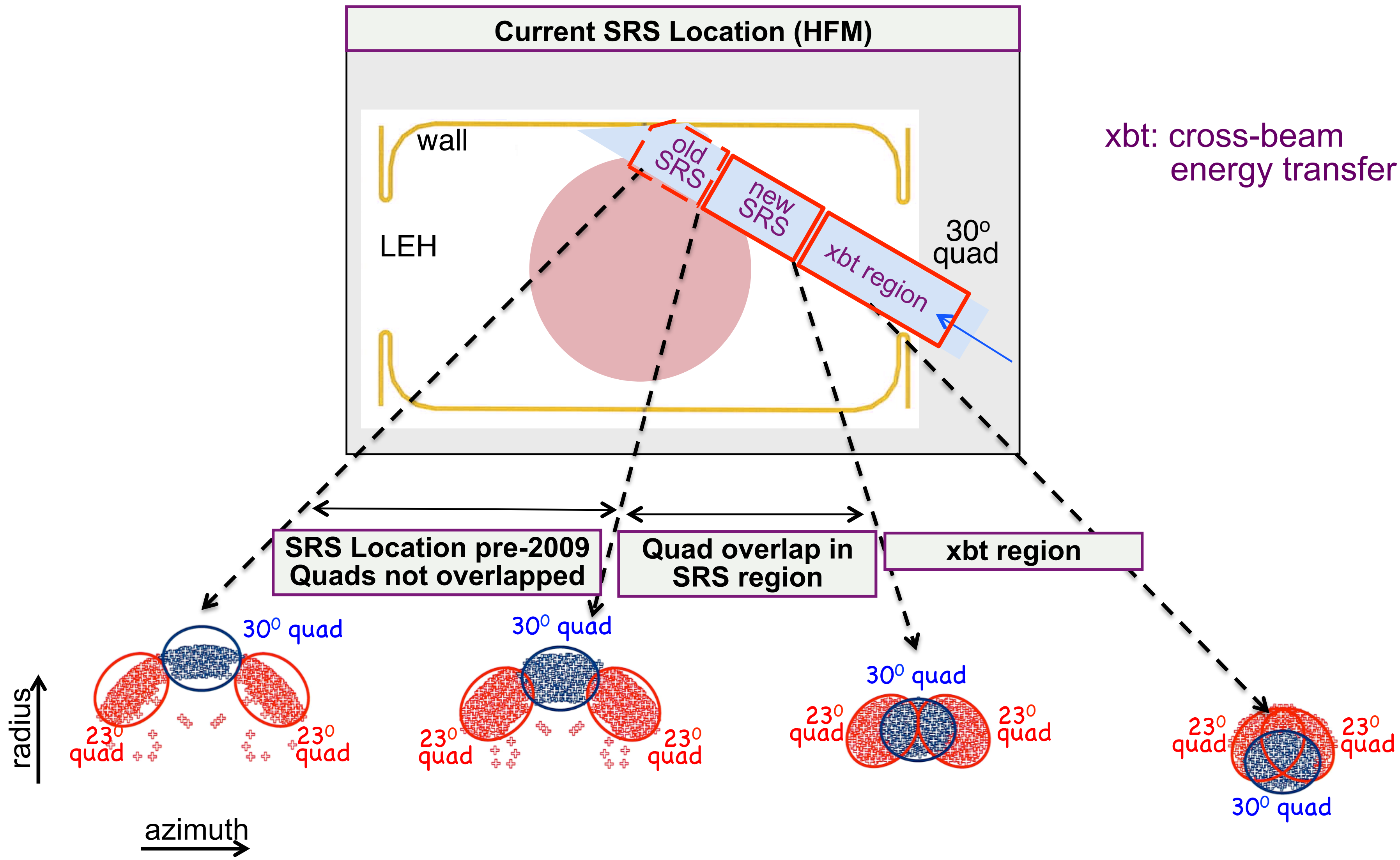


Current SRS Location (HFM)

