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Lawrence Livermore National Laboratory

Taxonomy: Computational Methods and Challenges in High Energy Density Physics

IPAM Computational Methods in High Energy Density Plasmas Tutorials

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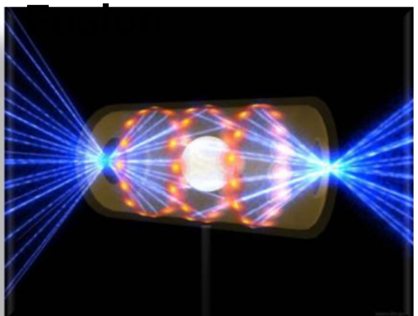
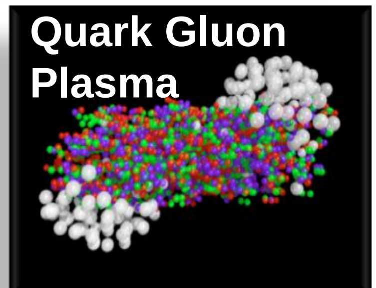
Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

The National Academy of Science report called the frontiers in High Energy Density Physics the X-Games of contemporary science

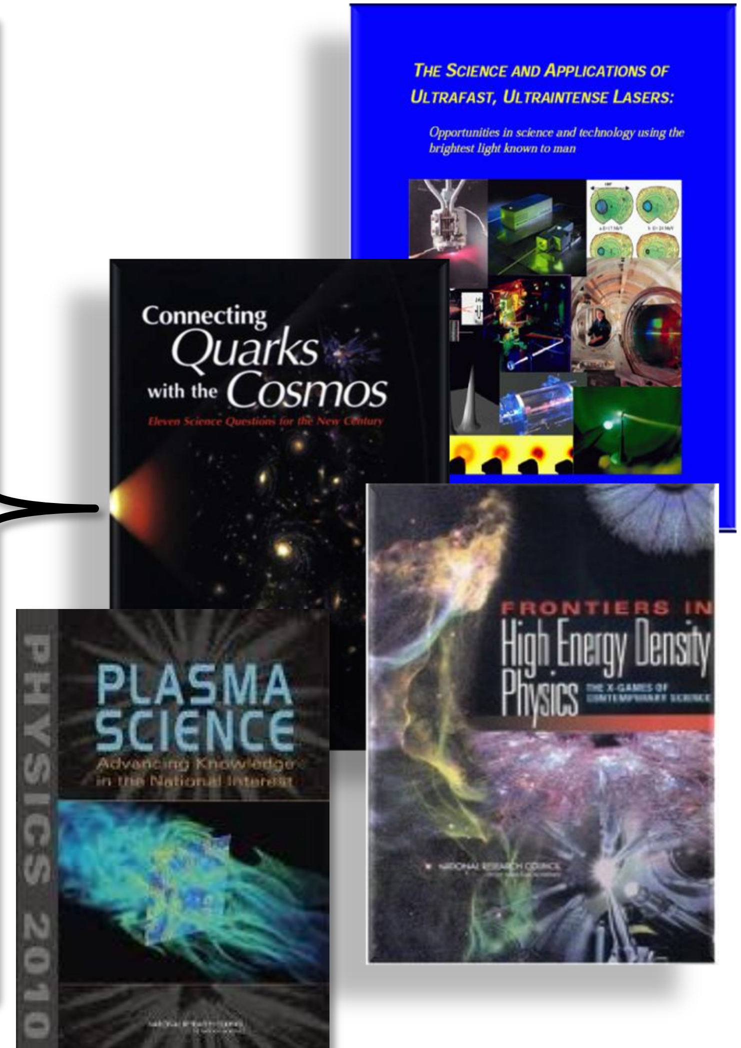
Inertial Confinement



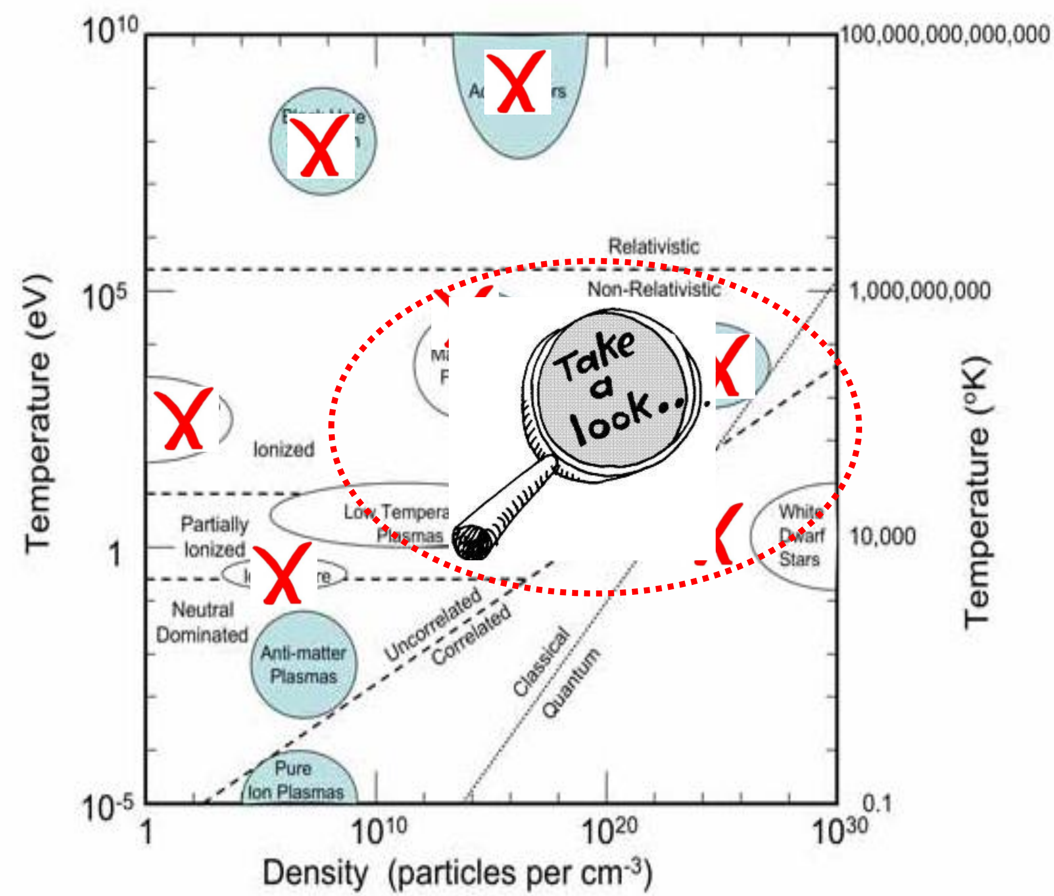
Astrophysics



Magnetic Fusion

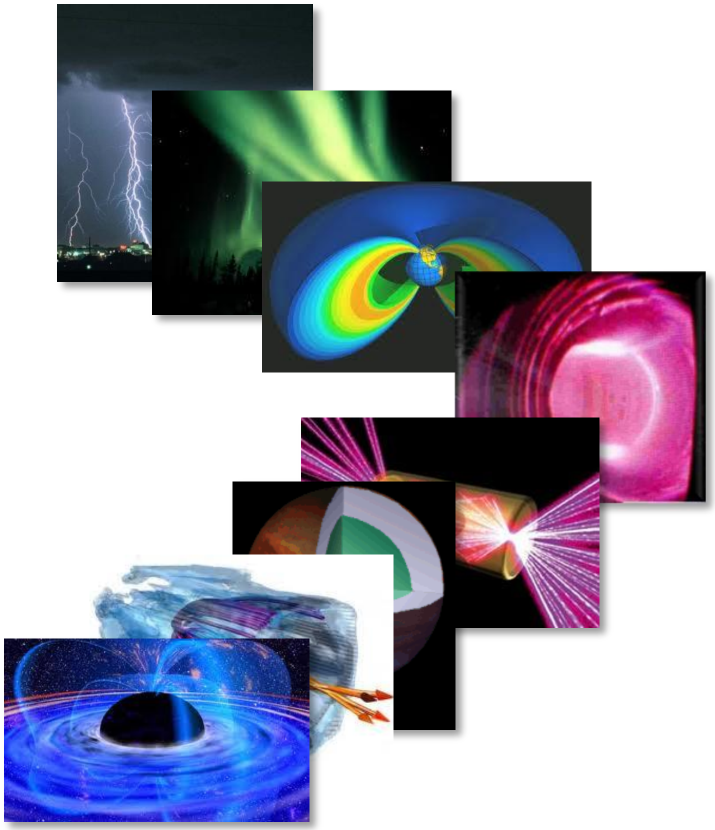


Plasmas consist of mobile charged particles (ions, electrons,..) interacting by long-range Coulombic N-body forces



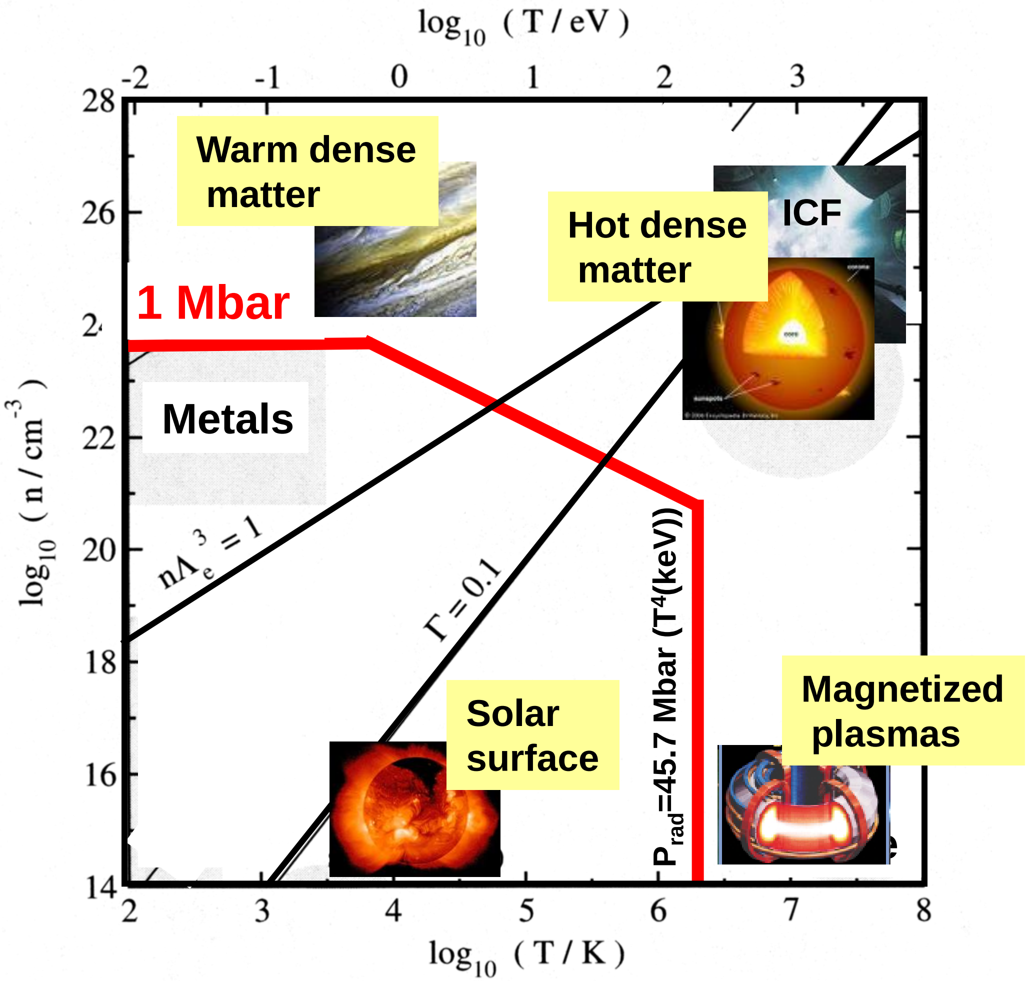
Our understanding of plasma behavior in each of these regimes differs widely

