SAND2018-9703PE

Developing Consistent Models for Matter in Extreme Conditions

S. Hansen, T. Nagayama, T. Gomez, A. Baczewski, and A. Cangi

Sandia National Laboratories

New Research Ideas Forum
Sandia National Laboratories (NM)
September 4, 2018

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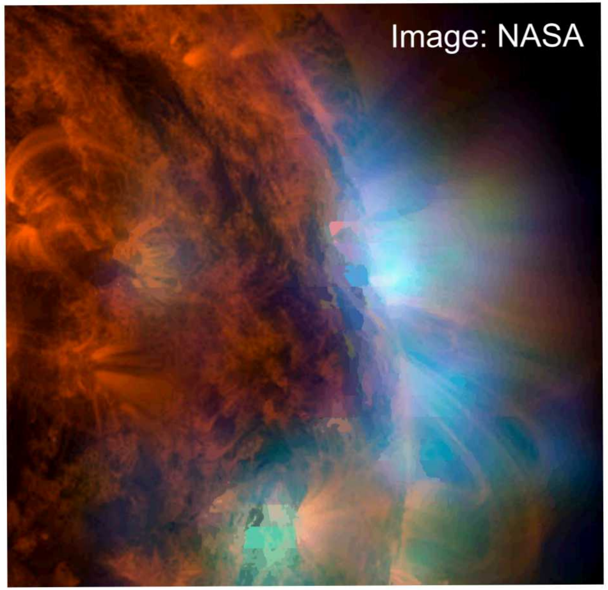
Context: we are interested in matter at extreme conditions relevant to fusion and astrophysical plasmas



10^{+9} meters
10^{+17} seconds

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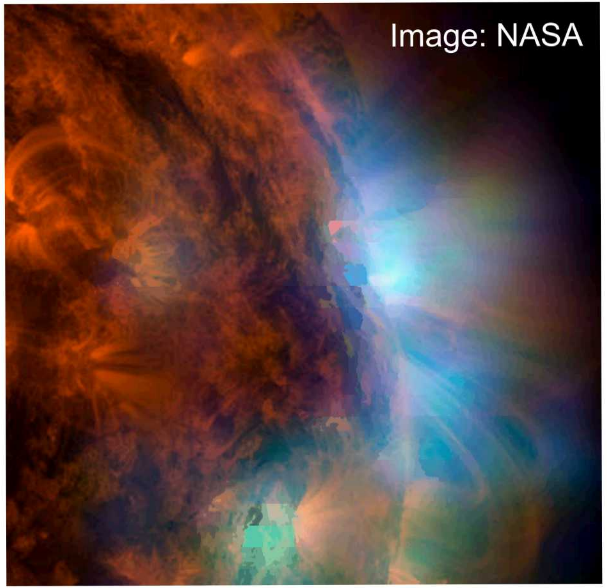

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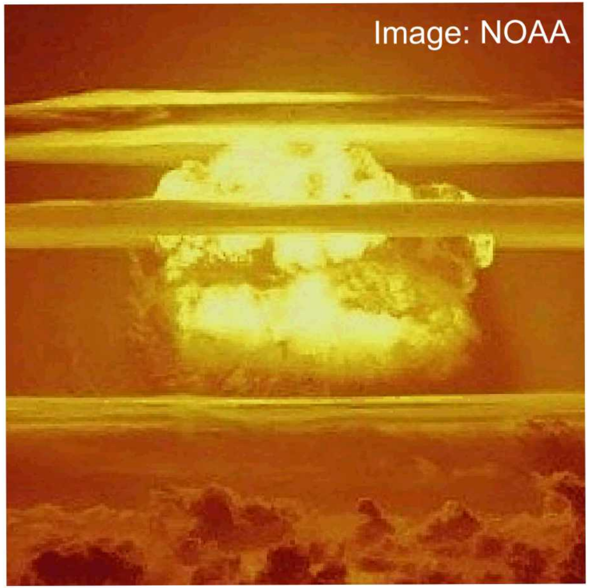

10^{+3} meters
10^{+2} seconds

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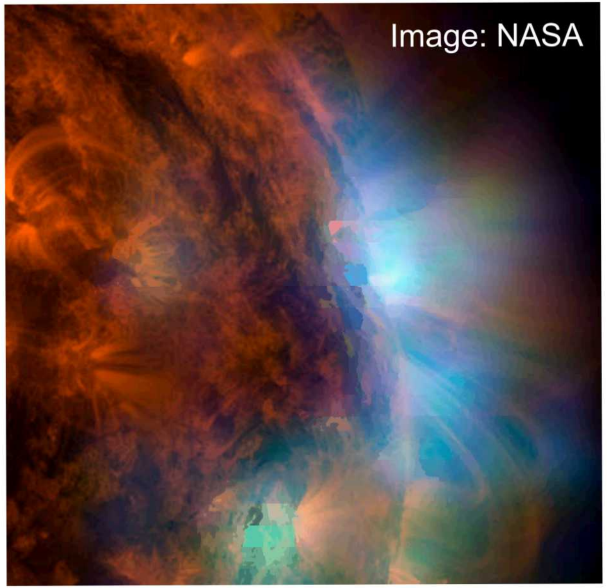

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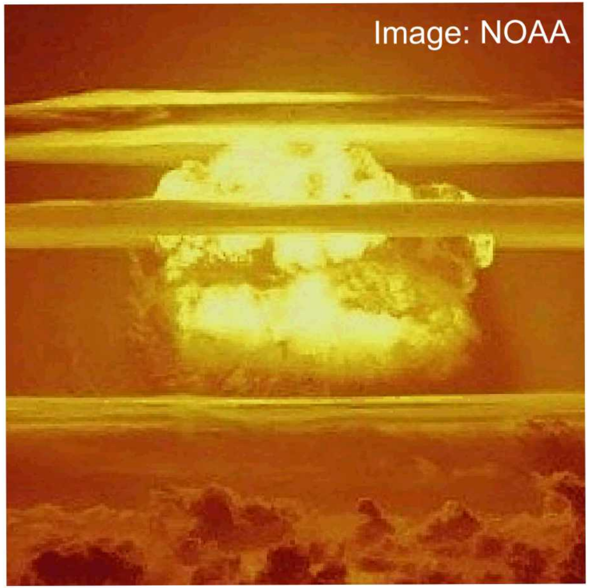

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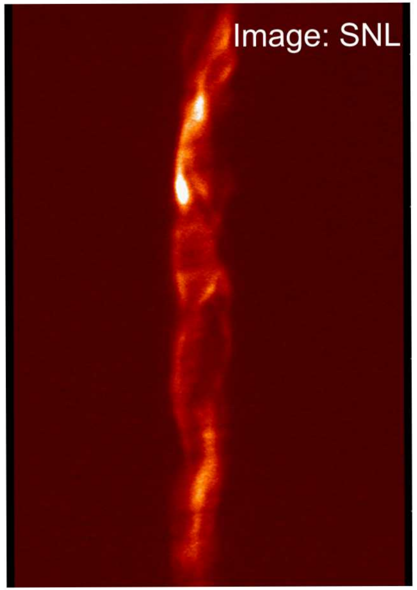

10^{-4} meters
10^{-9} seconds

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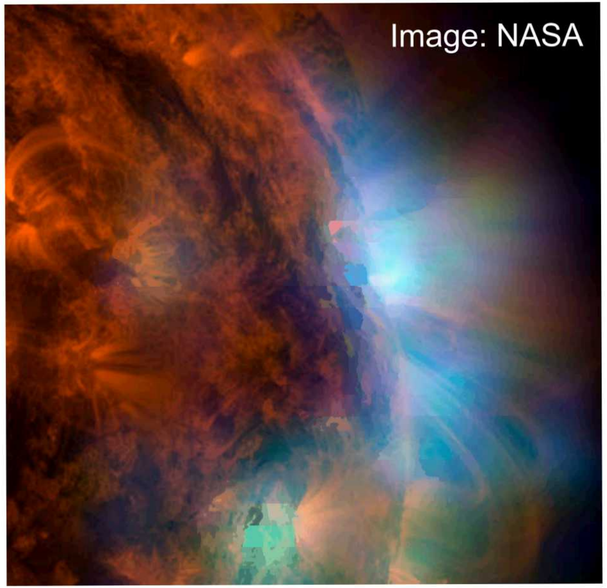

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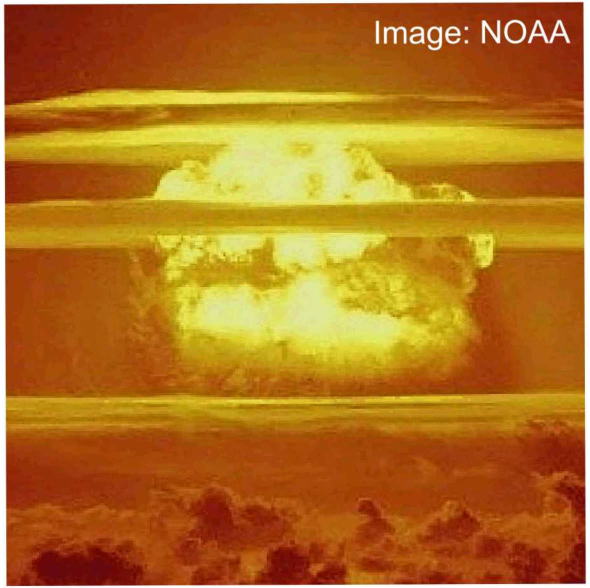

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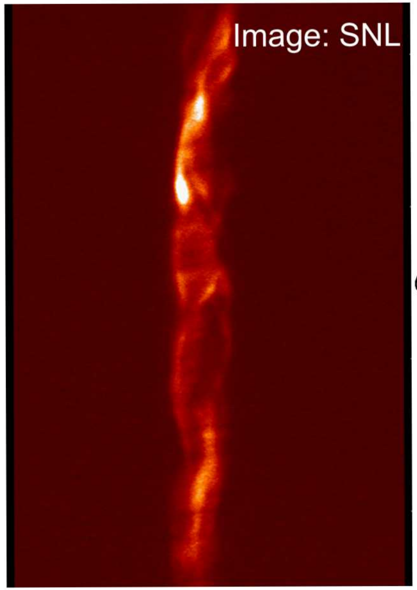
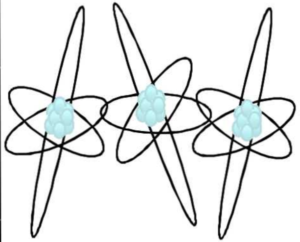


10^{-4} meters
10^{-9} seconds



10^{-10} meters
10^{-14} seconds

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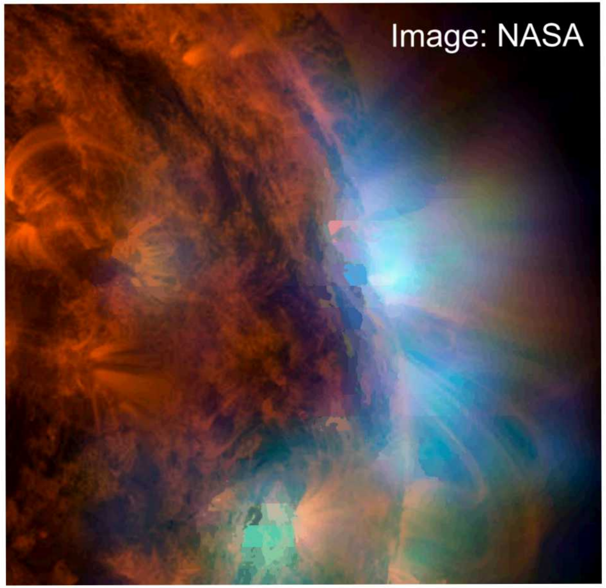