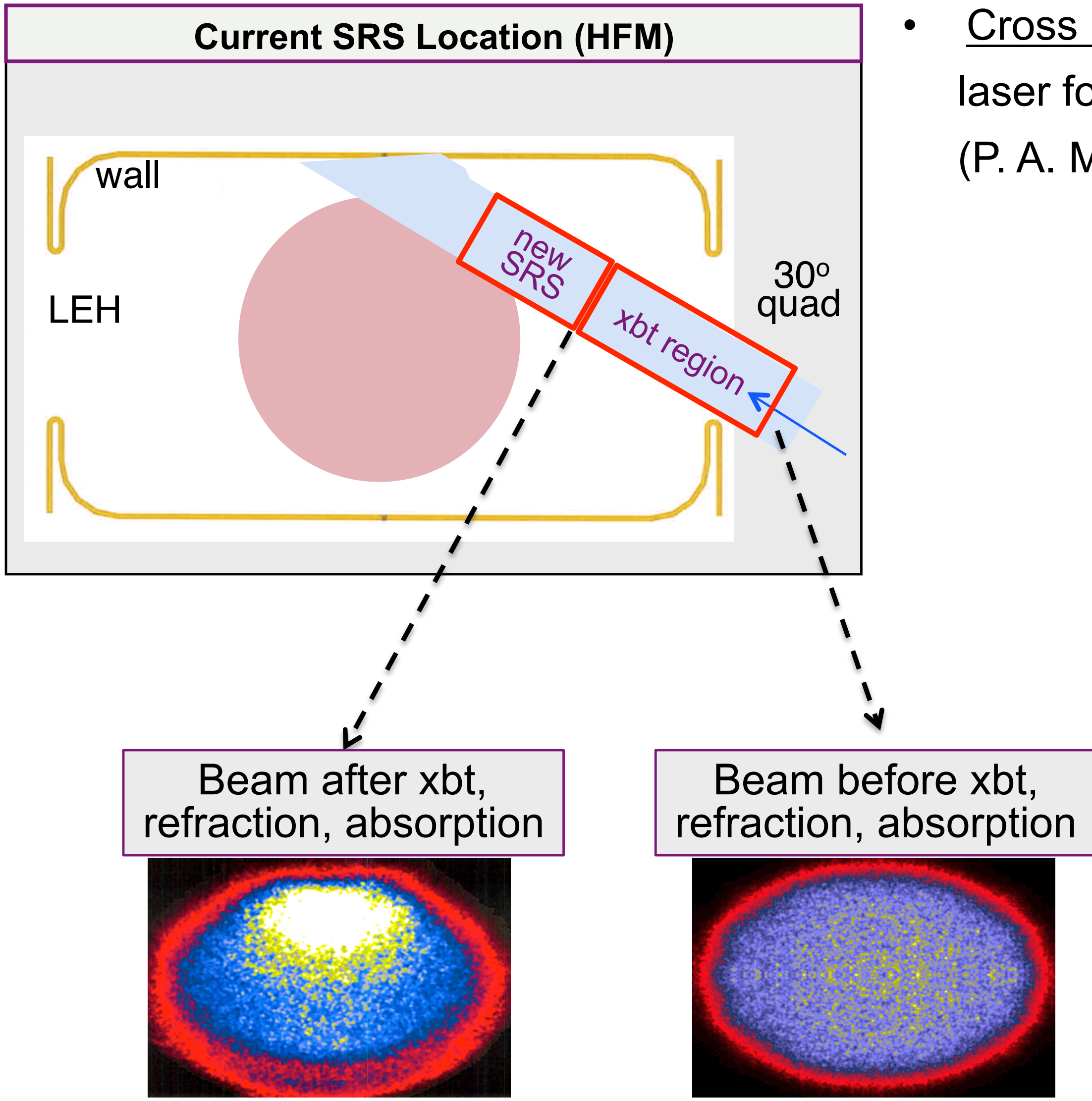


LPI: 30° SRS now occurs where there is overlap with nearest neighbor 23° quads

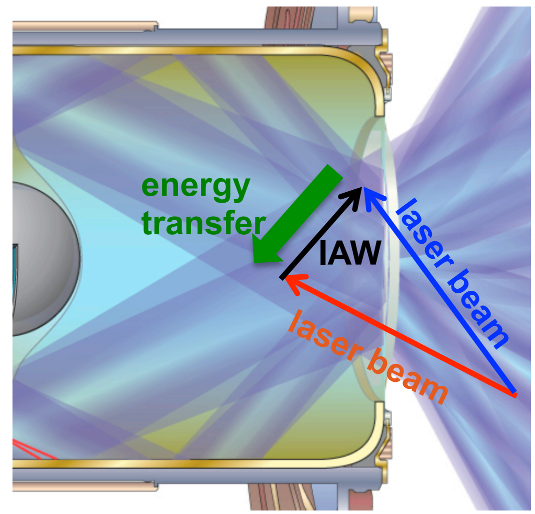
xbt: cross-beam energy transfer



LPI: Cross-beam energy near the LEH results in a spatially non-uniform intensity distribution



- Cross Beam Energy Transfer (xbt): laser forward scatters off ion acoustic waves (P. A. Michel *et al.*, PoP, May 2010)



We assess the impact of realistic plasma conditions and laser spots on reflectivity using pF3D

- pF3D provides beam transmission, reflectivity and energy deposition by numerically solving equations of the form:

$$\mathcal{L}_{prop} A_0 = C^* (\delta n_f A_0 + \boxed{\delta n_A A_1} + \boxed{\delta n_L A_2})$$