Matter in the plasma state exists in an unimaginable variety



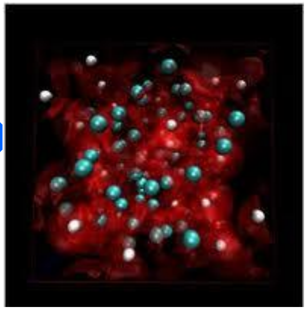
$$1\,\text{eV} = 1.16\times10^{4}\ \text{K}$$

Matter under high energy density conditions, 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**

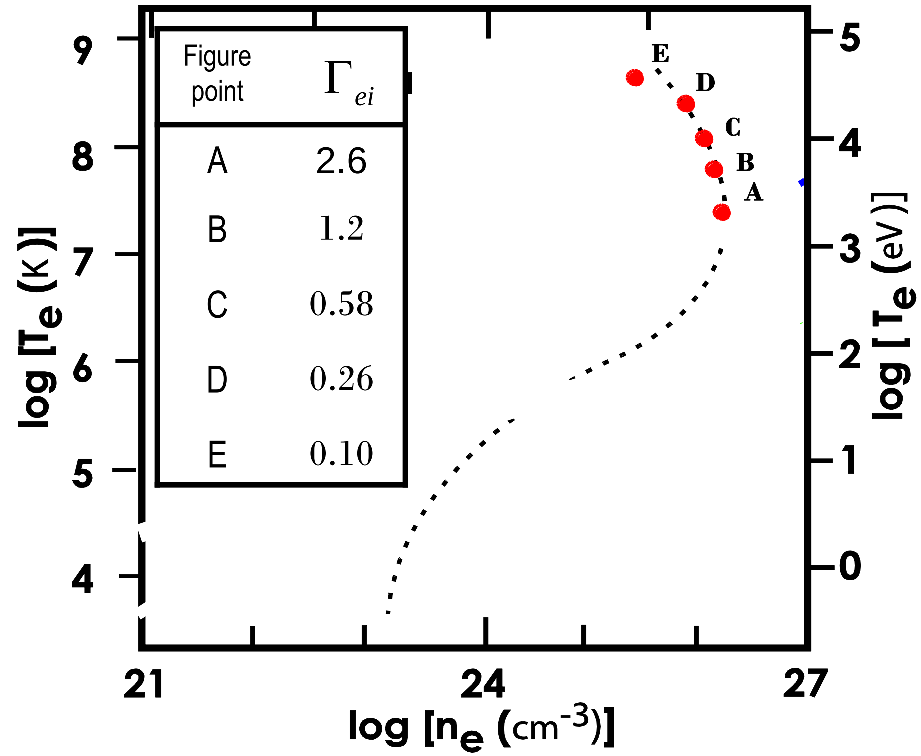
An ICF example: Spanning strongly coupled (large particle-particle correlations) to weakly coupled (Brownian motion like) regimes

Weakly coupled plasma: $\Gamma << 1$

- Collisions are long range and many body
- Weak ion-ion and electron-ion correlations
- Debye sphere is densely populated
- Kinetics is the result of the cumulative effect of many small angle weak collisions
- Theory is well developed $1/n\lambda_D^3 << 1$

Strongly coupled plasma: $\Gamma \geq 1$

- Large ion-ion and electron-ion correlations
- Particle motions are strongly influenced by nearest neighbor interactions
- Debye sphere is sparsely populated
- Large angle scattering as the result of a single encounter becomes important



density-temperature trajectory of the DT gas in an ICF capsule

HED plasmas of interest to this Long Program span a wide range of quantum/classical behavior, coupling and degeneracy

Debye length

$$\frac{1}{\lambda_D^2} = \frac{4\pi e^2 n_e}{kT_e}$$

Ion sphere radius

$$R_{ion} = \left(\frac{3}{4\pi n}\right)^{1/3}$$

Thermal deBroglie

$$\lambda_e = \sqrt{\frac{2\pi \hbar^2}{m_e kT}}$$

Landau length

$$\lambda_L = \frac{Ze^2}{kT}$$

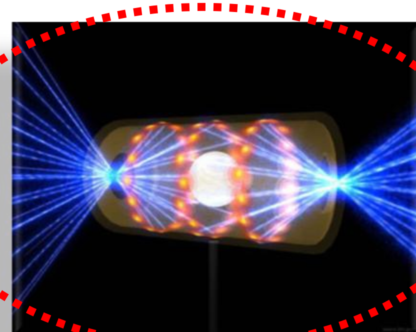
Plasma coupling

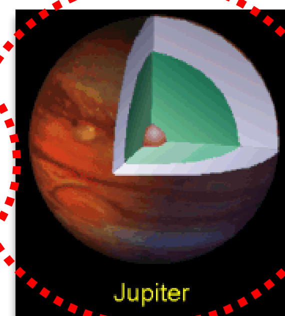
$$\Gamma_{ab} = \frac{Z_a Z_b e^2}{kT}\left(\frac{4\pi n}{3}\right)^{1/3}$$

$$n^{\gamma}_{1/cc} = 3.13\times10^{22} T^3_{keV}$$

$$T_{keV} \approx 2\rho^{1/3}_{gm/cc}$$

$$P^{\gamma}_{Mbar} = 45.7 T^4_{keV}$$





n	T	λ_D	R_{ion}	λ_e	λ_L	Θ	Γ
10^{25}	1keV	7.4×10^{-9}	2.9×10^{-9}	2.2×10^{-9}	1.4×10^{-10}	.17	.05
10^{25}	10eV	7.4×10^{-10}	2.9×10^{-9}	2.2×10^{-8}	1.4×10^{-8}	17	4.8
10^{15}	1 keV	7.4×10^{-4}	6.2×10^{-6}	2.2×10^{-9}	1.4×10^{-10}	3.6×10^{-8}	2.3×10^{-5}

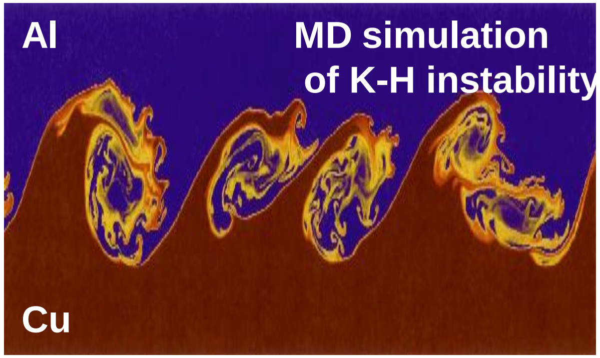
What are the computational and modeling advances needed to address the key questions confronting high energy density plasmas

Multi-scale modeling

Microscopic scale simulations to inform continuum models

A significant but fascinating challenge

On-going effort in material science



Computer hardware and architecture

Algorithmic R&D on efficient uses of new GPU machines

Visualization and data analysis

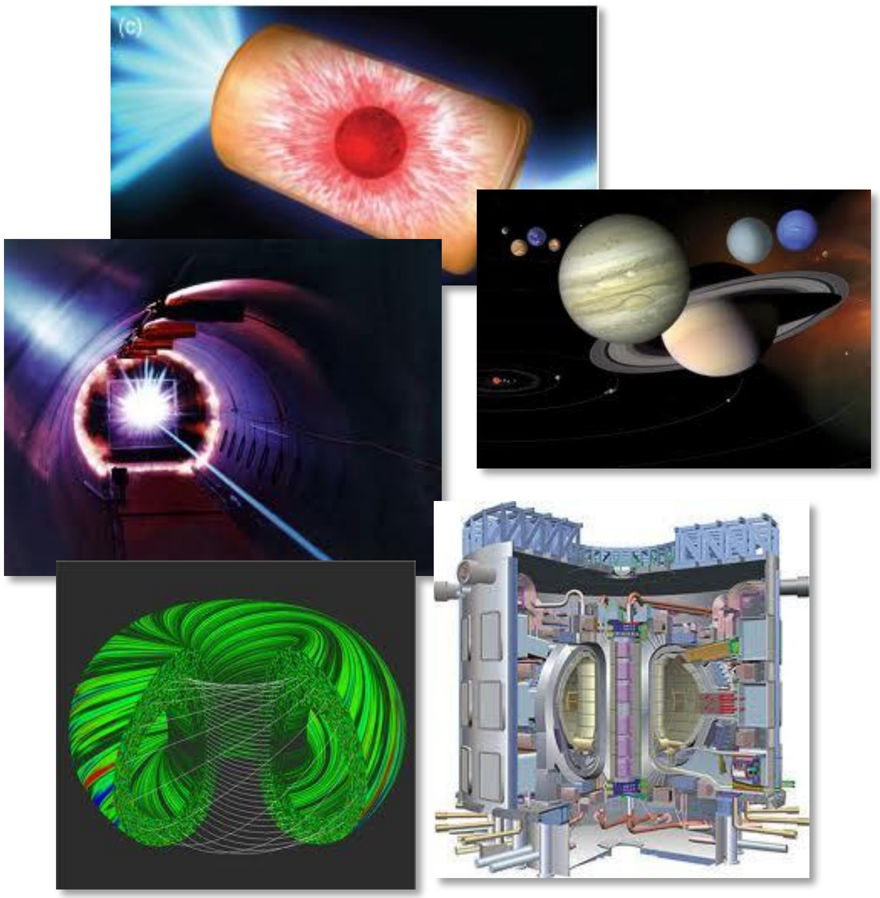
A national user facility for HEDP simulations (MD, QMD, PIMC, PIC, electronic structure)