10^{+9} meters
10^{+17} seconds

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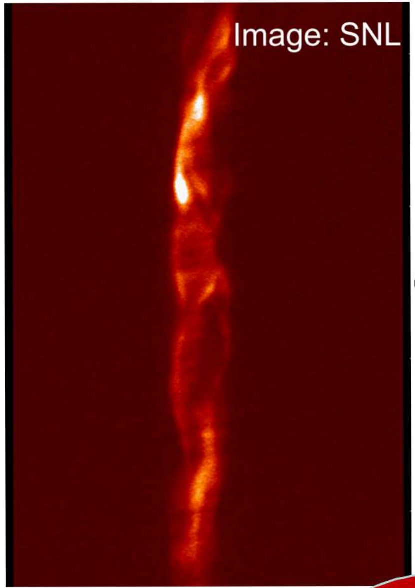
10^{+2} seconds



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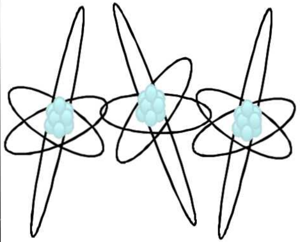
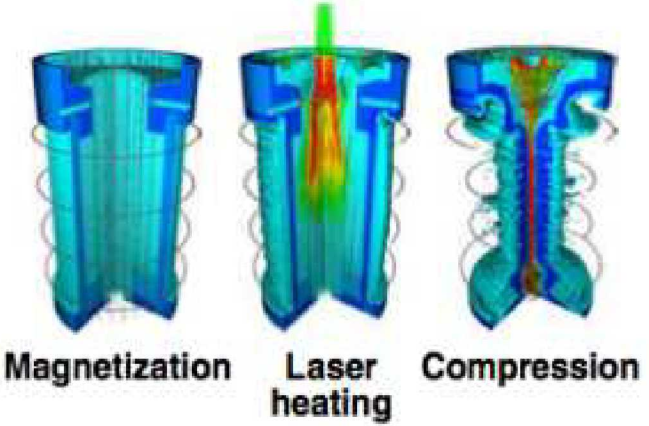
10^{-9} seconds



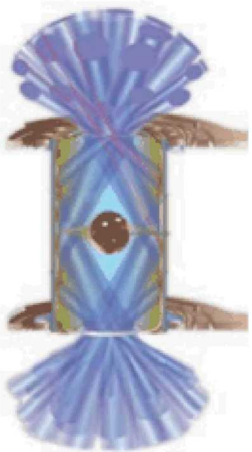
10^{-10} meters
10^{-14} seconds

When we say "high-energy-density", we don't mean gasoline

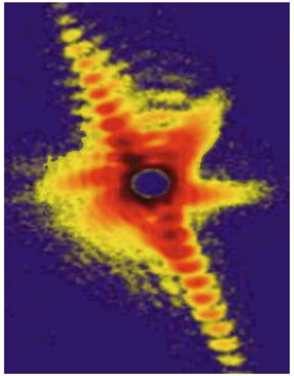
Context: How do we produce extreme conditions in the laboratory?



SNL's Z machine:
10 MJ → 10^{-9}s, 100-1000 μm
0.3 - 3 keV, 0.01 - 1g/cc
Fusion, Opacity, Rad. effects



LLNL's NIF:
2 MJ → 10^{-10}s, 10-100 μm
0.3 - 3 keV, 0.01 - 1g/cc
Fusion, Opacity, Rad. effects

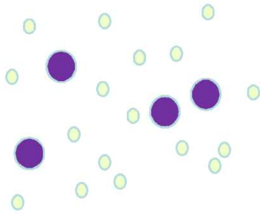


LCLS/ European XFEL:
2 mJ → 10^{-13}s, 1μm
10eV, 1g/cc
Fundamental material

We compress energy in space and time using pulsed power, lasers, or undulators

What’s so difficult about modeling extreme conditions?

- HED plasmas are (usually) not well described by classical plasma models
    - Partial ionization complicates simple ion + electron pictures
    - Degeneracy effects invalidate classical statistics
    - Density effects distort quantum orbitals
    - Ions can be strongly coupled



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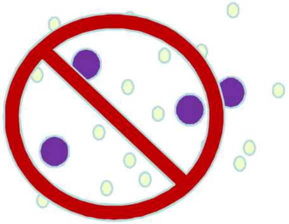
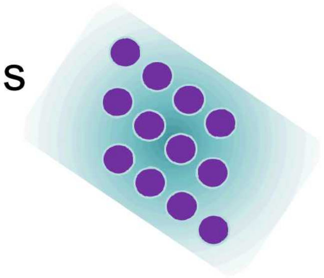


- HED plasmas are (almost) never well described by solid-state models
    - Even modest temperatures can open enormous state space
    - Simplifications of ionic and electronic behavior are suspect



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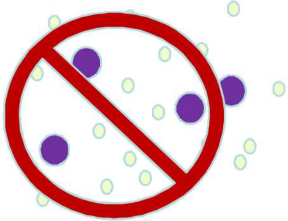

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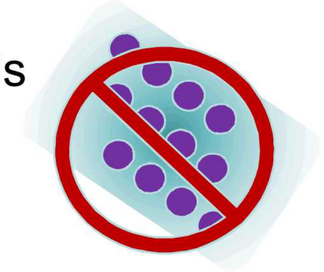
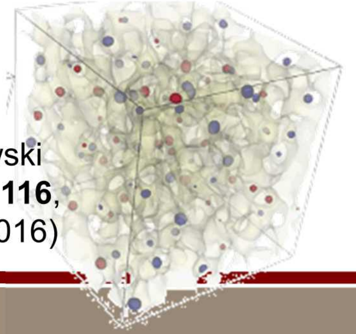


- Rigorous and reliable models exist, but…
  - Quantum Molecular Dynamics (QMD)
  - Time-dependent Density Functional Theory (TD-DFT)
  - Computationally expensive and difficult to extend to high temperatures, low densities, and complex ions



A. Baczewski *et al*, PRL **116**, 115004 (2016)

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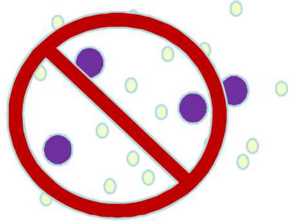

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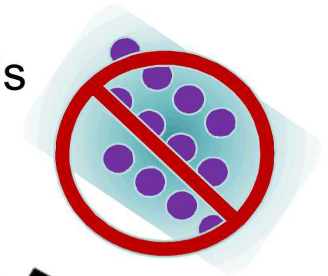

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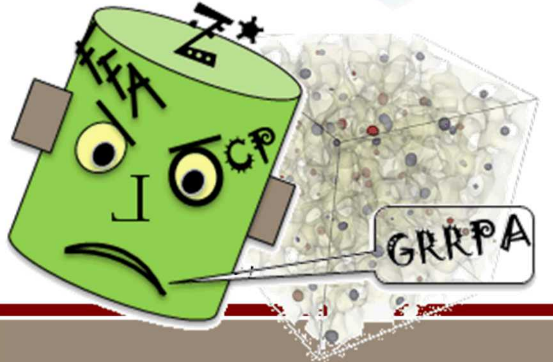

Central question: What happens to material when you squish it very hard and/or heat it quite a lot?

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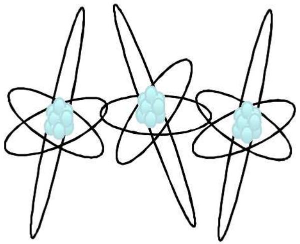
Experiments/Observables

Measurements from small, short-lived lab plasmas and large, distant astrophysical objects are inherently challenging

Observables (yields, images, spectra) can be difficult to interpret and may require both adequate material models and complex simulations



Simulations

"Magneto-radiation-hydrodynamic" simulations are used to design experiments and help interpret data from laboratory and astrophysical plasmas

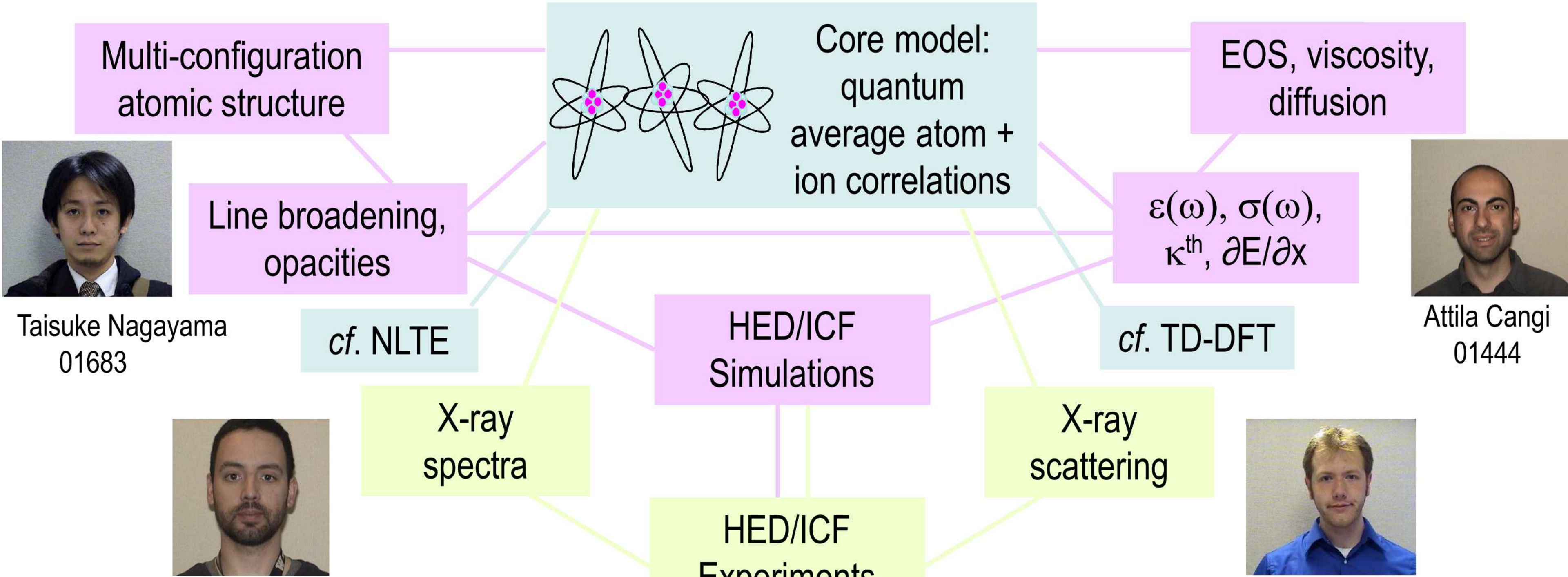
Reliable simulations themselves require extensive input from adequate material models (EOS, transport, opacity)

Additional questions:

How can we tell if our models are right?

How important is model consistency?

Our central goal: Develop a unified, tractable, and consistent model for matter in extreme conditions



Taisuke Nagayama
01683

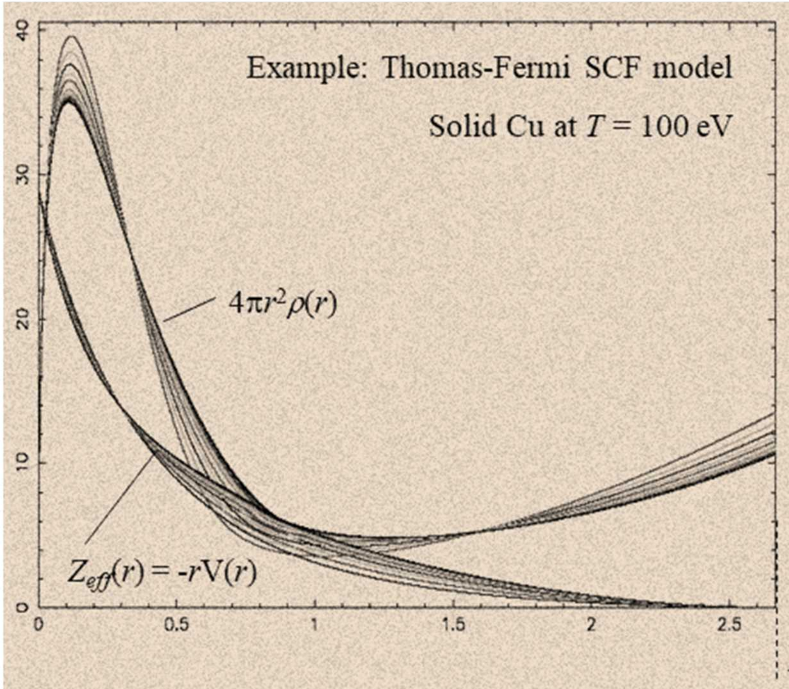
Attila Cangi
01444

Thomas Gomez
01684

Andrew Baczewski
01425

History: Thomas-Fermi fluid models developed in the 1920s still inform some present-day simulations

Fluid "Self-consistent field" models capture a lot of essential HED physics on the cheap!