advection
absorption
diffraction

refraction

SBS coupling

SRS coupling

Fields

A_0 : incident laser

A_1 : SBS; driven by $\delta n_A A_0$

A_2 : SRS; driven by $\delta n_L A_0$

Plasma Response

δn_A (iaw): driven by $A_0 A_1$

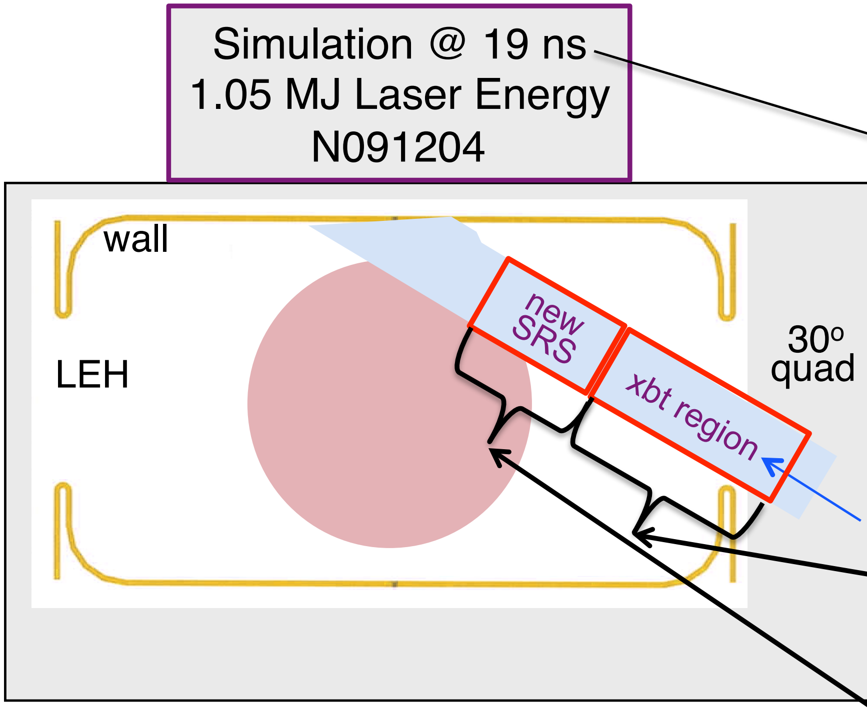
δn_L (epw): driven by $A_0 A_2$

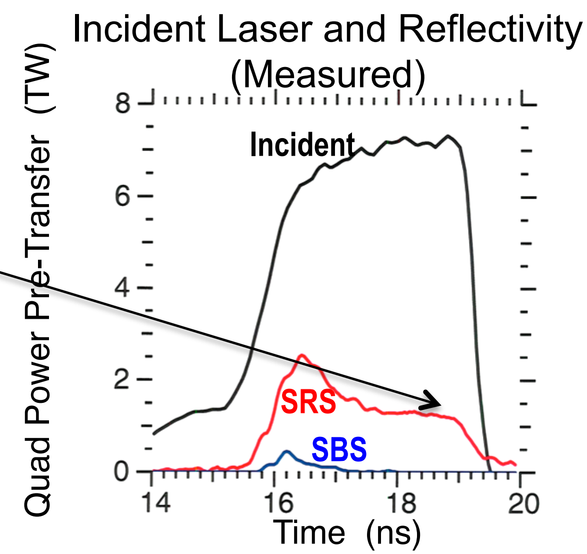
- satisfy respective wave equations

Background plasma:

- described by nonlinear fluid model (with multiple materials)
- couples to laser via ponderomotive (radiation) pressure, inverse brehmsstrahlung

Proof-of-principle simulation: propagate two quads (23°, 30°) through the resonance region





- Laser Input: use SLIP* to propagate quads through the LEH to the input plane (*E. A. Williams*)
- pF3D: propagate two quads of beams (23°, 30°) through SRS region (*A. B. Langdon*)

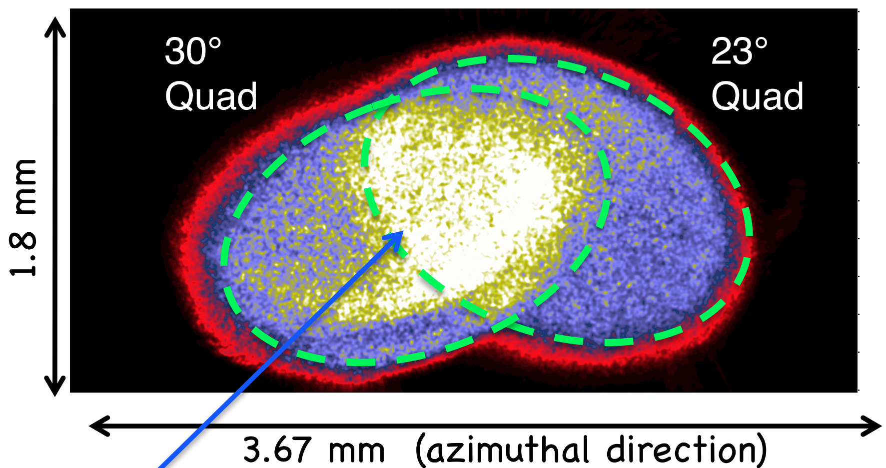
*SLIP code, P. A. Michel and L. Divol

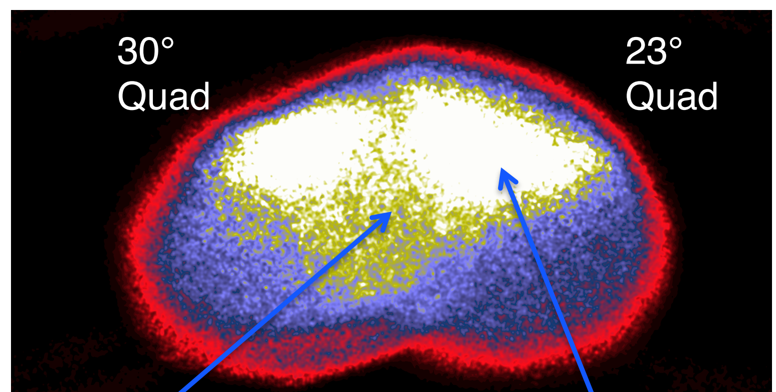
We have separated the effects of overlap and non-uniformity by performing different simulations

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2010 pF3D: high flux model plasma *spatially uniform* beams			1 Quad: 0.18 2 Quads: 0.62

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2011 pF3D: high flux model plasma *spatially non-uniform* beams			1 Quad: 0.43 2 Quads:0.67

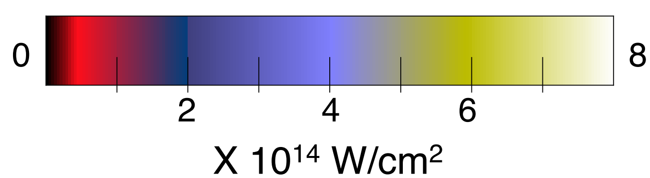
Laser Quads on Input Plane to "New SRS" Region