Verification and validation

Robust V&V program for computational tools

Validation of simulations below the continuum scale

The multi-scale problem: Applications require simulation at the macro-scale but need fundamental physics information from the micro-scale



Fluid Models

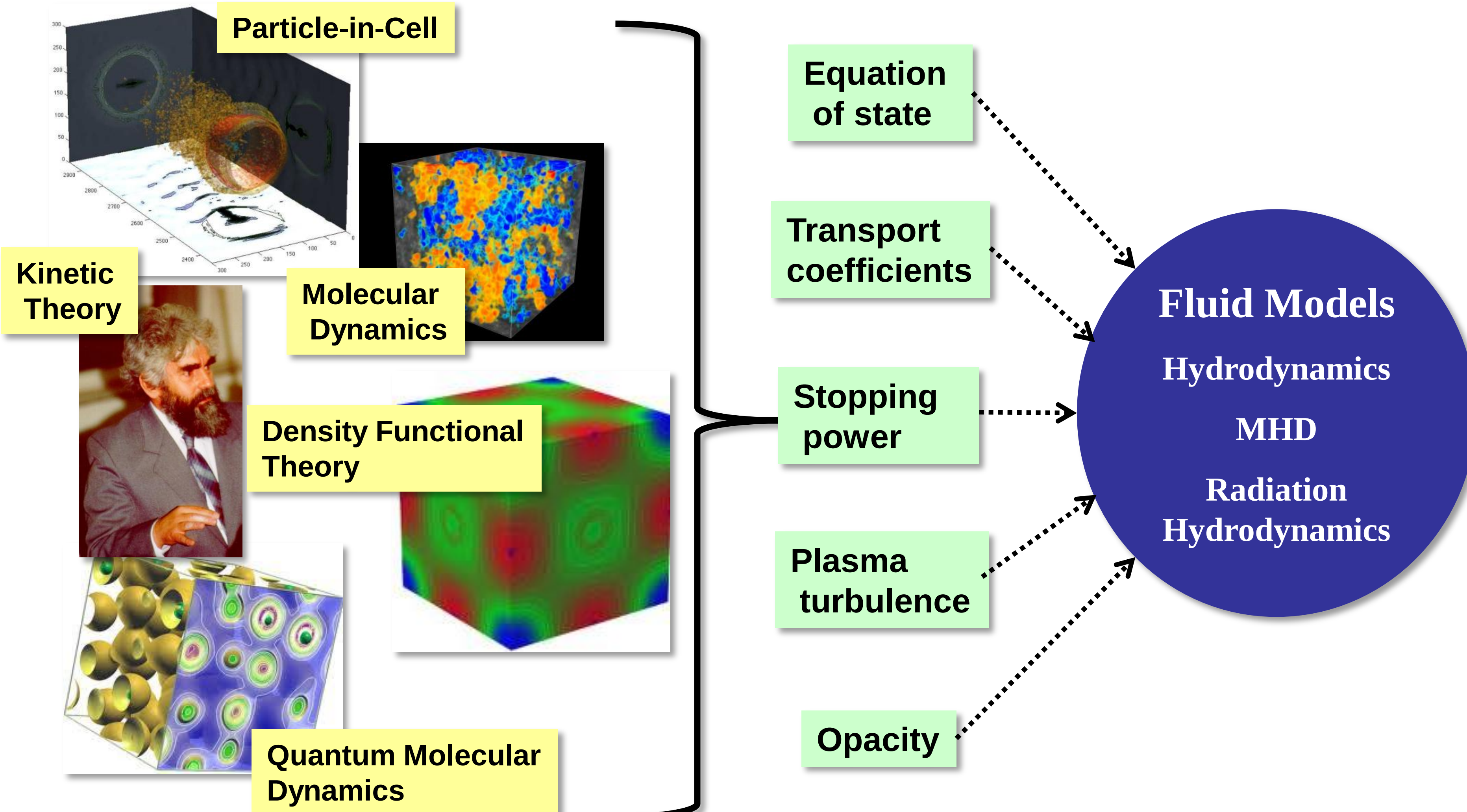
Hydrodynamics

MHD

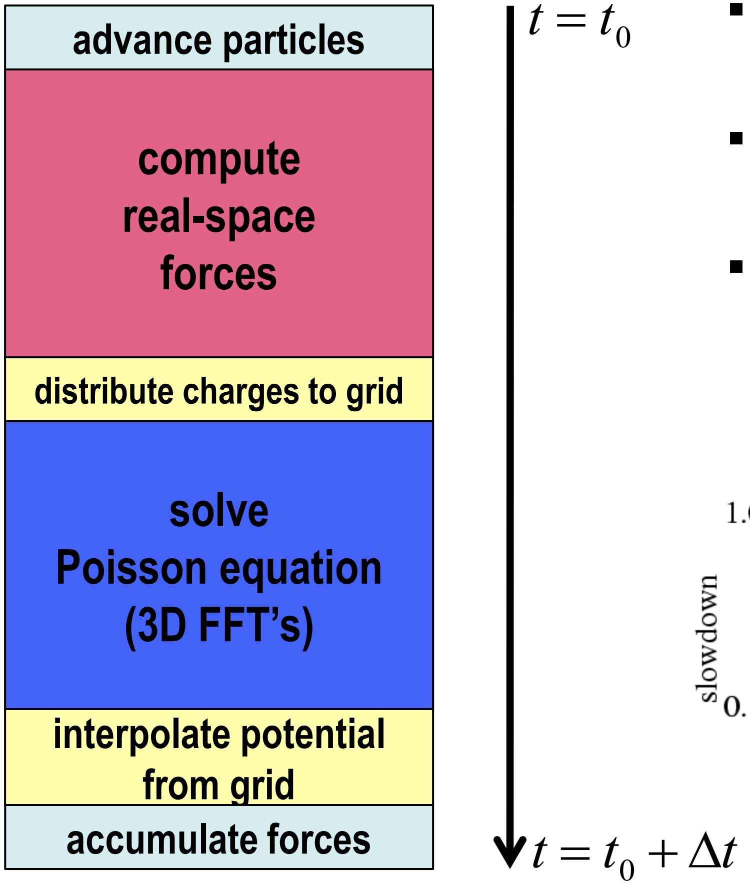
Radiation Hydrodynamics

- Equation of state
- Transport coefficients
- Stopping power
- Plasma turbulence
- opacity

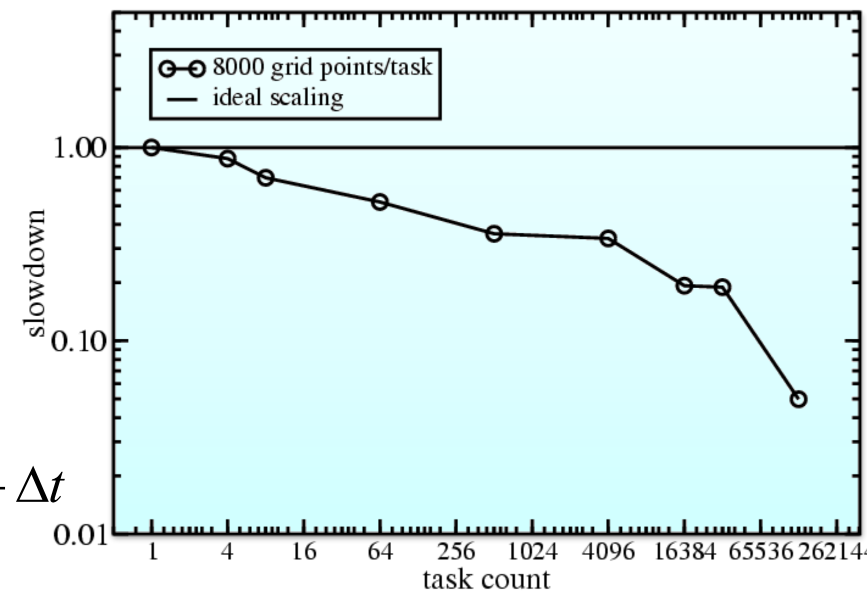
The multi-scale problem: Applications require simulation at the macro-scale but need fundamental physics information from the micro-scale



Traditional PPPM implementation for molecular dynamics is disastrously inefficient at large scale

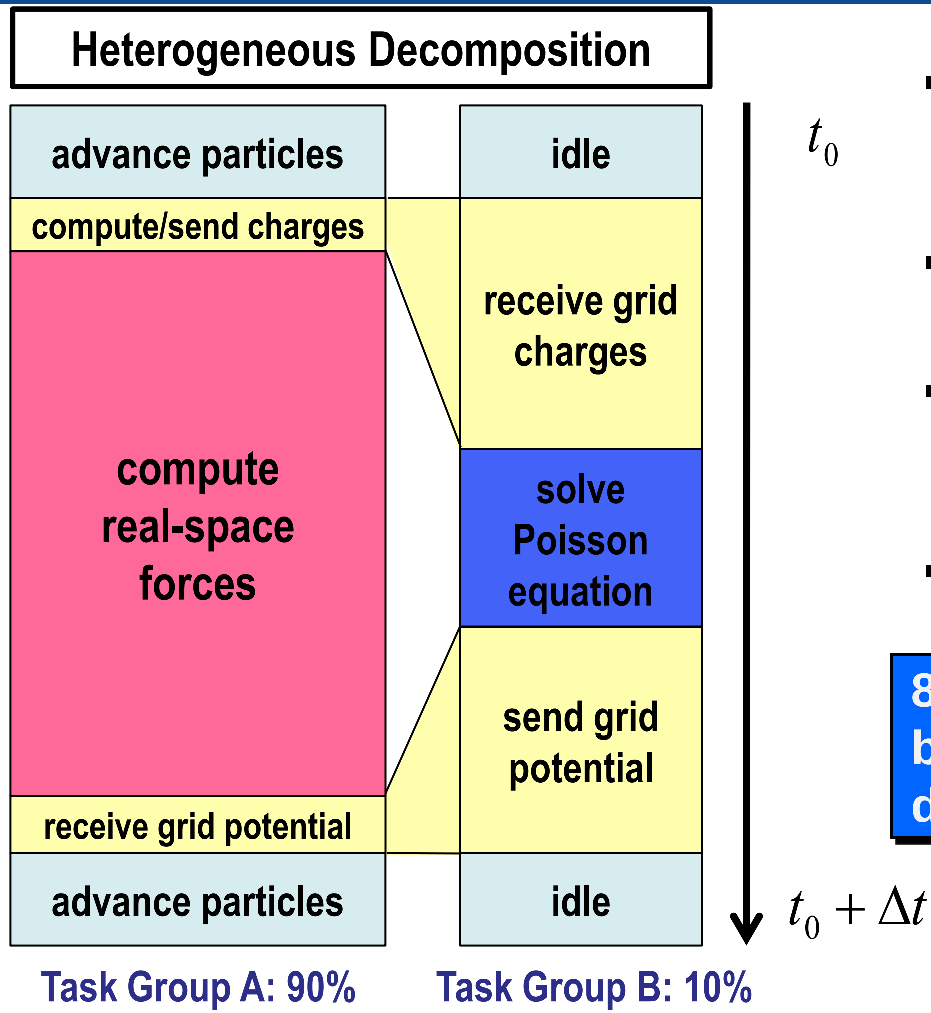


- **All tasks have an equivalent slice of the problem and work synchronously**
- **Width of screening charge balances work between pair and FFT parts**
- **Scaling breaks down due to global communication in 3D FFTs**