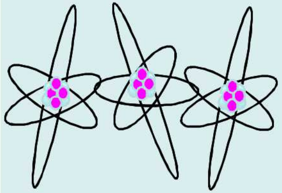


An initial guess is made for the electrostatic potential $V(r)$ in the ion sphere. This potential is used to determine an electron density distribution $\rho(r)$, which is in turn used to generate a new potential.

The procedure is iterated until self-consistent $V(r)$ and $\rho(r)$ are obtained, giving also Z_i and μ.

But they neglect electronic shell structure and treat other ions as a uniform "jellium"

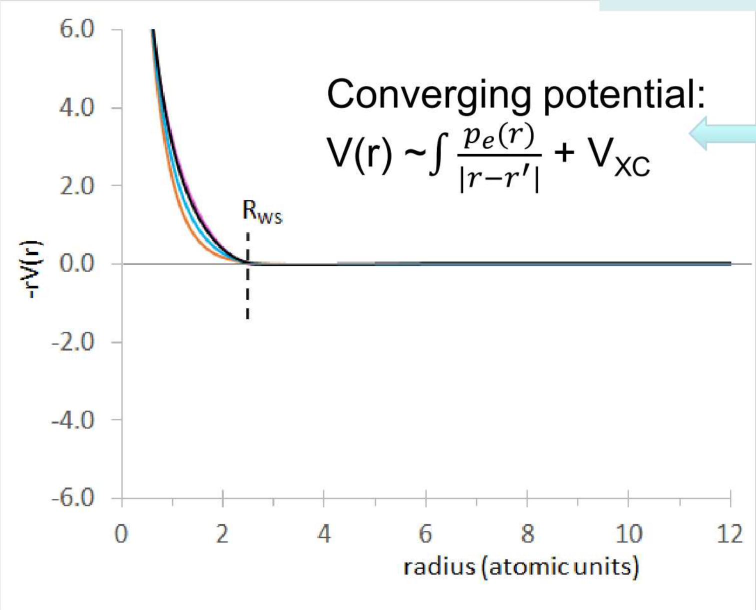
Our model builds on that history:
Fully quantum, semi-relativistic electrons for both the atom…

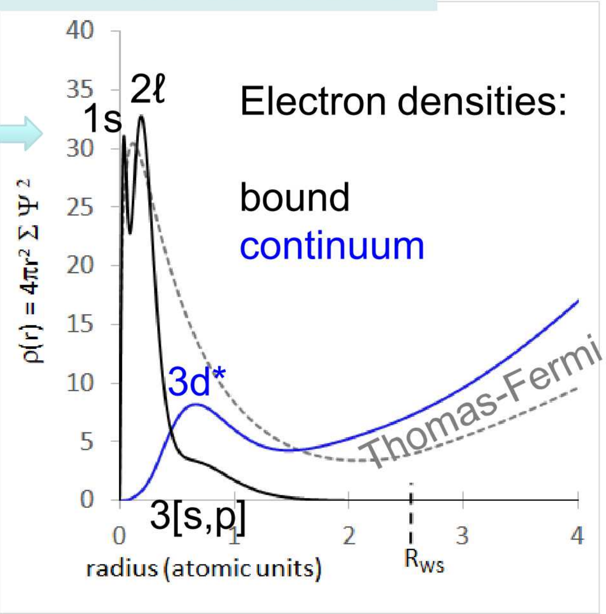


Core model: quantum average atom + ion correlations

Bound and free atomic wavefunctions are calculated in a self-consistent potential

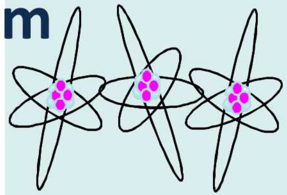
Solid-density iron, 10 eV





Liberman, *Phys Rev. B* **20**, 4981 (1981); Wilson, Sonnad, Sterne & Isaacs *JQSRT* **99**, 658 (2006)

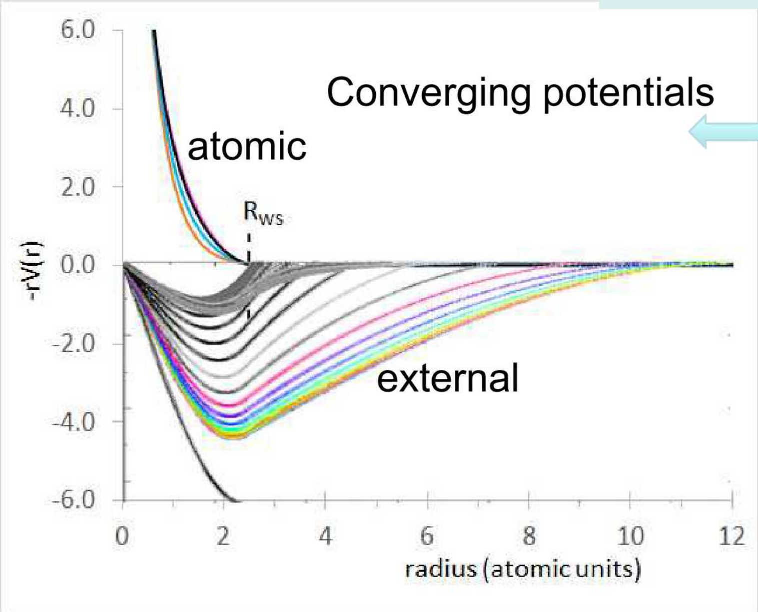
Our model builds on that history: Fully quantum, semi-relativistic electrons for both the atom and the external system

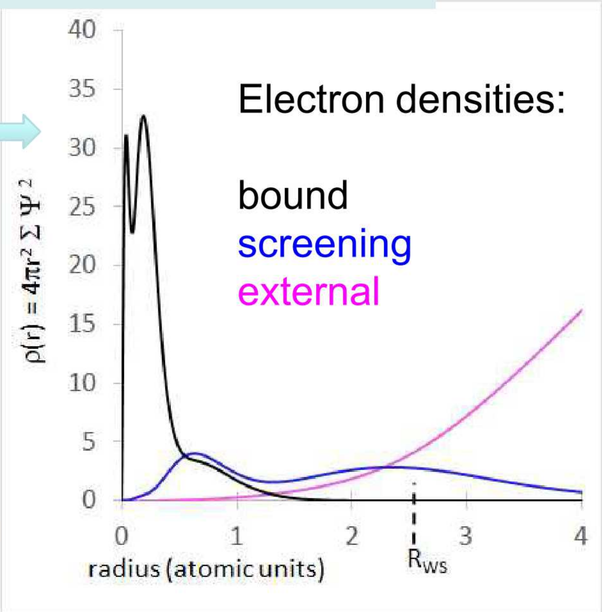


Core model: quantum average atom + ion correlations

The external system defines a neutral pseudo-atom (NPA) that extends beyond the Wigner-Seitz cell

Solid-density iron, 10 eV

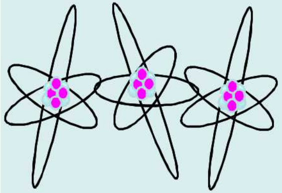




$$\rho^{NPA} = \rho^{atomic} - \rho^{external}$$

$$\rho^{screening} = \rho^{NPA} - \rho^{ion}$$

…which extends the model's self-consistency to ions:

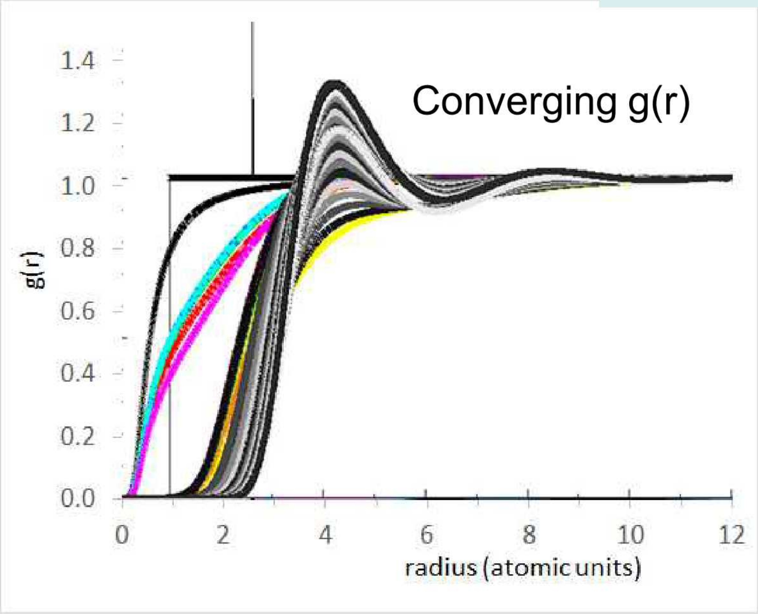


Core model: quantum average atom + ion correlations

The screening electron density determines the ion-ion interaction potential:

$$\beta V(k) = \frac{4\pi\beta}{k^2}\bar{Z}^2 - n_e^{scr}(k) C_{Ie}(k)$$

Solid-density iron, 10 eV



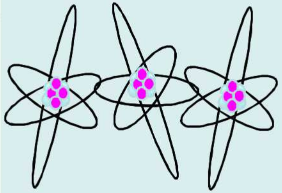
This potential constrains the ion distribution through the quantum Ornstein-Zernicke equations

Starrett & Saumon, *HEDP* **10**, 35 (2014)

This is our fully self-consistent core model, which is sensitive to a limited number of constraints

v_{XC}

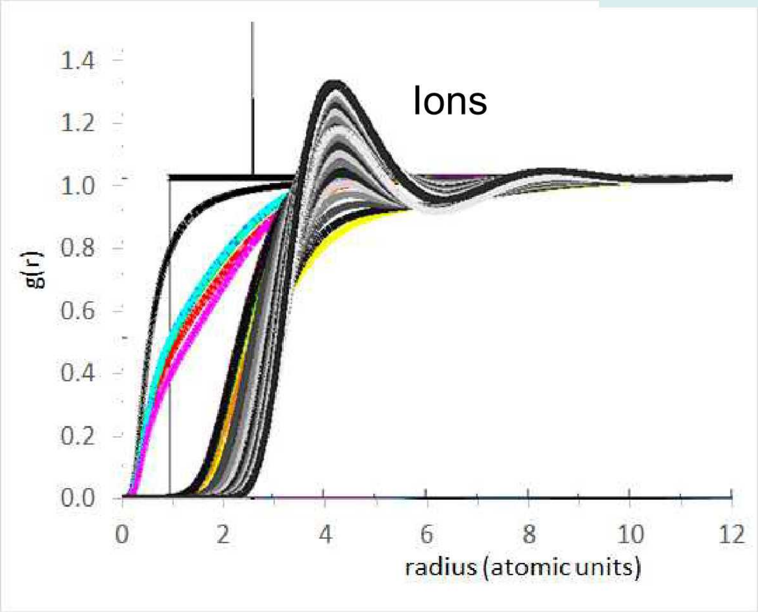
ρ_{scr}

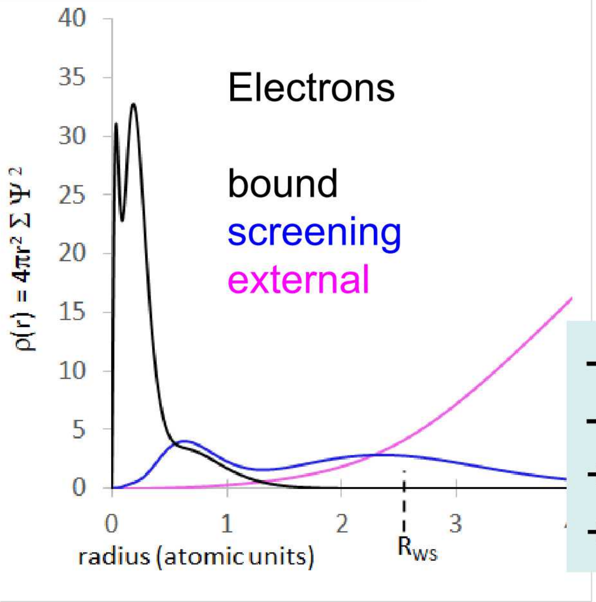


Core model: quantum average atom + ion correlations

Self-consistent $V_{ei}(r)$, $\Psi(r)$, $\rho(r)$, $V_{ext}(r)$. $\rho_{ext}(r)$, $V_{ii}(r)$, $\rho_{ion}(r)$