most intense portion of beam is in overlap region

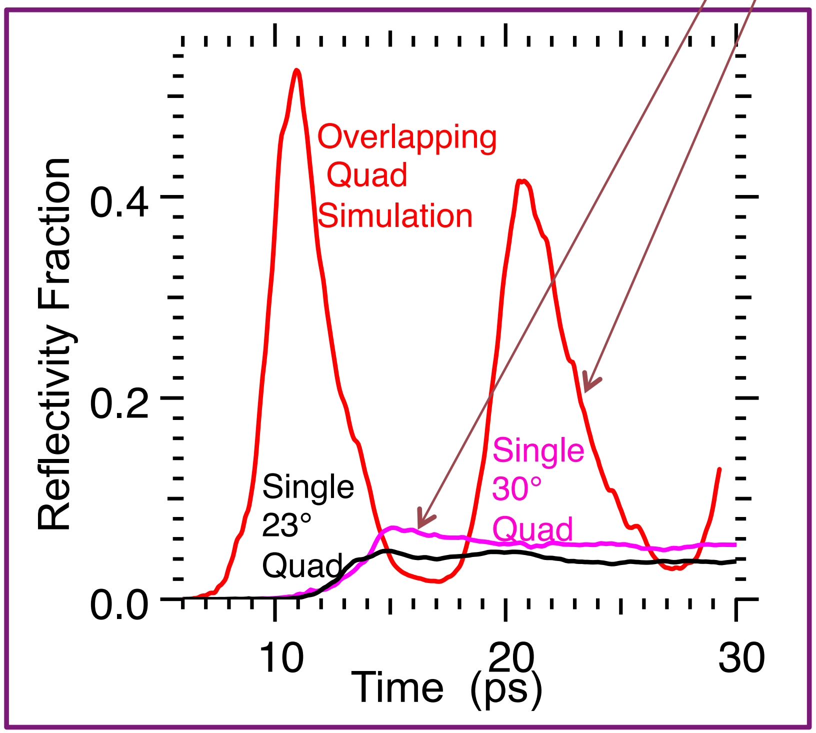
overlap region is less intense than xbt region

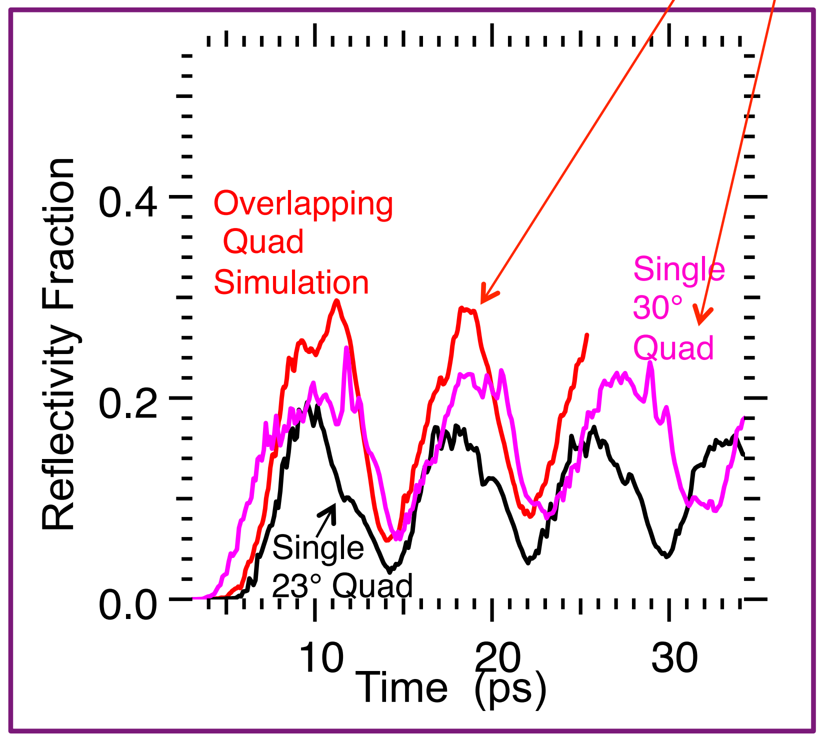


Both effects (overlapping quads and spatial non-uniformity) act to increase reflectivity

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2010 pF3D: high flux model plasma *spatially uniform* beams			1 Quad: 0.18 2 Quads: 0.62

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2011 pF3D: high flux model plasma *spatially non-uniform* beams			1 Quad: 0.43 2 Quads: 0.67





*We thank the Office of Science INCITE program for computational resources and the ALCF staff for computational support

<u>SRS light</u>: a "pre-amp" generated by the single quads is resonantly amplified in the overlap region

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2010 pF3D:	high flux model plasma *spatially uniform* beams		1 Quad: 0.18 2 Quads: 0.62