This problem appears to be un-scalable

By rethinking the decomposition strategy a scalable algorithm is obtained

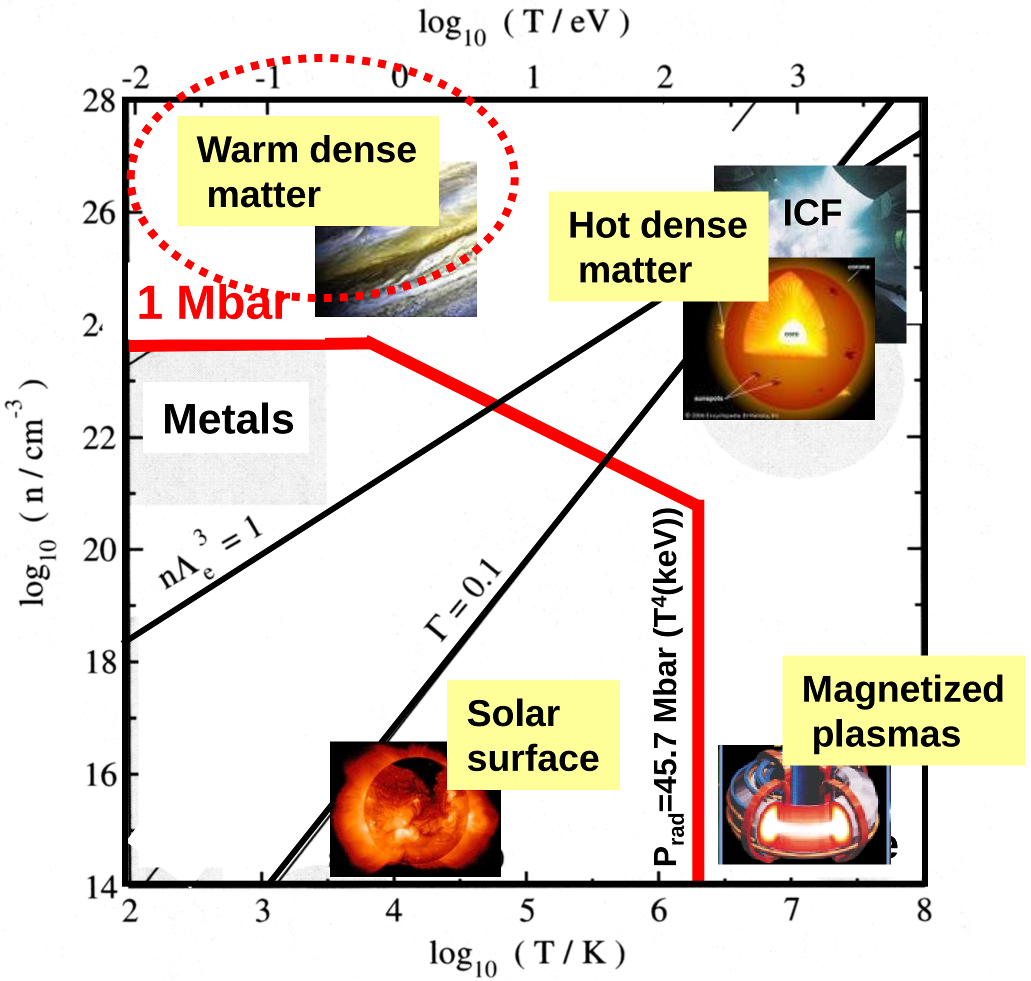


- **Short-range and long-range parts are independent and need not be serialized**
- **No need to distribute problem to all nodes evenly**
- **Applies to more than plasmas: biological, astronomical, and condensed matter systems**
- **Enabling technique for exascale**

80% parallel efficiency on a 2.4-billion particle simulation of a dense hydrogen plasma

Scale algorithms as much as necessary but no more

Why is matter in the high energy density regime so interesting: The warm dense matter regime



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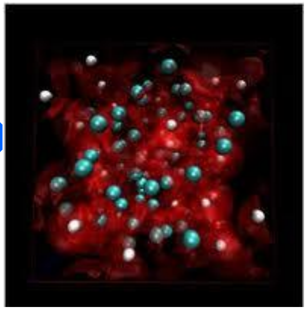
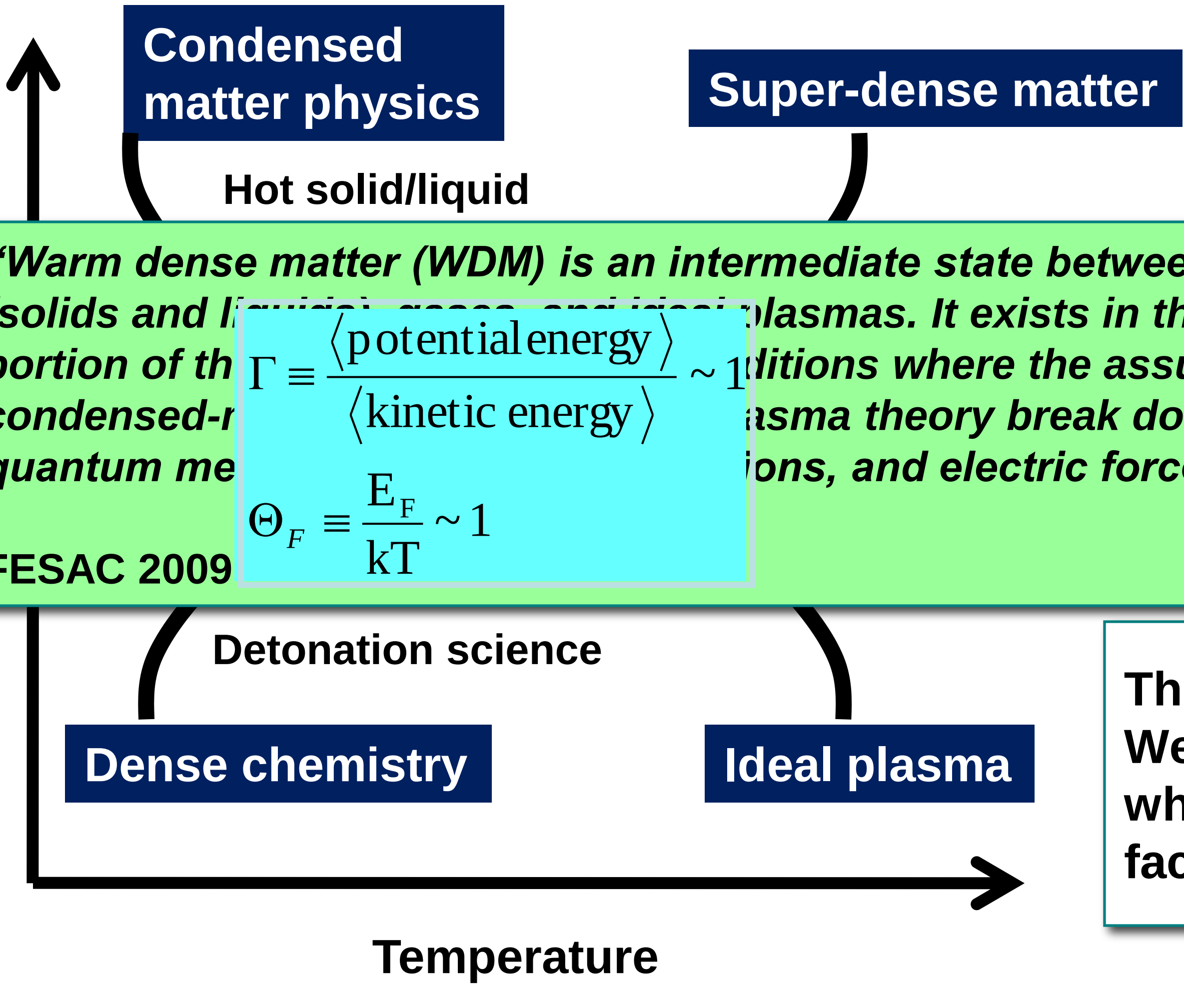


Bulk modulus ~ 1 Mbar

- Radiative processes **NO**
- Strong correlations **YES**
- Multiple species **NO**
- Fermi degeneracy **YES**
- TN burn **NO***
- Atomic processes **NO**

Warm dense matter regime is at the meeting point of several distinct physical regimes- a scientifically rich area of HEDP



"Warm dense matter (WDM) is an intermediate state between condensed matter (solids and l… plasmas. It exists in the lower-temperature portion of th… ditions where the assumptions of both condensed-m… asma theory break down, and where quantum me… ions, and electric forces are all important."