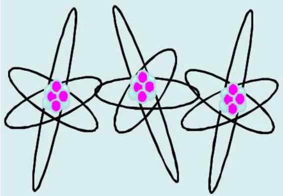
Observable and constitutive properties





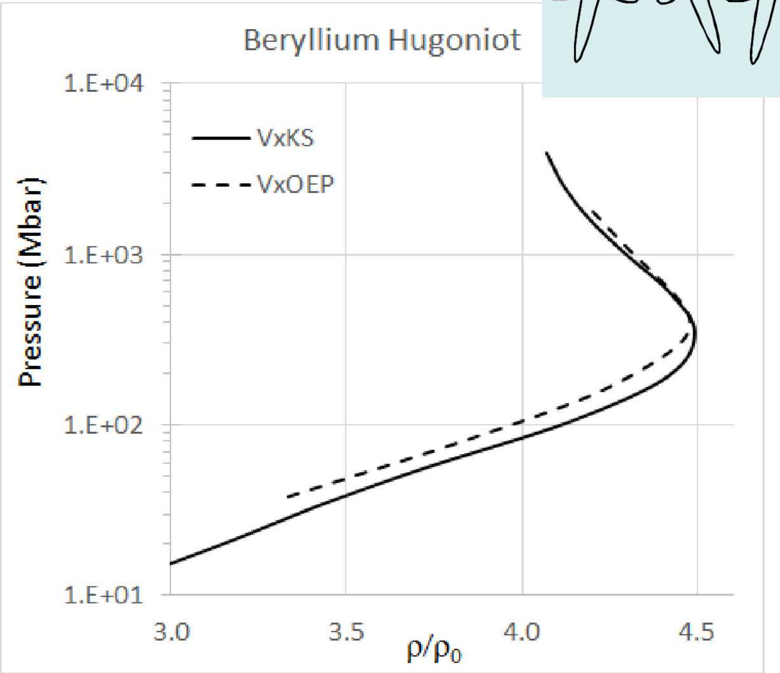
- Spherical
- semi-relativistic
+ orthonormal $\Psi(r)$
+ runtime ~ 3 minutes

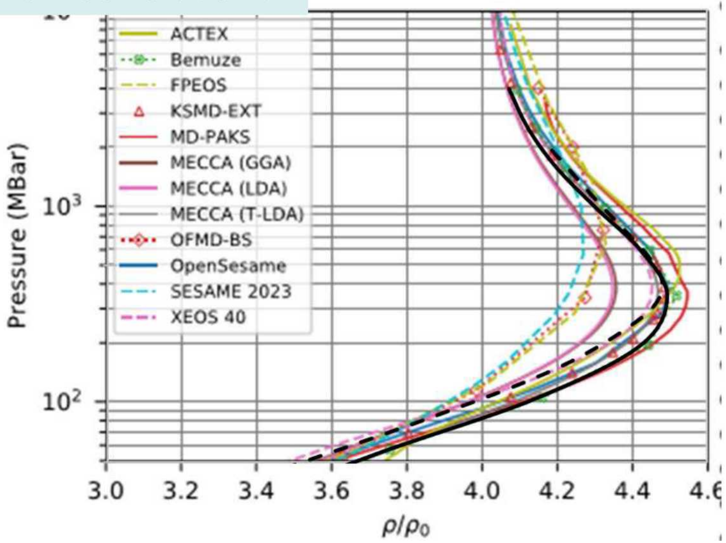
These constraints impact Equations of State and all other model-derived properties while preserving self-consistency



Core model: quantum average atom + ion correlations

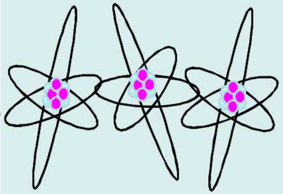
EOS, viscosity, diffusion





J. Gaffney, S. Hu *et al.*
LLE EOS code comparison

Screening from the core model drives PAMD simulations, which inform EOS & provide ionic transport coefficients



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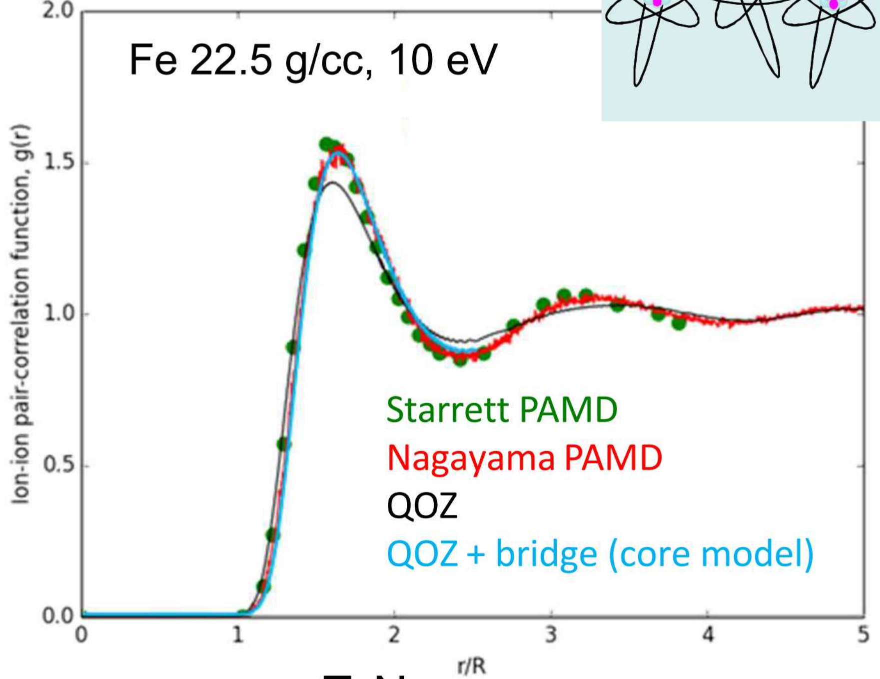
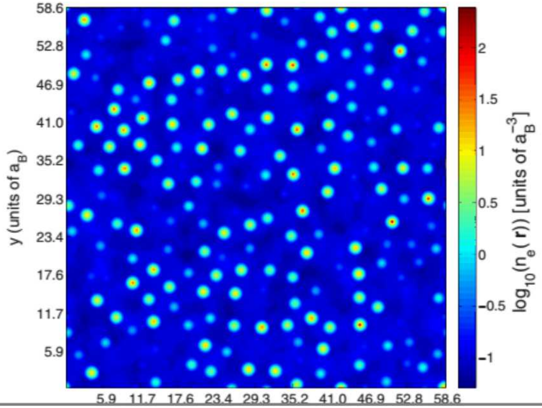


T. Nagayama

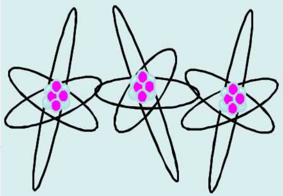


PHYSICAL REVIEW E **91**, 013104 (2015)

Pseudoatom molecular dynamics

C. E. Starrett,* J. Daligault, and D. Saumon

The core-model wave functions produce optical properties: conductivities, dielectric functions, & opacities



Core model: quantum average atom + ion correlations

Line broadening, opacities $\alpha(\omega)$

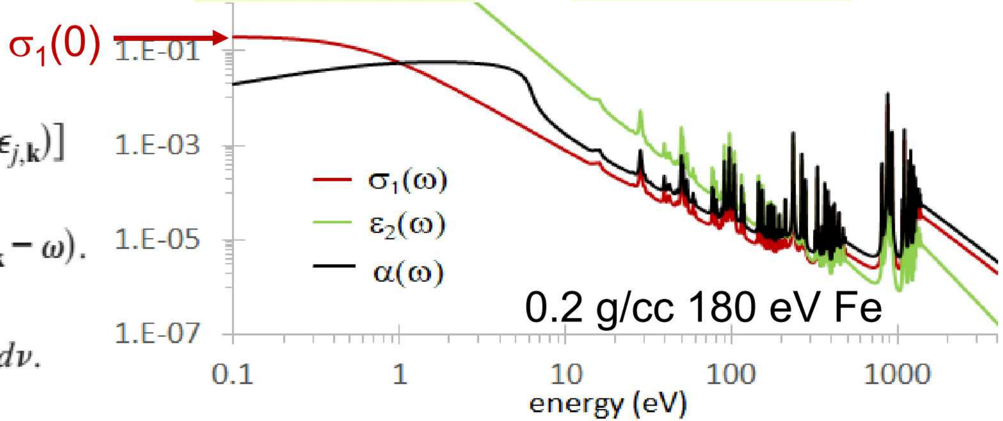
$\sigma(\omega)$, $\varepsilon(\omega)$, κ^{th}, $\partial E/\partial x$

X-ray spectra

X-ray scattering

$$\sigma_1(\mathbf{k},\omega) = \frac{2\pi}{3\omega\Omega}\sum_{j=1}^{n_b}\sum_{i=1}^{n_b}\sum_{\alpha=1}^{3}\left[F(\epsilon_{i,\mathbf{k}})-F(\epsilon_{j,\mathbf{k}})\right] \times \langle\Psi_{j,\mathbf{k}}|\nabla_\alpha|\Psi_{i,\mathbf{k}}\rangle^2\delta(\epsilon_{j,\mathbf{k}}-\epsilon_{i,\mathbf{k}}-\omega).$$

$$\sigma_2(\omega) = -\frac{2}{\pi}\mathrm{P}\int\frac{\sigma_1(\nu)\omega}{(\nu^2-\omega^2)}d\nu.$$



$$\epsilon_1(\omega) = 1 - \frac{4\pi}{\omega}\sigma_2(\omega),$$

$$\epsilon_2(\omega) = \frac{4\pi}{\omega}\sigma_1(\omega),$$

$$\alpha(\omega) = \frac{4\pi}{n(\omega)c}\sigma_1(\omega),$$

$$n(\omega) = \sqrt{\tfrac{1}{2}[|\epsilon(\omega)| + \epsilon_1(\omega)]}.$$

Kuchiev & Johnson, *PRE* **78**, 026401 (2008)

Thermal conductivities are derived from electrical conductivities $\sigma(0)$ with additional electron-electron scattering

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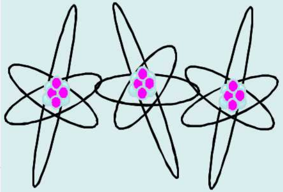
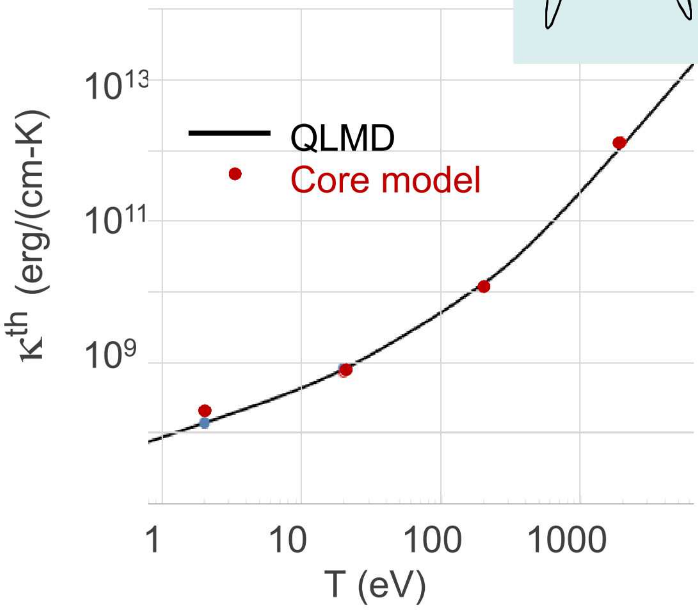