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
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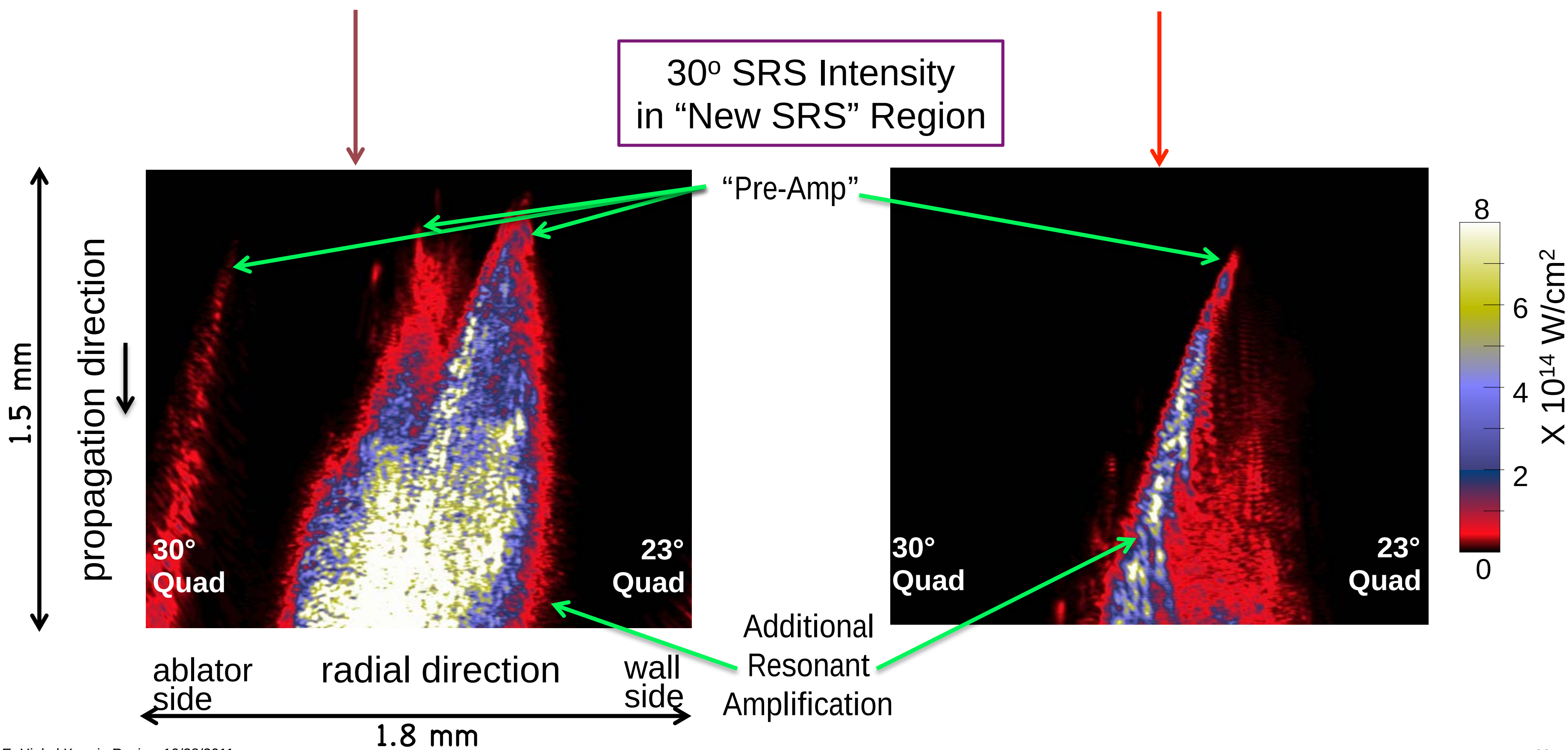
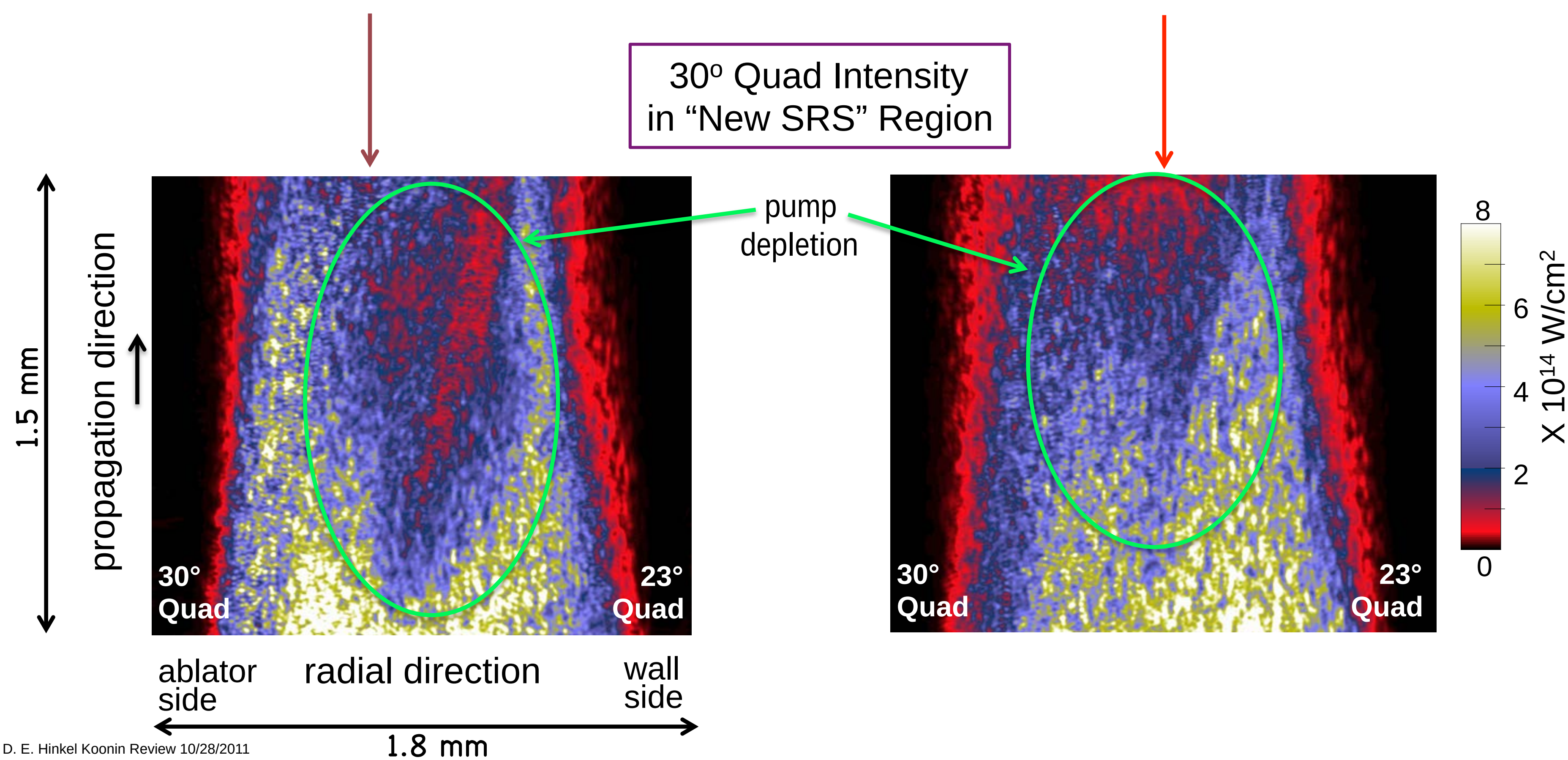