FESAC 2009

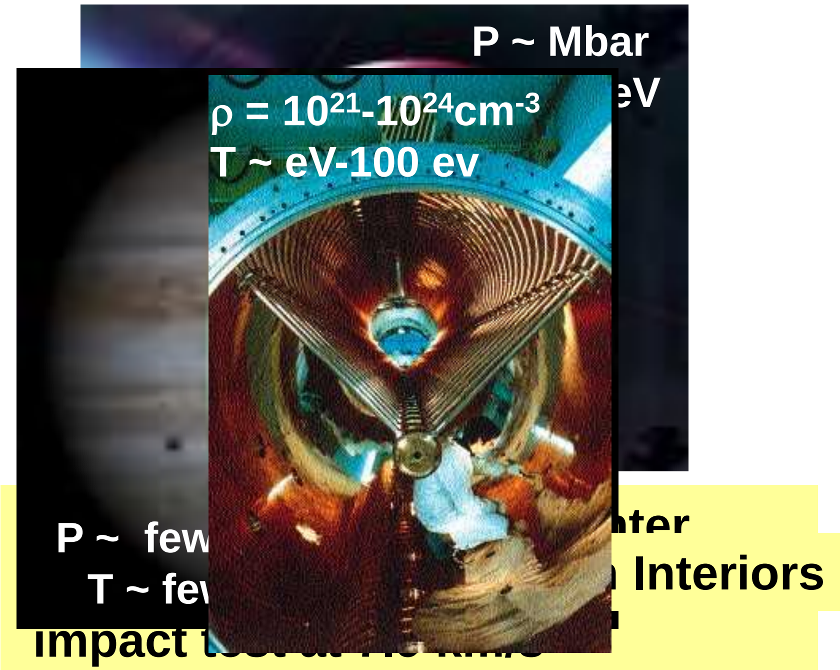
$$\Gamma \equiv \frac{\langle \text{potential energy} \rangle}{\langle \text{kinetic energy} \rangle} \sim 1$$

$$\Theta_F \equiv \frac{E_F}{kT} \sim 1$$

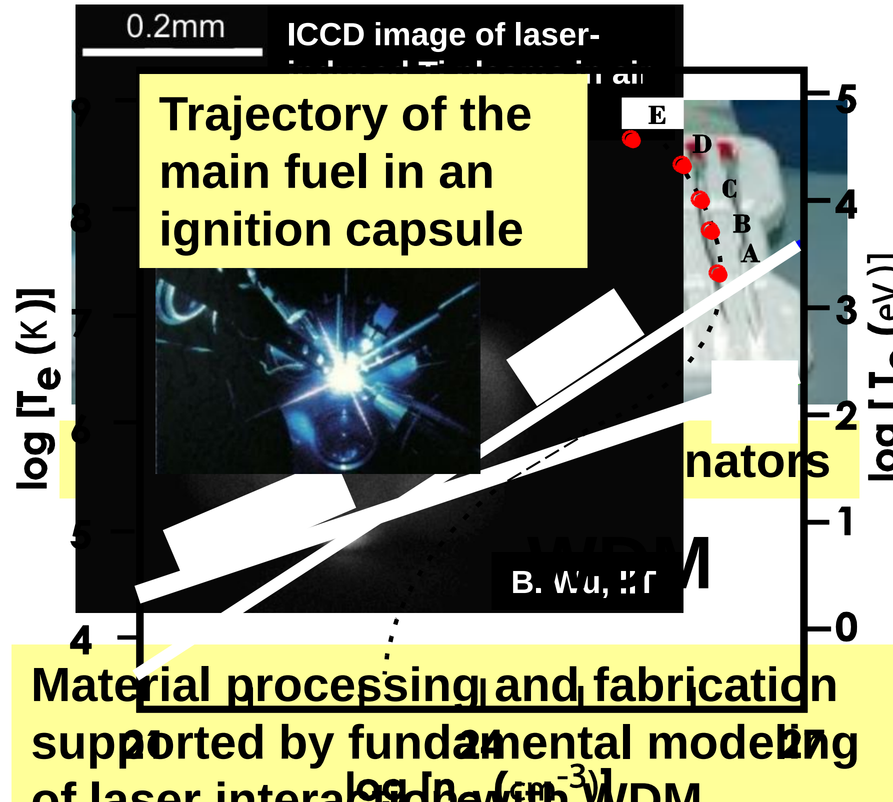
The WDM challenge: Well developed models when extended to WDM face severe problems

Adapted from R. More, WDM School, LBNL, 2008

Substantial progress in these critical areas will impact many customers of WDM research



Heavy ion inertial fusion



Material processing and fabrication supported by fundamental modeling of laser interaction with WDM

A subset of WDM conditions are attainable in the laboratory today

($0.1eV < T < 10eV$ and $0.1\ \rho_0 < \rho_0 < 10\ \rho_0$)

Surprising that many basic science questions are open

What are the major challenges facing each of the critical areas of warm dense matter ?

Phase Transitions in WDM

Melting, liquid-liquid phase transitions, plasma phase transitions

Metal-insulator transition

Equations of state and their dependence on formation history

Computation of EOS without decomposition of ionic and electronic contributions

EOS for mixtures

Transport properties of WDM

Viscosity, diffusivity, electric, ionic and thermal conductivity

Constitutive properties of warm solids

What is a solid at very high pressures?

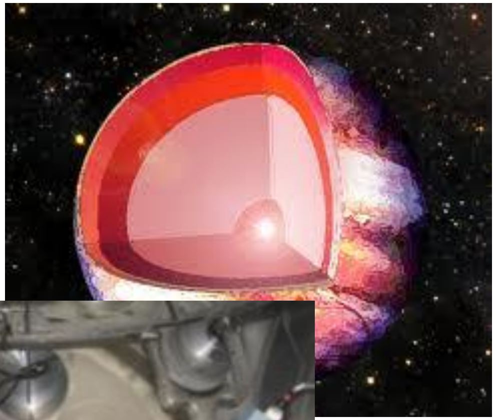
Deformation and dissipation mechanisms (strength)

Comprehensive theory connecting WDM regions

DFT: Orbital-free, exact exchange, going beyond Born-Oppenheimer, high B fields

Particle simulation methods

What are the theoretical and computational advances that enable key questions in WDM to be answered



Orbital free (OF) DFT

Development of OF free-energy functionals

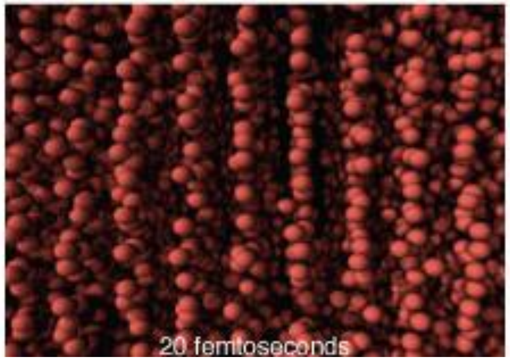
Development of density-based quantum dynamics

Exact exchange (EXX) DFT

Suite of atomic potentials and pseudo-potentials

Develop compatible correlation for EXX

Pursue MD in the EXX framework



Exploration of alternative theoretical approaches

Non-equilibrium statistical operator (Zubarev)

Keldysh formalism and Kadanoff-Baym approach

Particle methods (Molecular dynamics)

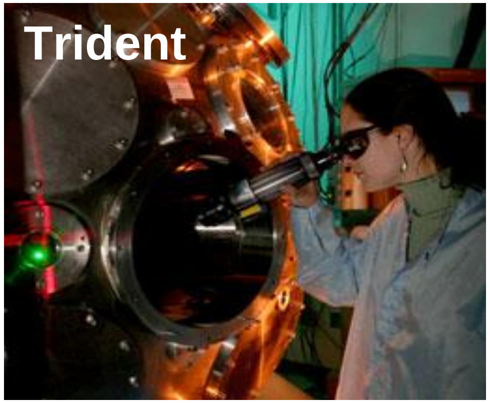
Self-consistent electronic structure MD

Hybrid techniques

What are the experimental advances needed to address the key challenges confronting WDM ?

Small scale laser facilities

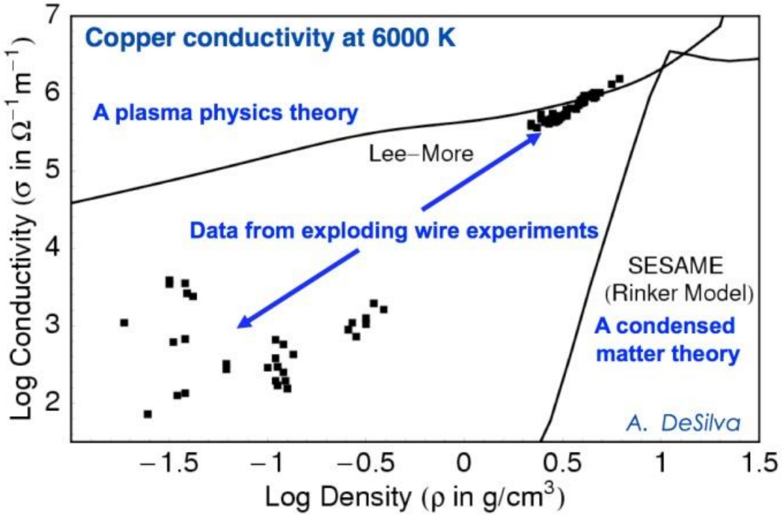
- *Vast majority are well-controlled, intense short pulse laser sources*
- *Provide the training ground for people and proving ground for techniques*
- *Ion stopping in WDM*



Small scale pulsed-power facilities

- *University setting (Cornell, Imperial College, Nevada-Reno, Michigan, UCSD, Texas Tech, Missouri,…)*
- *WDM regime is readily reached*
- *Much-needed data is accessible*
- *Great place to develop/improve diagnostics*
- *Exploding wires for transport and EOS studies, radiographic studies of liquid-vapor region, …*

Small scale , big impact



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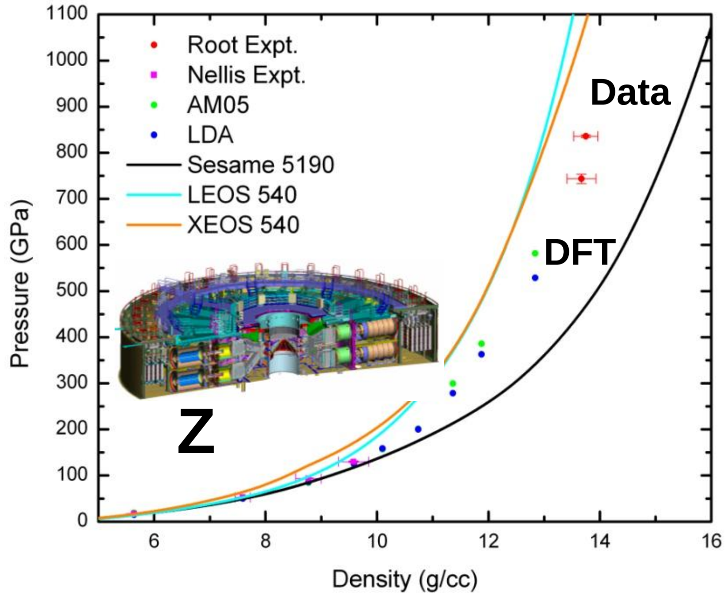