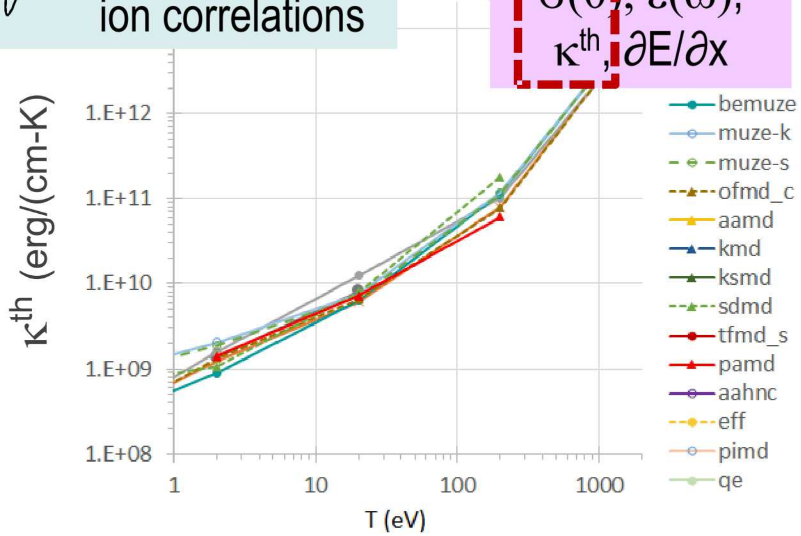
Core model: quantum average atom + ion correlations

$\sigma(0)$, $\varepsilon(\omega)$, κ^{th}, $\partial E/\partial x$

10 g/cc hydrogen



M. Desjarlais



P. Grabowski, A. Baczewski *et al.*
SNL transport code comparison workshop

The dielectric function and electron density inform stopping powers (dE/dx) relevant to self-heating in fusion plasmas

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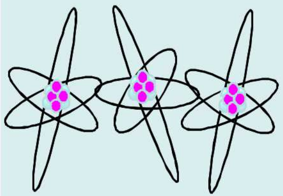
$$L(\rho,V)=\frac{i}{\pi\omega_0^2}\int_0^\infty\frac{dk}{k}\int_{-kV}^{kV}\omega dw\left(\frac{1}{\varepsilon(k,\omega)}-1\right)$$

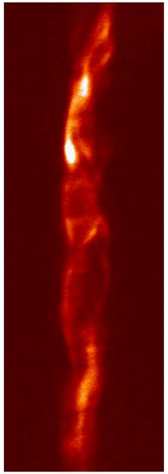
$$\left(\frac{dE}{dx}\right)=-\frac{4\pi}{m}\left(\frac{Ze^2}{V}\right)^2\int_0^\infty\rho(r)L(\rho,V)4\pi r^2dr$$

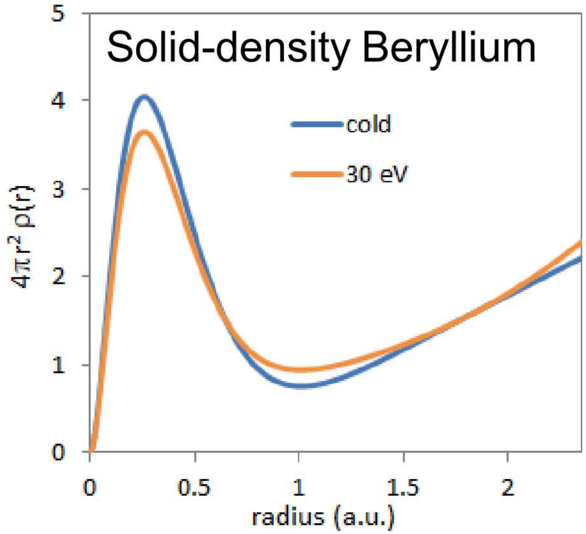


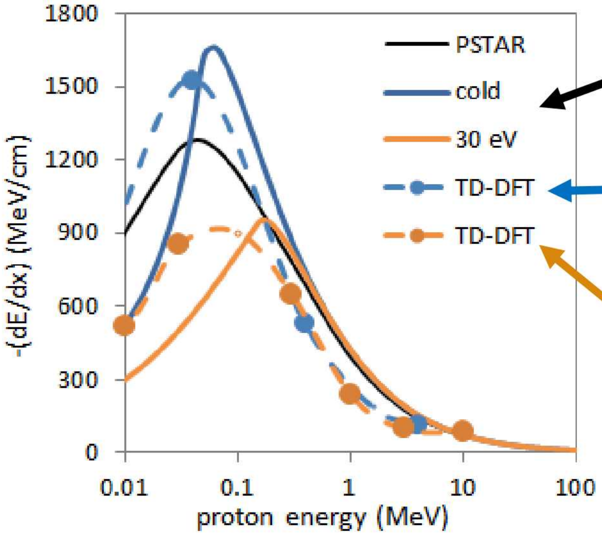
Core model: quantum average atom + ion correlations

$\sigma(\omega)$, $\varepsilon(\omega)$, κ^{th}, $\partial E/\partial x$

MagLIF







Core model:
~3 minutes on desktop

cold TD-DFT
(5 x 32 cores, 1 day)

32 eV TD-DFT
(3000 x 16 cores, 1 day)

A. Cangi, A. Baczewski

Wang *et al.*, *Phys Plas* **5**, 2977 (1998); Magyar *et al.*, *C. Plas Phys*. 56 459 (2016)

The dielectric function is also related to X-ray scattering, which is used as a diagnostic for laboratory plasmas

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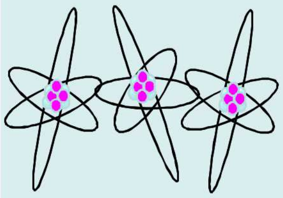
$$S(\omega) \propto \mathrm{Im}\left[\frac{1}{\varepsilon(\omega)}\right]$$

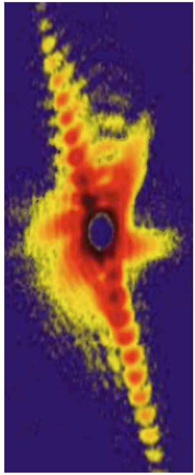


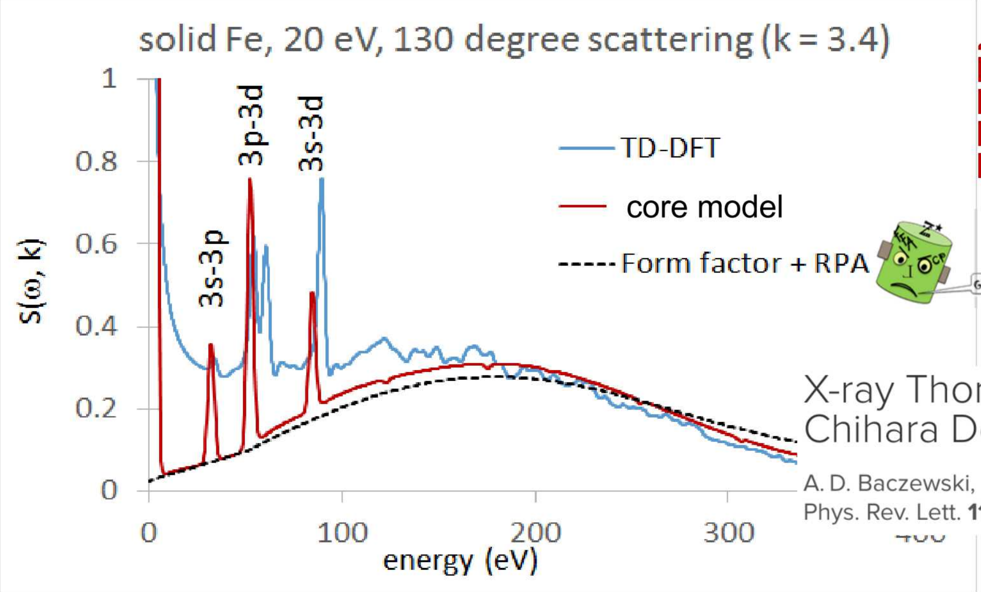
Core model: quantum average atom + ion correlations

$\sigma(\omega)$, $\boxed{\varepsilon(\omega)}$, κ^{th}, $\partial E/\partial x$

X-ray scattering

XFEL



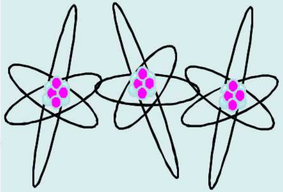


X-ray Thomson Scattering in Warm Dense Matter without the Chihara Decomposition

A. D. Baczewski, L. Shulenburger, M. P. Desjarlais, S. B. Hansen, and R. J. Magyar
Phys. Rev. Lett. **116**, 115004 – Published 18 March 2016

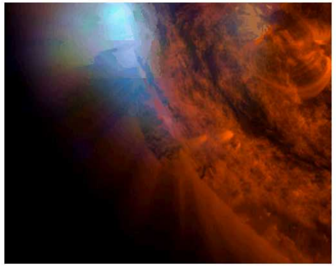
Johnson *et al*, *PRE* **86**, 036410 (2012); Chihara, J. Phys. Cond. Matt. **12**, 231 (2000)

The optical properties that inform transport and scattering also provide opacities – but they're not very good



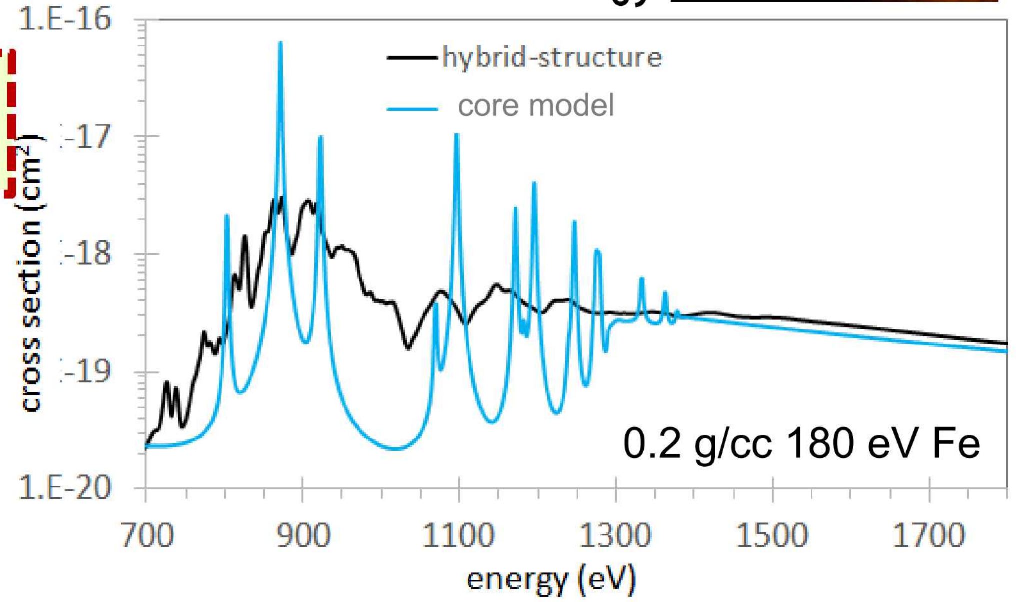
Core model: quantum average atom + ion correlations