Incident light: pump depletion in region where SRS is amplified

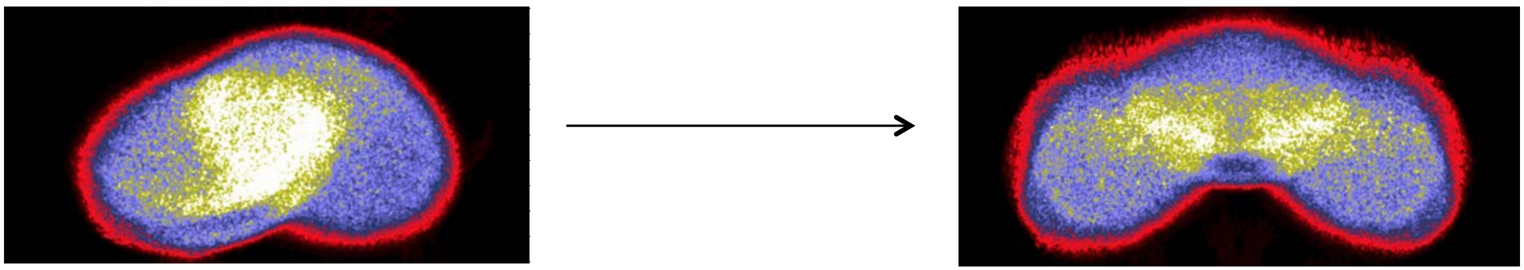
Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2010 pF3D: high flux model plasma *spatially uniform* beams			1 Quad: 0.18 2 Quads: 0.62

Shot	Energy (MJ)	Time (ns)	30° SRS (TW)
N091204	1.05	19	1.3
2011 pF3D: high flux model plasma *spatially non-uniform* beams			1 Quad: 0.43 2 Quads:0.67



Future pF3D simulations would focus on more recent shots/new designs – for (hopefully) a triplet of quads

- Simulations of a triplet of quads to determine whether reflectivity increases as expected
  - -- SRS/SBS competition
  - -- increases azimuthal extent of simulation
  - -- *targeted machines*: Cielo(?); TLCC2(?); Sequoia(?); ???



- Increase axial length, to better capture SBS reflectivity
  - -- would like to simulate 3.5 mm with a triplet
  - -- *targeted machines:* TLCC2(?); Sequoia(?); ???

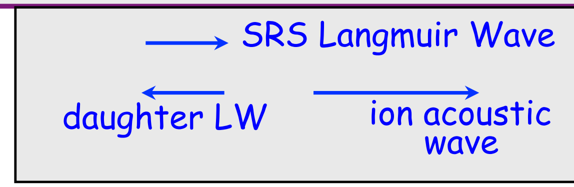
- Simulate five quads as early science users on Sequoia?
  - -- we are currently determining if this is feasible

To simulate a triplet of quads: > 100 billion zones and ~ 1 month on a BGP machine

Microscale simulations are a necessary ingredient in accurately modeling the interactions of LPI

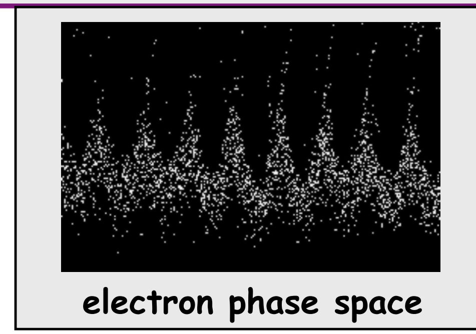
- *Langmuir Decay Instability (LDI):*
  - -- likely occurring in NIF sub-scale targets
  - -- or over capsule in full-scale targets

LDI depletes SRS Langmuir Wave



- *Electron Trapping:*
  - -- can "inflate" reflectivity via damping reduction
  - -- can "deflate" reflectivity via de-tuning, incoherence …

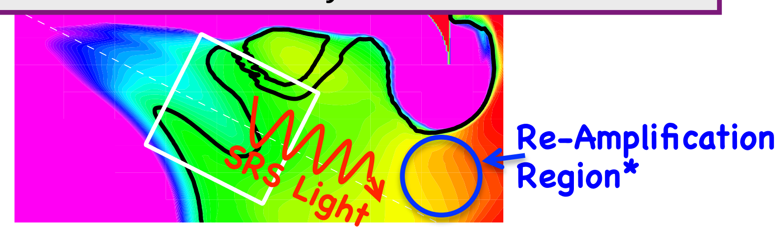
Electron trapping in Langmuir Wave



- *Re-scatter?*

SRS light further amplified non-resonantly near LEH?