Z

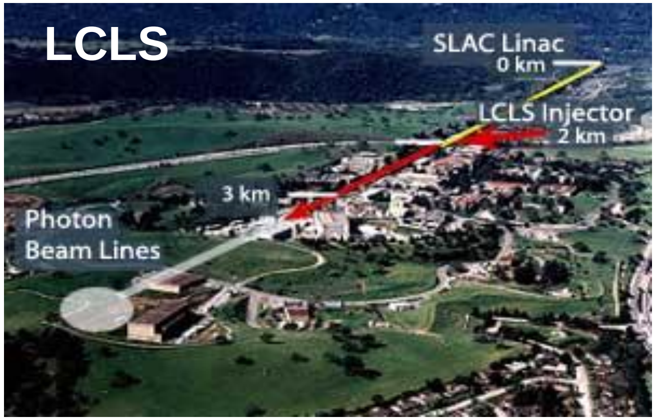
WDM materials platform
Ramp loading up to 5 Mbar,shock loading up to 40 Mbar

Validation quality data in WDM regime

Long time scales and large sample sizes

EOS and optical properties of elements and mixtures in WDM, Strength, Shock and release to WDM states

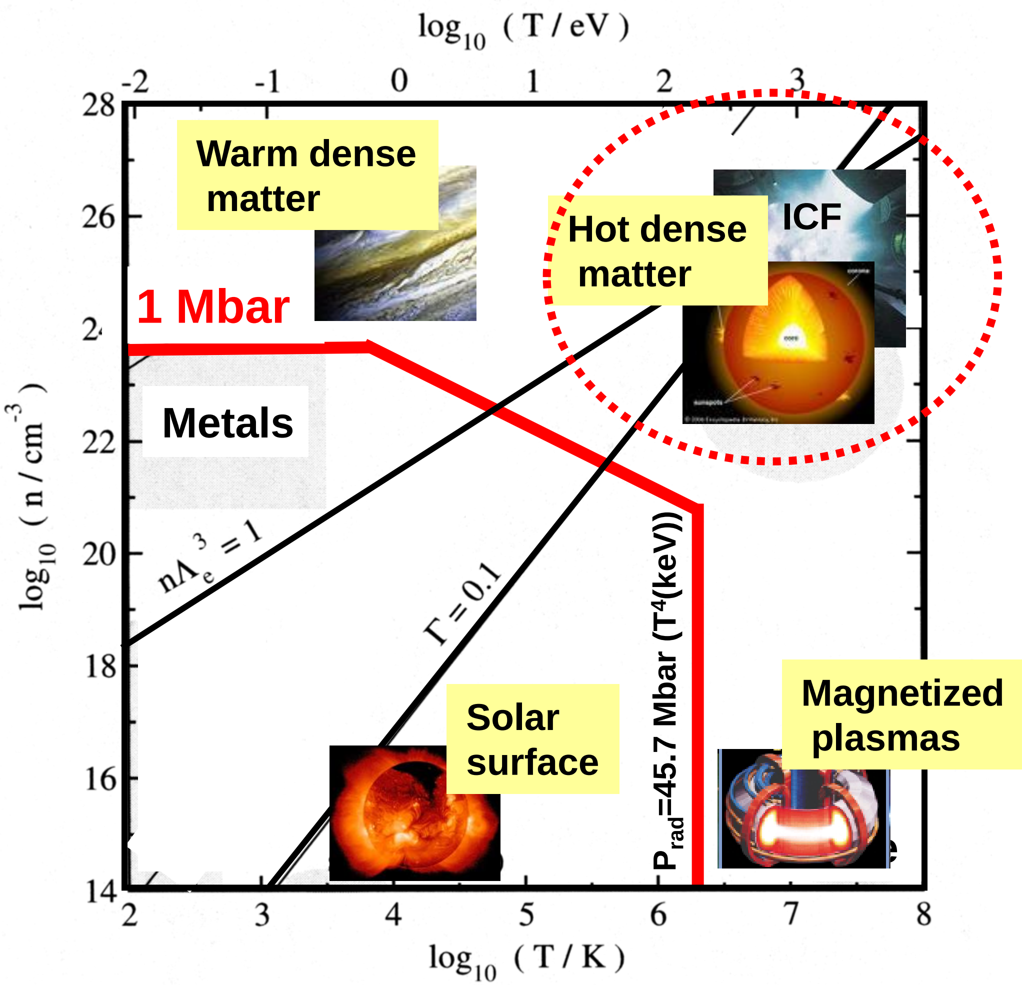
Linac Coherent Light Source



WDM states can be made in a controllable manner
Employs a rapid heating source that creates WDM conditions and measures it prior to disassembly

Dynamic structure factor and electron-ion thermalization- <u>validation data</u>

Why is matter in the high energy density regime so interesting: The hot dense matter regime



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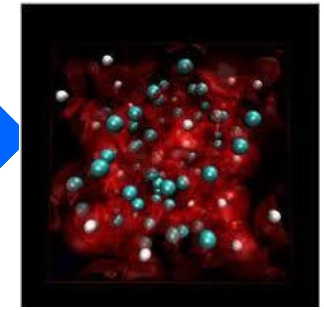


Bulk modulus ~ 1 Mbar

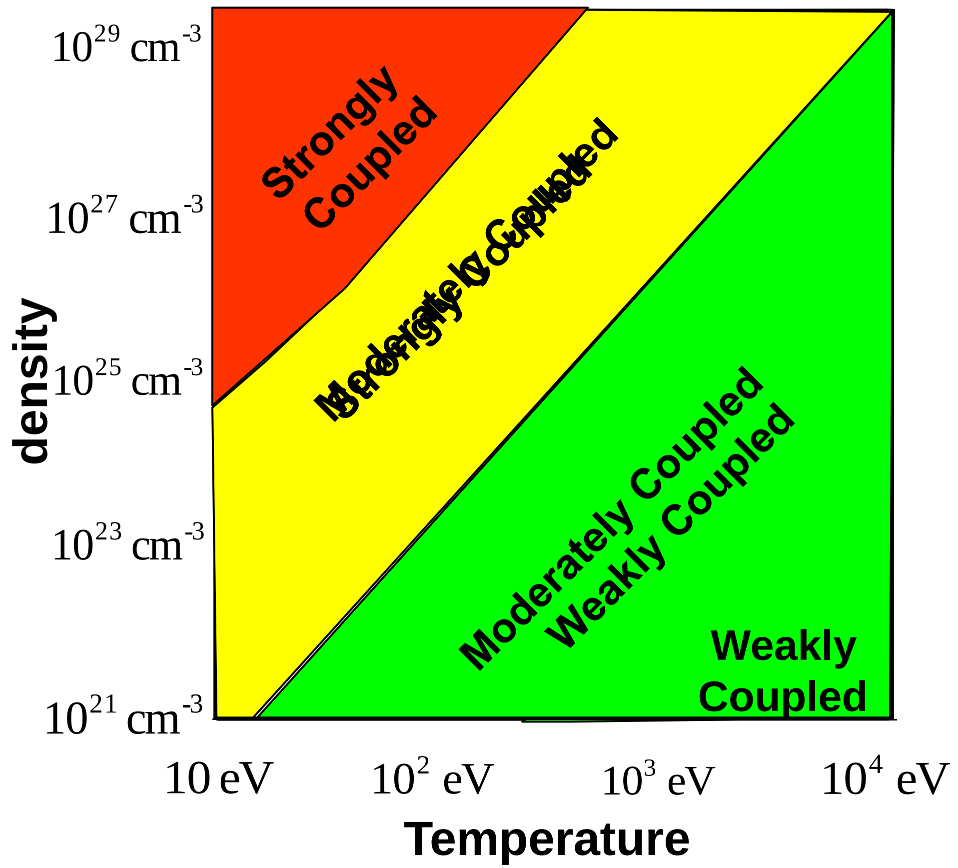
- **Radiative processes** YES
- **Strong correlations** MAYBE
- **Multiple species** YES
- **Fermi degeneracy** NO
- **TN burn** YES
- **Atomic processes** YES

Hot, dense matter is multispecies and involves a variety of radiative, atomic and thermonuclear processes

Characteristics of hot dense radiative plasmas:

- Multi-species
  - Low Z ions (p, D, T, He3..)
  - High Z impurities (C, N, O, Cl, Xe..)
- Radiation field undergoing emission, absorption, and scattering
- Non-equilibrium (multi-temperature)
- Thermonuclear (TN) burn
- Atomic processes
  - Bremsstrahlung, photoionization
  - Electron impact ionization

Hydrogen+3%Au



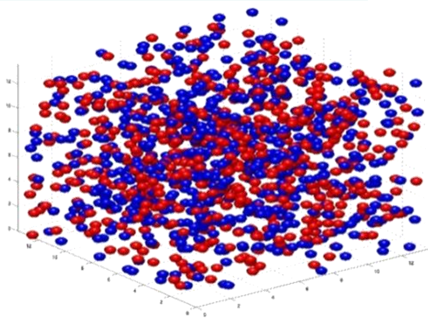
Iso-contours of Γ_{ei}

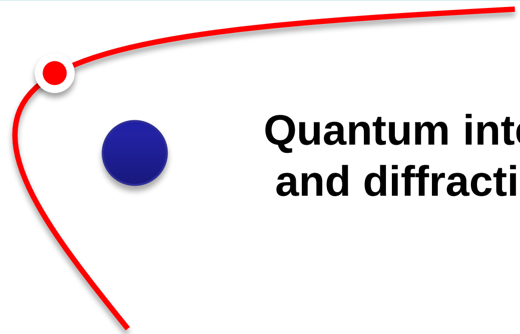
Hot dense matter challenge: Long range collective phenomena are classical while short range collisions can be quantum mechanical

$$\frac{1}{\lambda_D^2} = \frac{4\pi e^2 n_e}{kT_e} + \sum_i \frac{4\pi Z_i^2 e^2 n_i}{kT_i}$$

$$\lambda_e = \sqrt{\frac{2\pi \hbar^2}{m_e kT}} > \lambda_L = \frac{Ze^2}{kT}$$

Debye screening





Quantum interference and diffraction

How do we use a particle based simulation to capture short distance QM effects and long distance classical effects?