Solar opacity*



Line broadening, opacities $\alpha(\omega)$

X-ray spectra



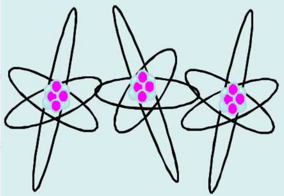
Average-atom opacities are strictly complete – which is not trivial for more complex models* – but they do not capture line splitting due to multiple configurations

*Iglesias and Hansen, *Ap. J* **835**, 284 (2017); ****Bailey *et al*, *Nature* 517, 56 (2015)**

The opacities can be significantly improved by splitting the average atom into detailed configurations

Multi-configuration atomic structure

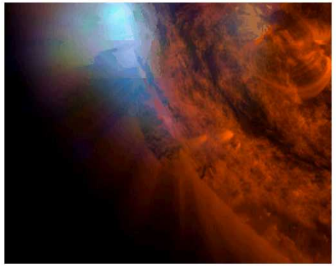
Line broadening, opacities $\alpha(\omega)$



Core model: quantum average atom + ion correlations

X-ray spectra

Solar opacity

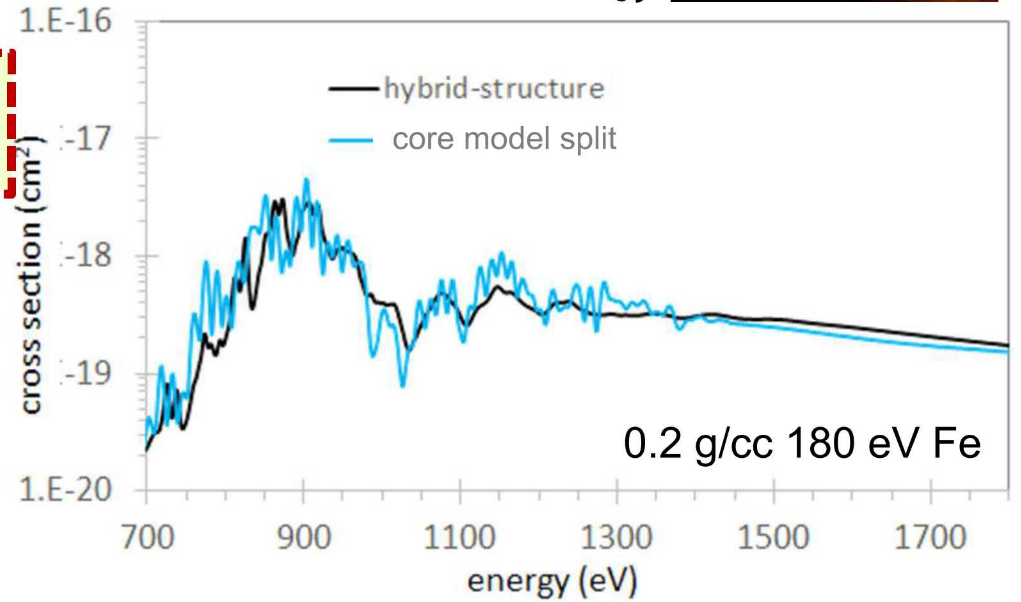


$$E_i = Ec_{onfig} + Ec_{orr} + Ep_{las} + ES_O$$

E_{config} from Slater coefficients/ Ψ

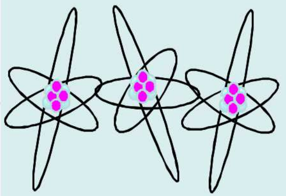
E_{plas} from ion distribution & Ψ_{config}

$$X_i = g_i w_i \exp\left(\beta\left(m(\bar{\mu} - \bar{E}_p) - E_i\right)\right)$$

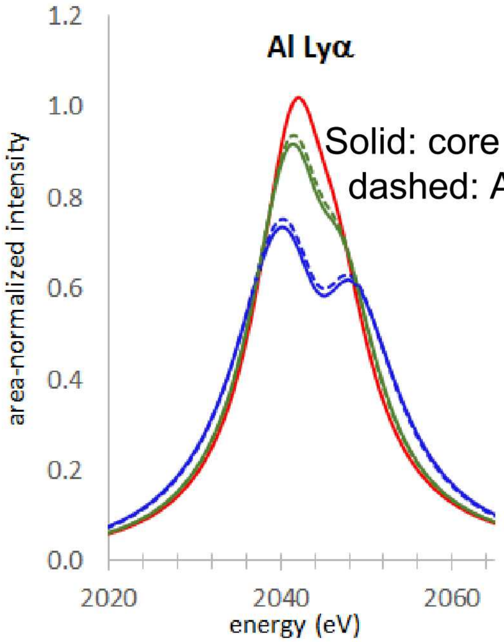


Opacities will be further refined using self-consistent line broadening from core-model PAMD & collision models

Line broadening, opacities

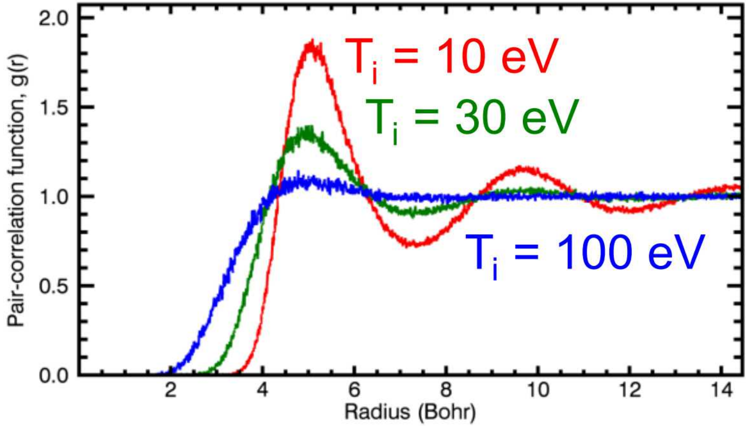


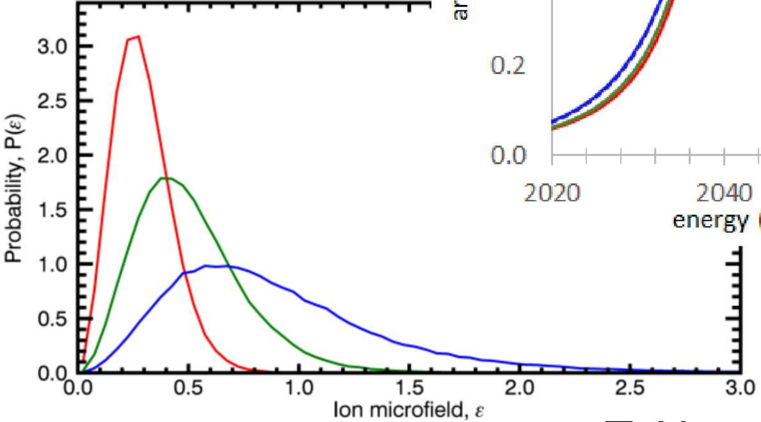
Core model: quantum average atom + ion correlations



T. Gomez

Solid-density Al, T_e = 250 eV





T. Nagayama

APEX: Iglesias *et al.*, *Phys Rev A* **31**, 1698 (1985)

Conclusions

We are working to build a self-consistent model of material at extreme conditions with:

- Constitutive properties adequate for use in simulations
  → Enforced consistency can improve sensitivity studies & increase constraints

- Observable predictions adequate for comparison with experiment
  → Enforced consistency means that if part of this model is wrong, the whole thing is wrong – and its wrongness should be detectable

For complex systems, internally consistent models that can be falsified by comparison to detailed data have more epistemic value than tunable models made to fit integrated data

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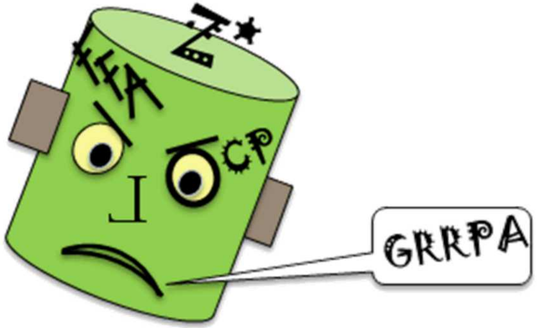
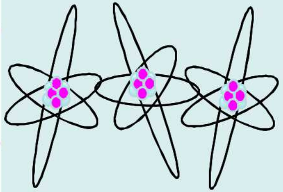


Summary & acknowledgements

Sandia National Laboratories

v_{XC} ρ_{scr}



Core model: quantum average atom + ion correlations

Multi-configuration atomic structure

EOS, viscosity, diffusion

Line broadening, opacities

$\varepsilon(\omega)$, $\sigma(\omega)$, κ^{th}, $\partial E/\partial x$

cf. NLTE

HED/ICF Simulations

cf. TD-DFT

X-ray spectra

X-ray scattering

HED/ICF Experiments

Taisuke Nagayama

Attila Cangi

Thomas Gomez

Andrew Baczewski

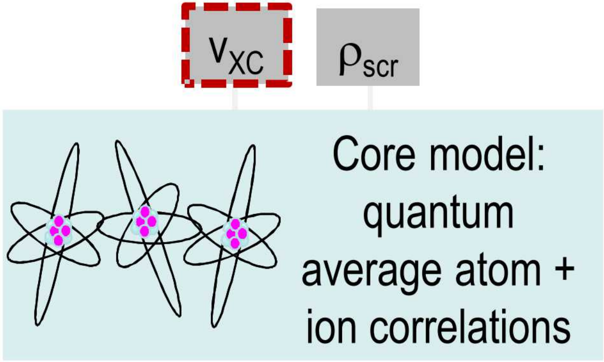
Thanks to:

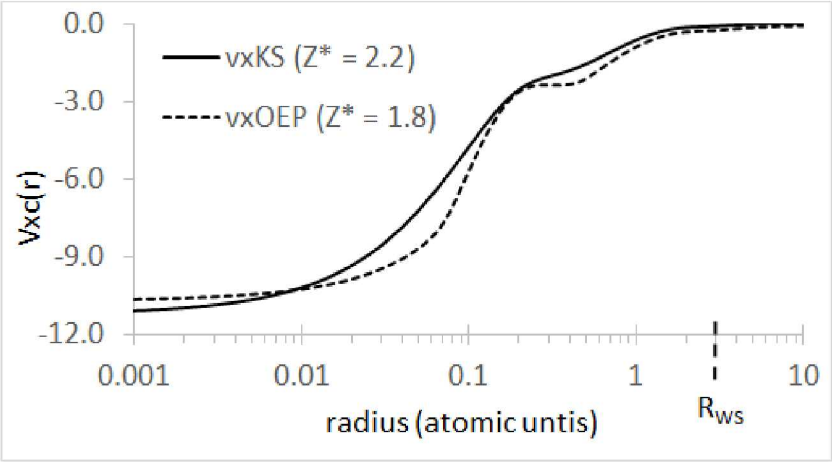
Charles Starrett, David Kilcrease (LANL), Carlos Iglesias, Brian Wilson, Phil Sterne, Paul Grabowski (LLNL), Richard More