- *Re-amplification of SRS Light:*

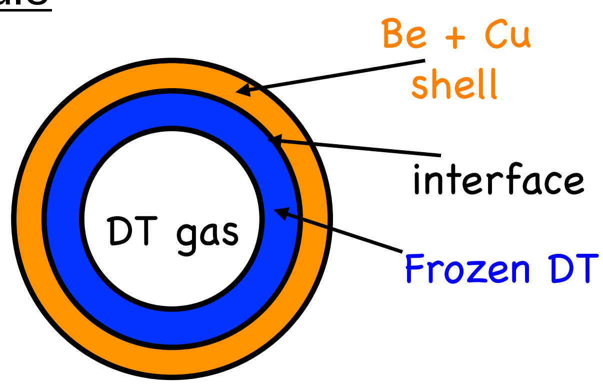


Incorporating these effects into pF3D allows for their interplay with geometry

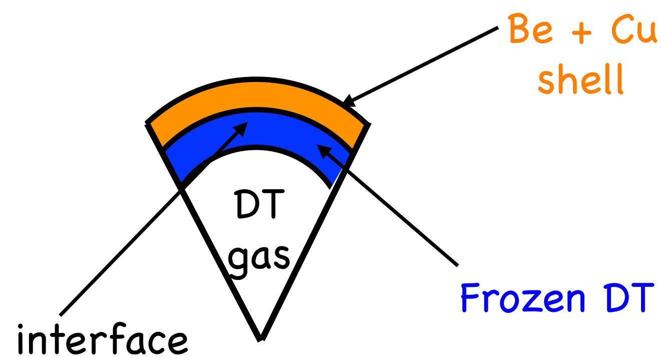
*P. A. Michel *et al.*, PoP **17**, 056305 (2010)

High resolution capsule-only simulations address implosion stability

Capsule



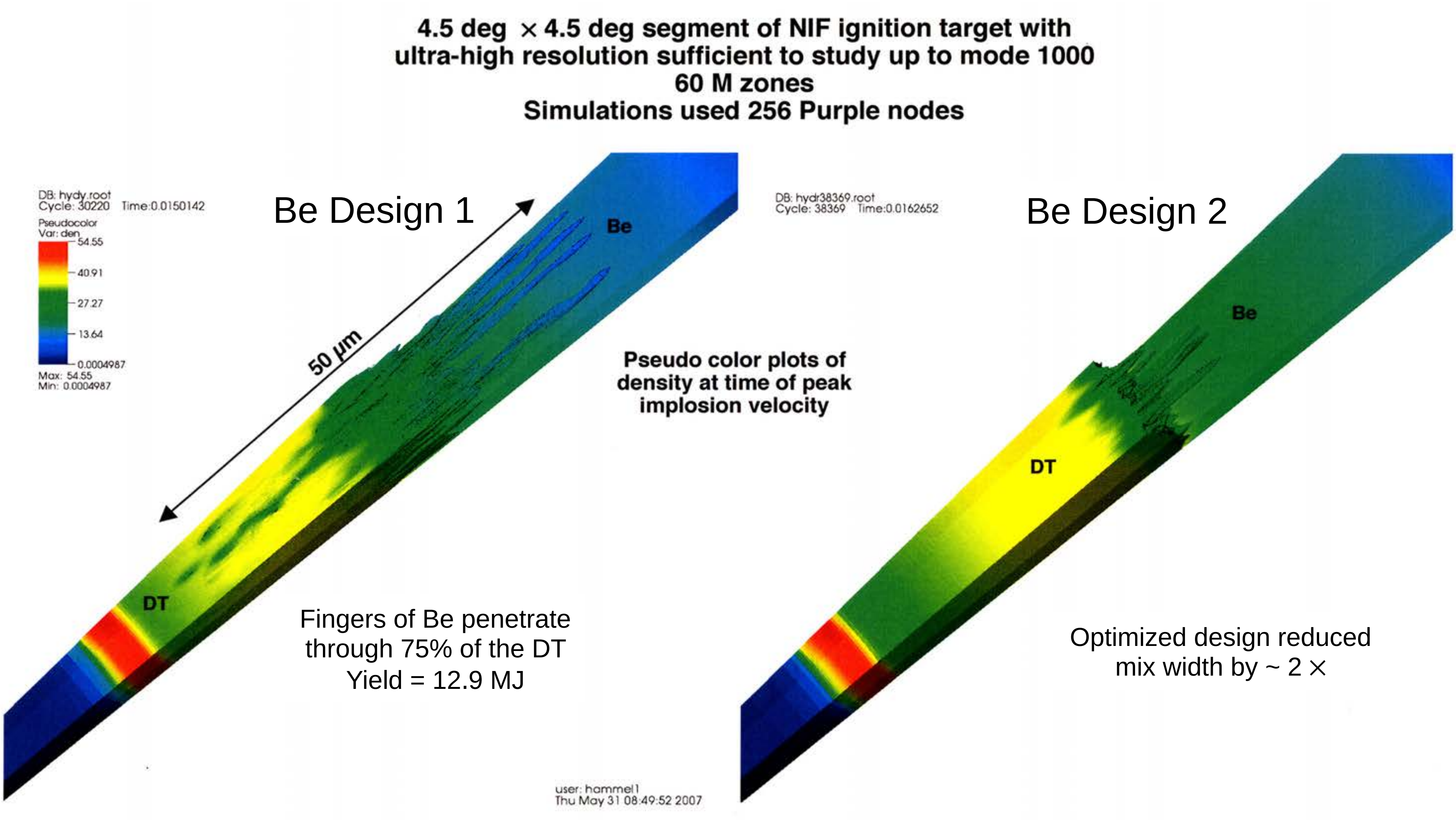
Hydra simulates a wedge of the capsule



- During implosion:
  - -- perturbations due to surface roughness grow at the interface
  - -- may become large enough to reduce fusion yield if not controlled

Macroscale simulations of hydrodynamic instabilities are another important multi-scale ingredient for the ignition campaign

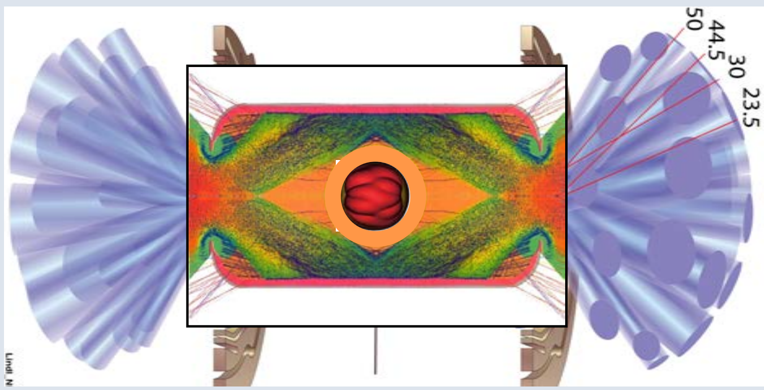
Design optimization reduces high mode growth, as verified with 3D simulations*