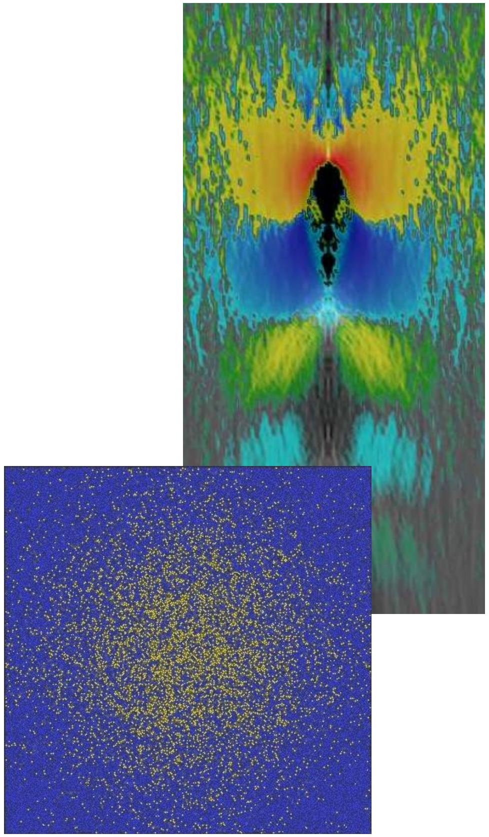
Kinetic equations

- Classical KE with cut-offs
- Quantum kinetic theory

Particle methods

- PIC with specified collision models
- MD with statistical potentials
- MD with momentum dependent potentials
- Wave packet MD
- Kinetic theory MD

What are the major challenges facing each of the critical areas of hot dense matter ?



Thermonuclear burn

Particle spectra (do D and T distributions remain Maxwellian?)
Electron, ion and radiation T(t)
The role of high Z impurities

Equations of state

Thermal conductivity
Species diffusivity

Transport properties of hot dense matter

Thermal conductivity
Species diffusivity
The role of high Z impurities

Momentum and energy exchange rates

Stopping power
Electron ion coupling
The role of high Z impurities

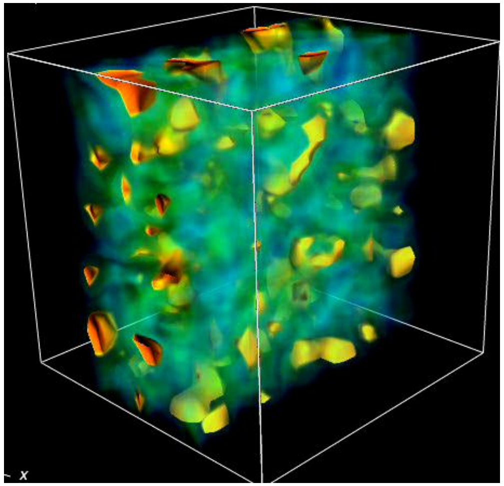
Comprehensive theory describing hot dense matter plasmas with impurities

Strongly coupled high Z component and weakly coupled low Z component

What are the theoretical and computational advances that enable key questions in hot dense matter to be answered

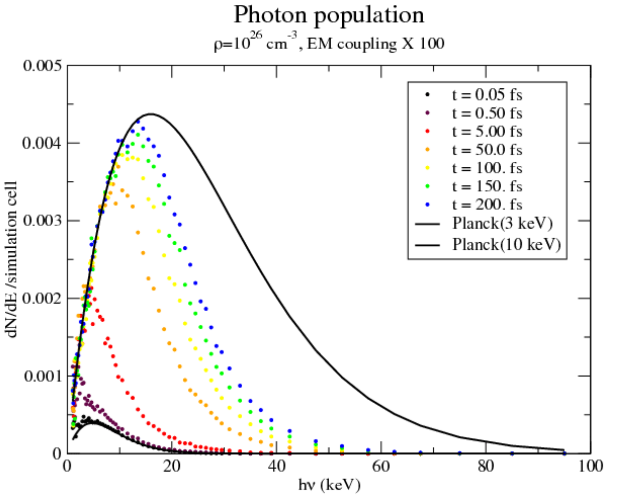
Molecular dynamics

Incorporating quantum effects
Kinetic theory MD
Wave packet MD
Multi-scale simulation
Algorithms for new architectures



Particle-in-Cell

Accurate collision models
Multi-scale simulation
Algorithms for new architectures



Kinetic theory

Plasma mixtures of a weakly coupled low Z component and a strongly coupled high Z impurity

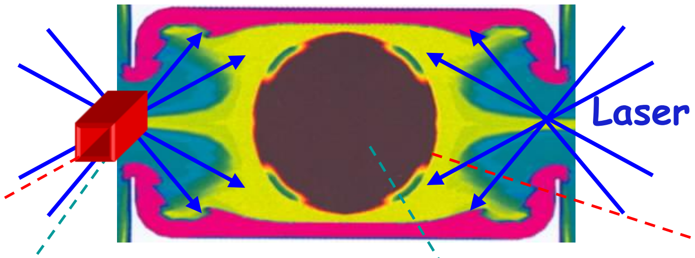
Exploration of alternative computational approaches

Quantum Langevin methods
Wigner trajectories
Quantum hydrodynamics

Ignition targets span a wide range of length and time scales

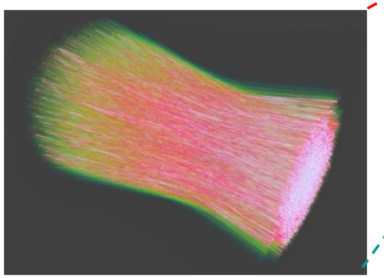
macroscale

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



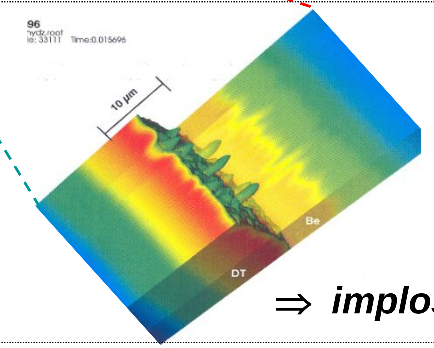
⇒ environment -- plasma parameters and scale lengths

mesoscale



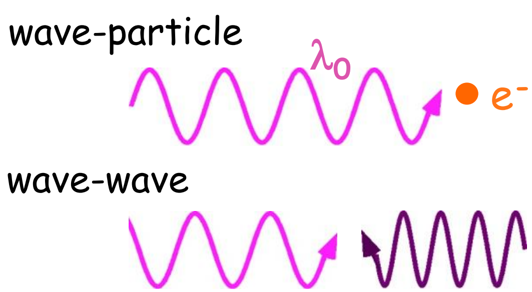
⇒ beam propagation

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



⇒ implosion stability

microscale



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

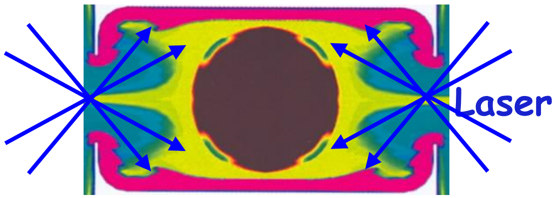
⇒ kinetic effects

Our challenge: incorporate all necessary physics at all relevant length and time scales

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

macroscale

Lasnex/Hydra

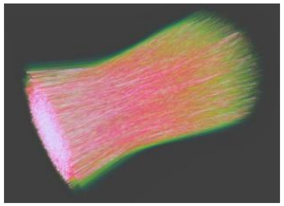


Radiation/Hydrodynamics simulations

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

mesoscale

pF3D

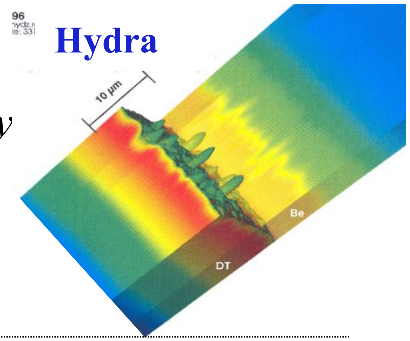


Wave propagation simulations

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

High resolution implosion stability simulations

Hydra

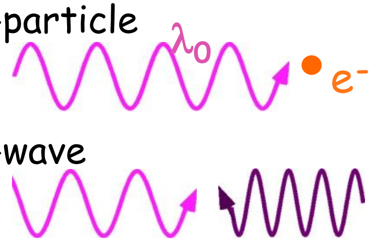


microscale

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

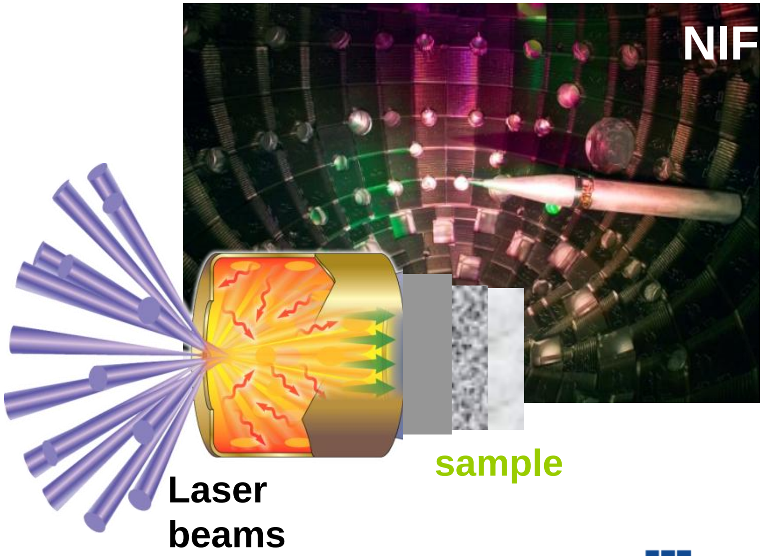
What are the experimental advances needed to address the key challenges confronting hot dense matter?