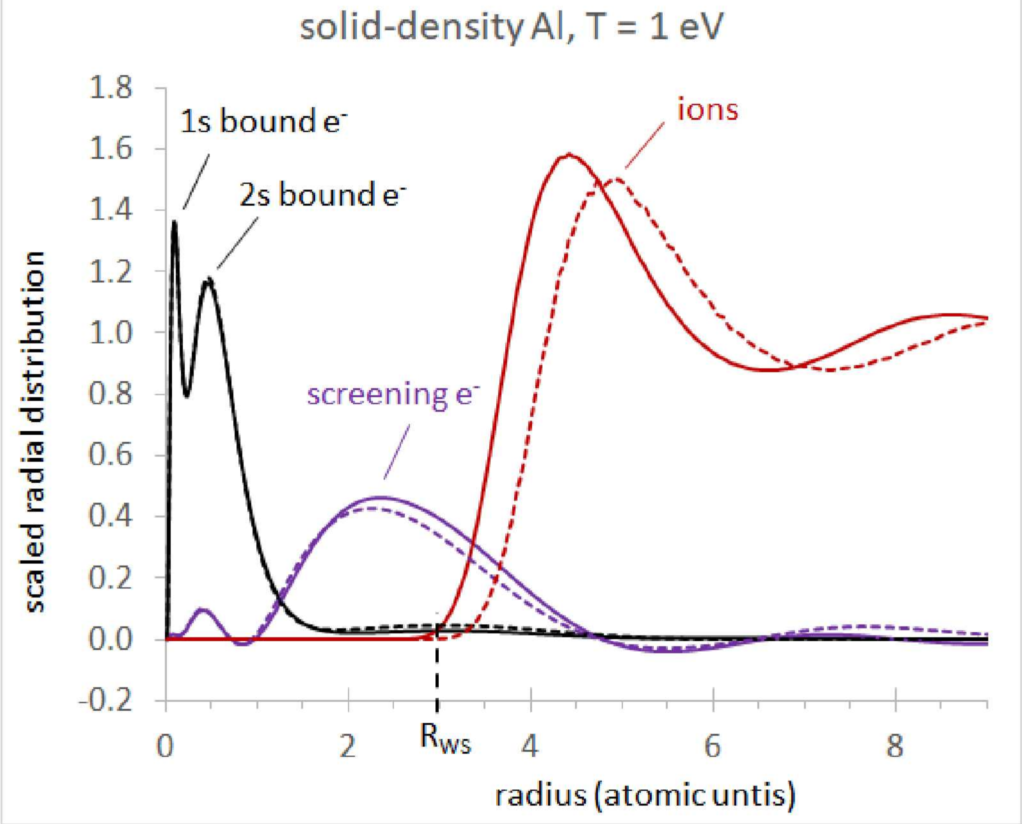
Primary funding: U.S. DOE, Office of Science Early Career Research Program, OFES FWP-14-017426

Thank you!

The core model is sensitive to the choice of exchange potential

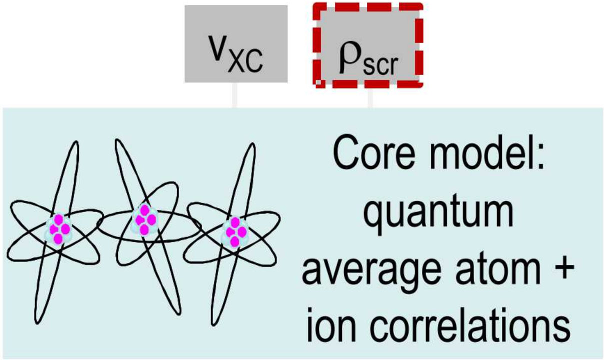


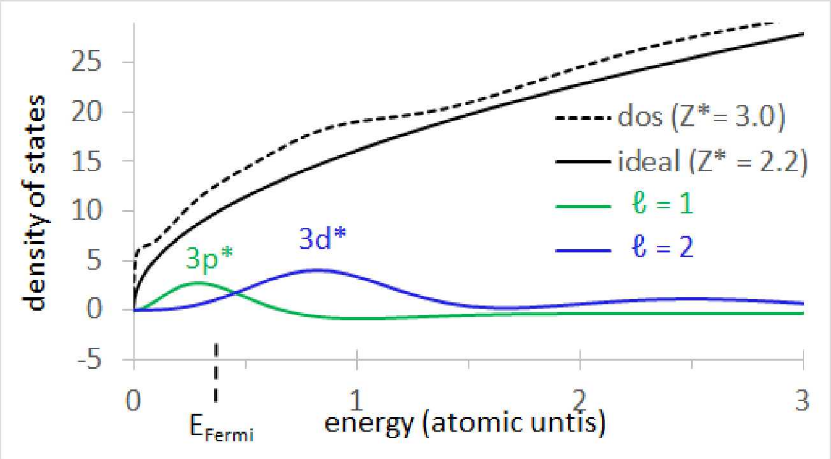


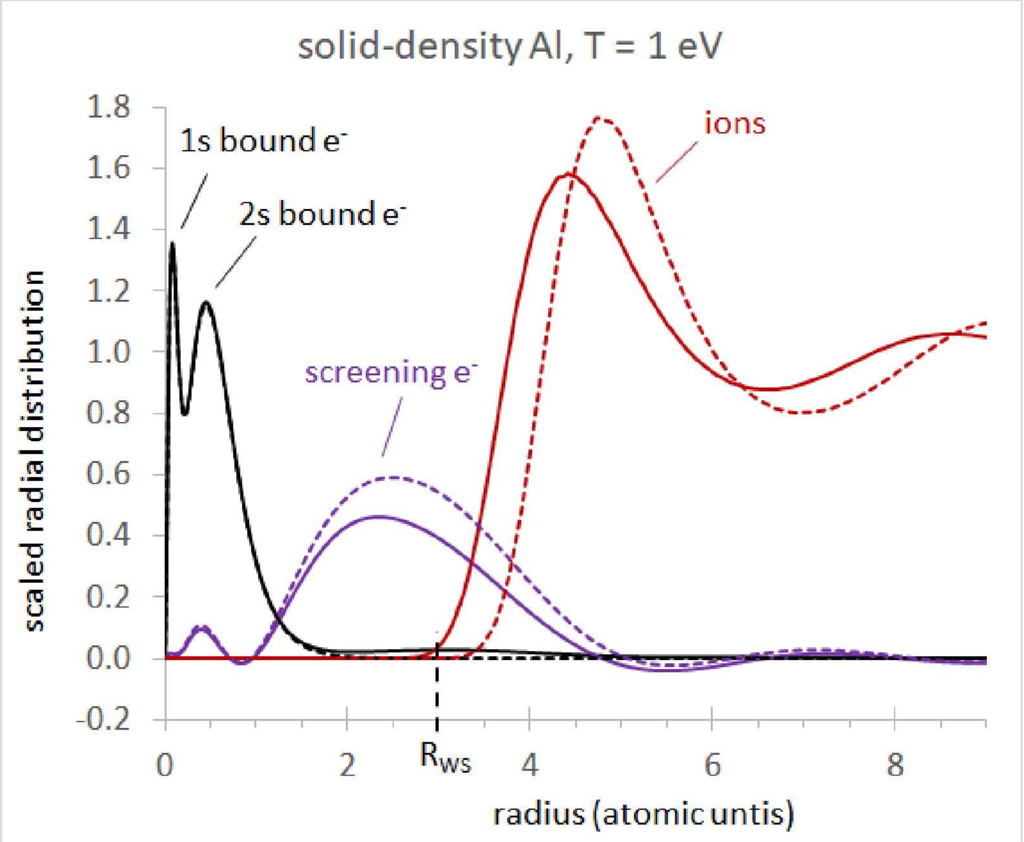


Becke & Johnson J Chem Phys **124**, 221101 (2006); Wilson & Liberman, JQSRT **54**, 427 (1995)

The core model is sensitive to whether the screening density includes the pressure-ionized “scars” of bound states





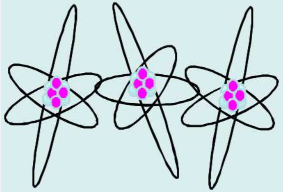


Examining the full dielectric function indicates a missing piece in the standard Chihara decomposition

Chihara decomposition:

$$S(k,\omega) = \underbrace{|f_I(k) + q(k)|^2 S_{ii}(k,\omega)}_{\text{elastic}} \cdot$$

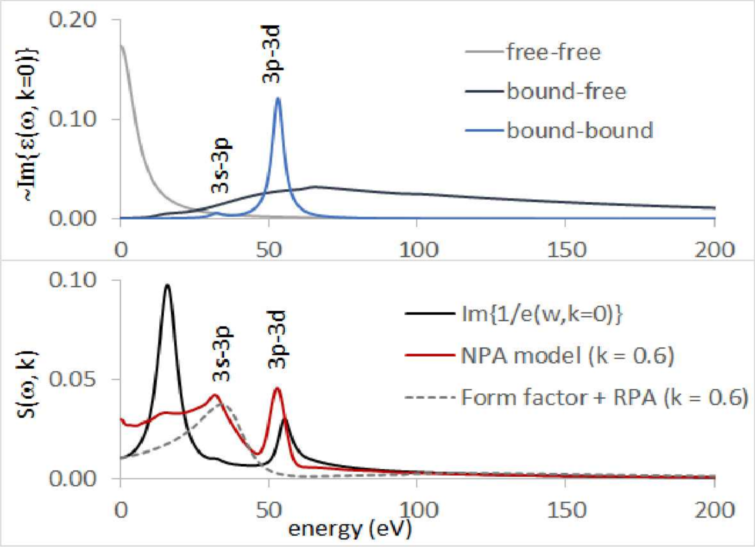
$$+ \underbrace{\bar{Z} S_{ee}(k,\omega)}_{\text{free-free}} + \underbrace{S_{bf}(k,\omega)}_{\text{bound-free}} + \underbrace{S_{bb}(k,\omega)}_{\text{bound-bound}}$$



Core model: quantum average atom + ion correlations

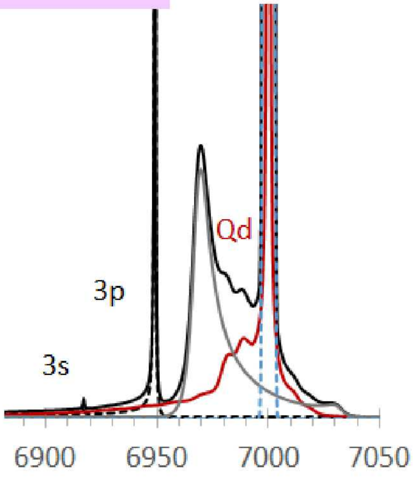
$\sigma(\omega)$, $\boxed{\varepsilon(\omega)}$, κ^{th}, $\partial E/\partial x$

X-ray scattering



The bound-bound features in $\mathrm{Im}\{1/\varepsilon_{bb}(\omega)\}$ are reminiscent of sharp bound-free features previously noted by Johnson *et al.* and Souza *et al.**

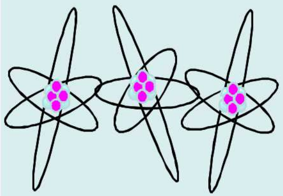
5 g/cc Fe, 10 eV



8 g/cc Fe, 1 eV

*Johnson *et al*, *PRE* **86**, 036410 (2012); Souza, Starrett *et al*., PRE **89**, 023108 (2015)

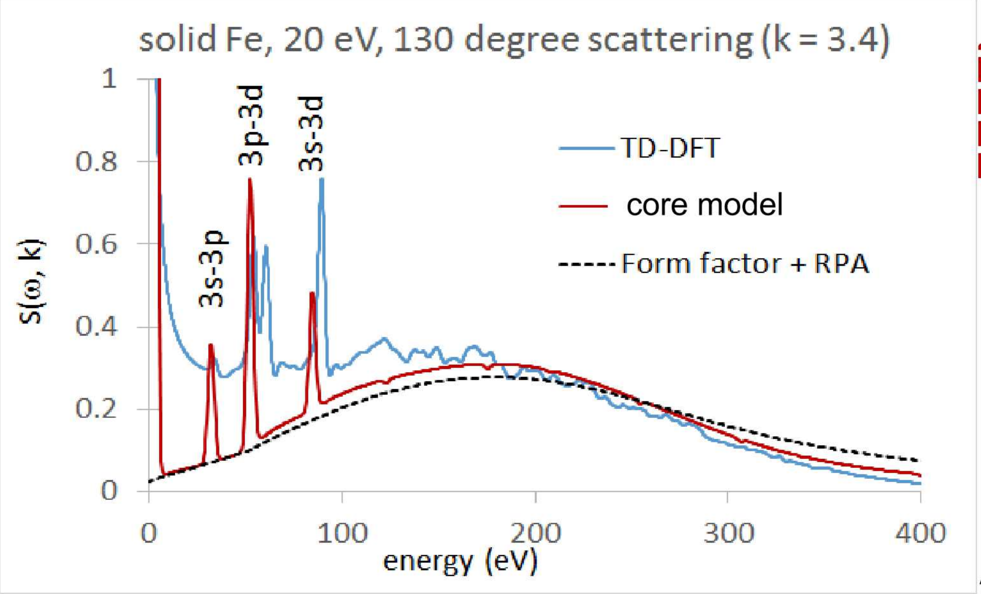
Both the core model and TD-DFT capture bound-bound scattering features in S(ω, k)