*simulations performed by B. A. Hammel, AX Division, WCI

At ~ 10 petaflop-days, we can begin to integrate mesoscale and macroscale physics

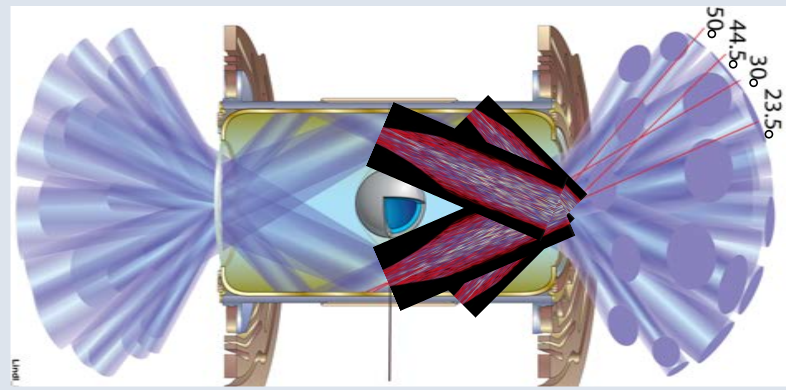
Ignition / Uses of Ignition



- resolve radiation flux asymmetry simultaneously with intermediate-mode hydrodynamic instabilities (up to ~ mode 100)

15 - 30 petaflop-days

Ignition / Uses of Ignition



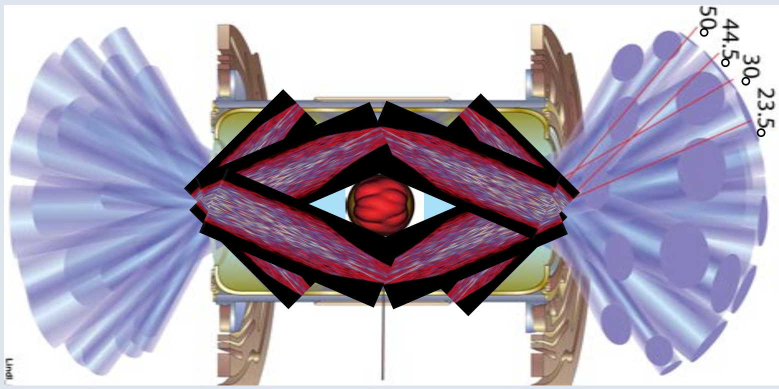
- 4 “letterbox” pF3D simulations (1/cone)
- 5 different time slices circa peak power
- feedback to rad-hydro simulations

6 - 12 petaflop-days

Full integration requires in excess of 1000’s of exaflop-days

At ~ 1 exaflop-day and beyond, we can integrate macroscale, mesoscale and microscale physics

Uses of Ignition



3D integrated macro-microscale simulations:
hohlraum, beams, capsule:

Dodge Viper Version:
~ 2 exaflop-days

Porsche Version:
~ 8,000 exaflop-days

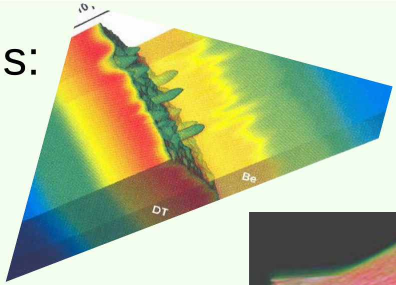
- Uses of ignition:
  - -- operate where nonlinear LPI matters
  - -- integration of macro- to micro-scale is key
- Viper Version:
  - -- rad-hydro simulations, hi-rez capsule
  - -- multi-quad beam propagation simulations at a few times
  - -- multiple PIC simulations at a few times
- Porsche Version:
  - -- rad-hydro simulations, hi-rez capsule, enhanced physics
  - -- many multi-quad beam propagation simulations with enhanced physics at many times
  - -- many PIC simulations at many times

Integrating macroscale to microscale physics enlarges NIF operations parameter space

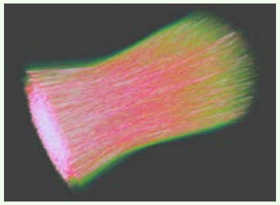
Simulation of multi-scale phenomena is a true challenge for HED physics

TODAY

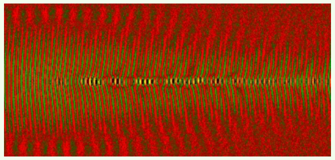
- High-resolution radiation-hydrodynamics simulations:
  -- continue to optimize capsule implosion stability



- Laser beam propagation simulations:
  -- guide focal spot size decisions for NIF beams
  -- guide ignition design optimization

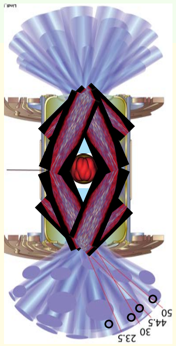


- Micro-scale kinetic simulations:
  -- investigate laser reflectivity saturation



FUTURE

- With a larger number of processors:
  -- "more of the problem" at high resolution
  -- simulations with higher fidelity physics
  -- integration of today's capabilities



2019 Uses of Ignition Target:
2 – 8,000 exaflop-days
(Viper vs Porsche version)

How can we best ensure this future vision?


NIC