Omega

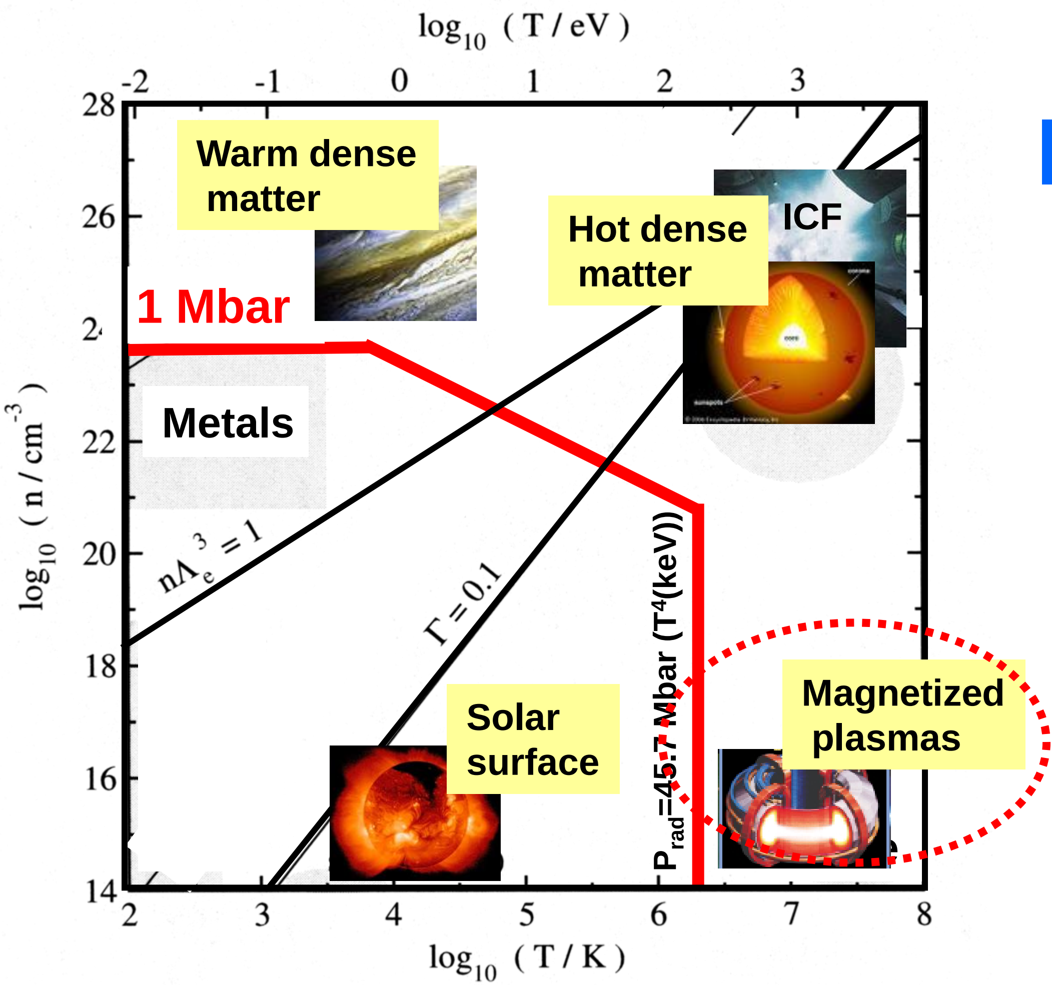
Important HEDP work continues
Diagnostic and target development
Develop time and space resolved spectroscopy techniques
Target design and physics platform

National Ignition Facility

Opens new areas of HED science
100's of Mbar to many Gbars
Key questions NIF can address:
High pressure strength and EOS
Transition from WDM to hot dense matter and what that means
Electron ion coupling
Dense plasma effects on σ
Plasma mixtures

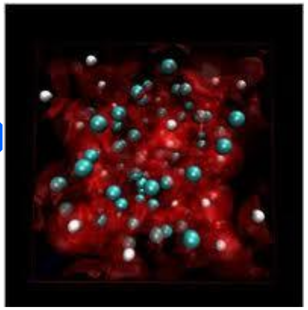


Why is matter in the high energy density regime so interesting: The magnetized plasma regime



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

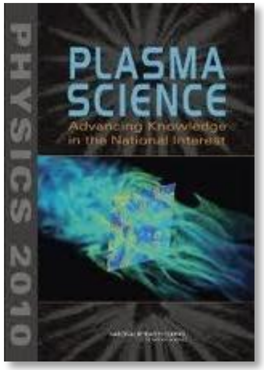
1 Mbar = 10^{12} erg/cm^3



Bulk modulus ~ 1 Mbar

- **Radiative processes** YES
- **Strong correlations** NO
- **Multiple species** NO
- **Fermi degeneracy** NO
- **TN burn** YES
- **Atomic processes** NO

What are the major challenges facing each of the critical areas of magnetized plasmas ?



Macroscopic stability and dynamics

Raising the critical pressure to attain better fusion performance
Developing methods to control the slower instabilities

Cross-field transport from microscopic processes

Understanding and predicting turbulence
Elucidating the transport mechanisms for heat, particles, and momentum
Regimes of low heat loss from the combination of collisional and turbulent processes

Boundary physics

Understanding edge turbulence and transport
Controlling instabilities in the edge
Spreading heat loads over larger areas of material surfaces

Wave-particle interactions

The nonlinear evolution and interaction of multiple unstable modes and their effect on fast particle confinement
Understanding and preventing energetic particle instabilities

What are the theoretical and computational advances that enable key questions in magnetized plasmas to be answered

Macroscopic stability and dynamics

Hybrid MHD modeling that includes very low collisionality kinetic effects
Interaction of the micro-instabilities and turbulence with the macro-instabilities
Interfacing fast timescale micro-turbulence codes with macro-instability codes

Cross-field transport from microscopic processes

Accurate predictive models of turbulence and transport, especially electron dynamics
Better understanding of transport barrier physics
Advance the science of low collisionality plasma turbulence
Turbulence with multiple scales in all dimensions of phase space

Boundary physics

Reduced physics model, derived from first principles, capable of describing the full range of plasma boundary phenomena

Wave-particle interactions

Extend the modeling of launched wave excitation and propagation to 3D
Improved understanding of wave heating and fast-ion transport

What are the experimental advances needed to address the key challenges confronting magnetized plasmas ?

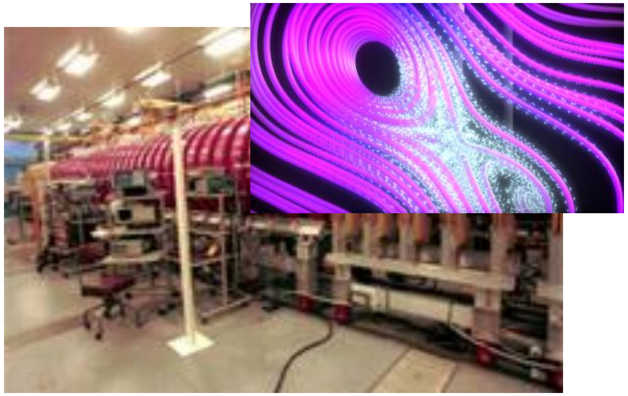
BaPSF

Frontier-level experiments that require physical conditions not suitable for small devices

Heat and particle transport under a wide variety of heating conditions

Electrostatic and electromagnetic turbulence

Behavior of edge plasmas



ITER

Opens new areas of magnetic fusion science

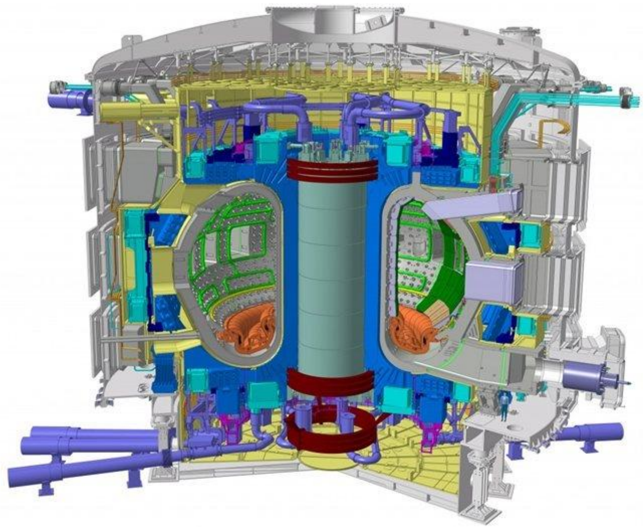
First magnetic fusion device to make substantial levels (< 500 MW) of thermal fusion power for hundreds of secs

Key questions ITER can address:

Experiments explore magnetically confined fusion burning plasmas

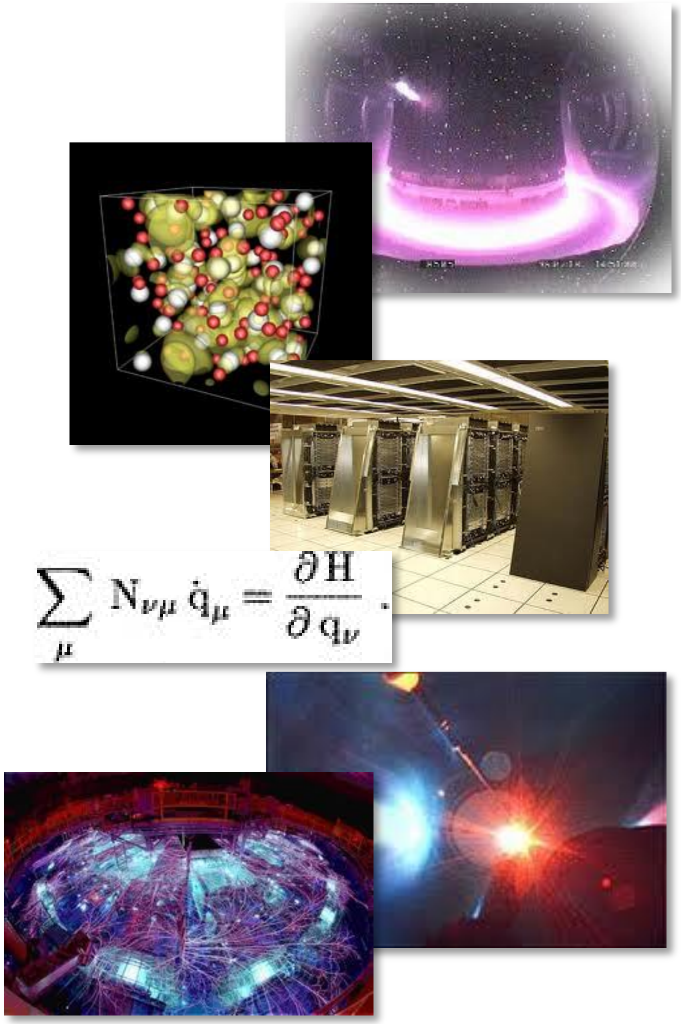
Improvements in diagnostics that reveal global structure and mesoscale correlation

Exploration of energetic particle driven instabilities



The goal of the Long Program is to acquaint you with the physics and computational challenges of HEDP

- What are the challenges facing HEDP ?
- What are the theoretical and computational tools ?
- What are the experiments that are providing key data
  - Integration of application drivers and data with simulation tools (algorithms and hardware)
- Communicate various methods successes and failures



$$\sum_{\mu} N_{\nu\mu}\,\dot{q}_{\mu} = \frac{\partial H}{\partial q_{\nu}}\,.$$