Core model: quantum average atom + ion correlations

X-ray scattering

While $S(\omega,0) \sim \mathrm{Im}\{1/\varepsilon(\omega,0)\}$ roughly describes edges and line, a more general $S(\omega,k)$ can be obtained directly from core-model wavefunctions



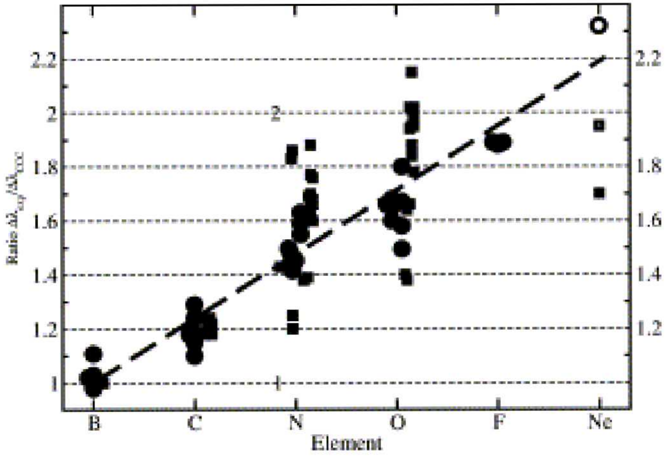
Experimental diagnostics benefit from consistent and complete atomic-scale models

A. Baczewski

Baczewski *et al*, PRL **116**, 115004 (2016)

A persistent puzzle: isolated line broadening for multi-electron atoms

- Efforts to model simple multi-electron atoms (low-Z Li-like ions) show a disturbing disagreement with experiment
- These are not exotic conditions ($T_e \approx 15$eV; $n_e \approx 2x10^{18}$ e/cm^3)
- This indicates that there might be some missing physics or something that the community is doing incorrectly
- In order to model more complex atoms, we must resolve this discrepancy with simple 3-electron atoms

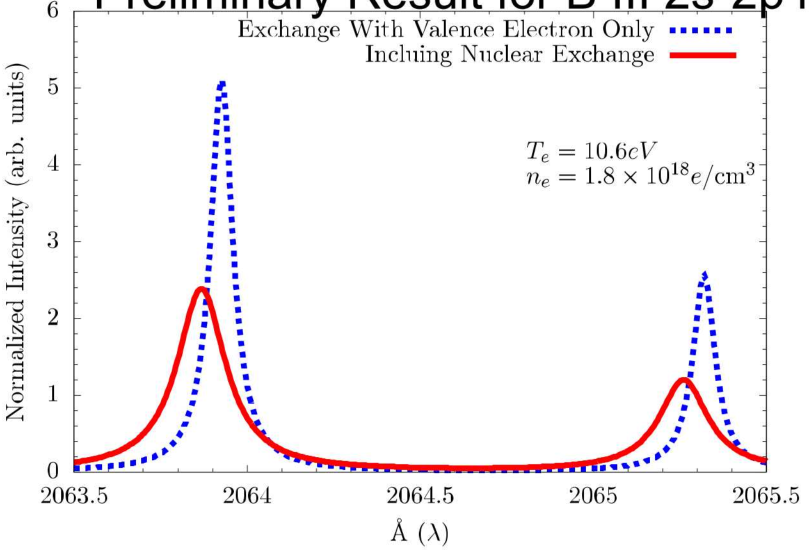


Ralchenko et al.
JQSRT 81, 371 (2003)

Interaction Between Radiator and Plasma

- We need to use a complete Coulomb interaction (rather than the simpler dipole approximation)
- We also need to include the effects of the anti-symmetry between atomic and plasma electrons
- Approximations about wavefunctions can neglect some exchange interactions
- These neglected interactions have large consequences

*Preliminary Result for B III 2s-2p line



More work is needed to complete this project, but we have identified some physics that requires careful attention because it has a significant effect on line shapes

These calculations (AA-LDA) described Zylstra's recent measurements of 14 MeV proton stopping reasonably well

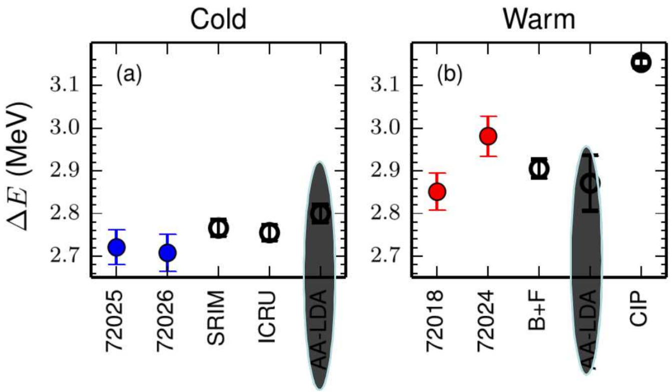


FIG. 4 (color online). Downshift (ΔE) for cold (a) and warm (b) shots compared to theory. The solid points are data (denoted by shot number), and theories are hollow points. The uncertainties in theoretical calculations are due to uncertainties in ρL and plasma conditions.

The downshift of 14 MeV protons is determined by integrating calculated dE/dx over measured path length

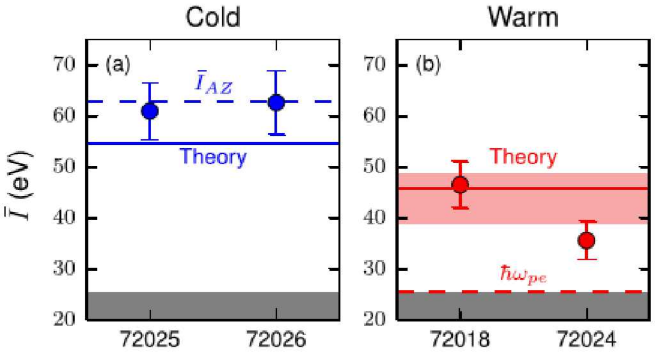
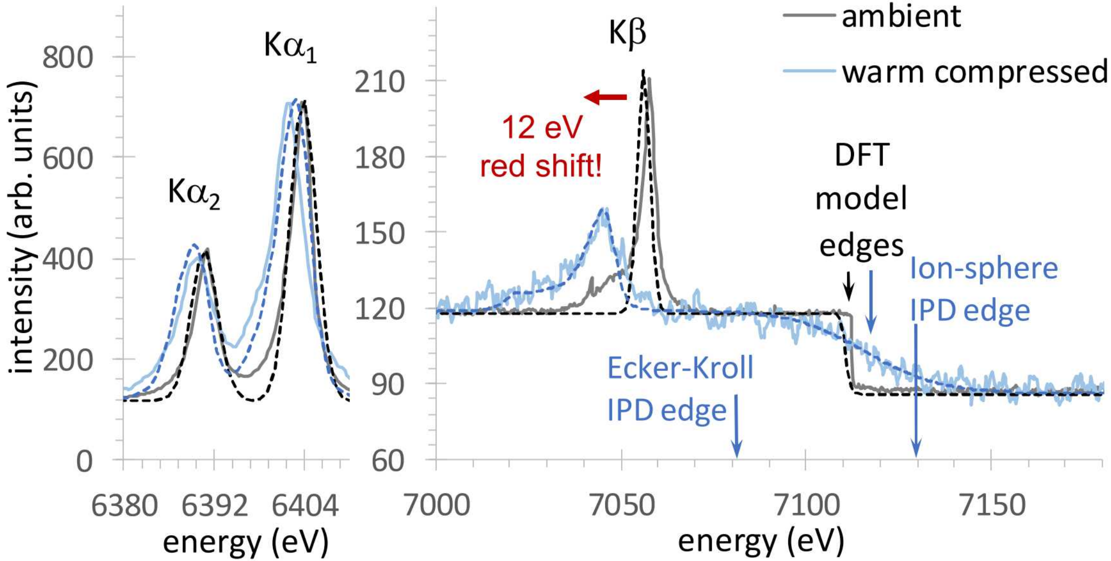
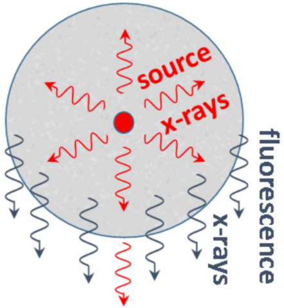


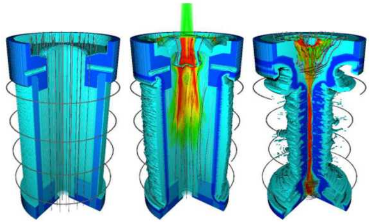
FIG. 5 (color online). Mean ionization potential ($\bar{I}$) inferred from the stopping-power data in the cold (a) and warm (b) cases compared to the Andersen-Ziegler empirical fits ($\bar{I}_{AZ}$), the ideal plasma case ($\hbar\omega_{pe}$), and electronic structure theory.

Mean ionization potential can be calculated simply by averaging $E_{binding}$ + E_{Fermi} for all electrons in the Average Atom calculation

Observables in extreme WDM: absorption edges and fluorescence lines





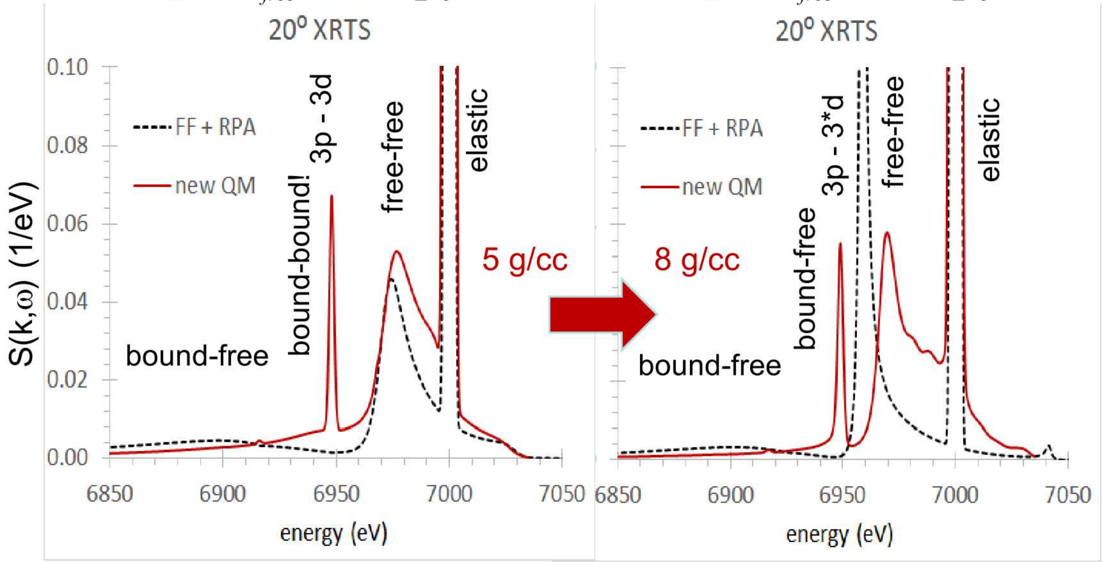


Calculations (dashed lines) anchored to the K-edge of ambient data (solid gray) show good agreement with line and edge shifts and broadening due from a warm compressed MagLIF liner backlit by stagnation emission (solid blue) with T ~ 10 eV and n_e ~ $2x10^{24}$ e/cc.

This agreement indicates that self-consistent DFT models describe electronic structure in extreme conditions with better fidelity than ad-hoc models of density effects.

Scattering calculations are also fully constrained

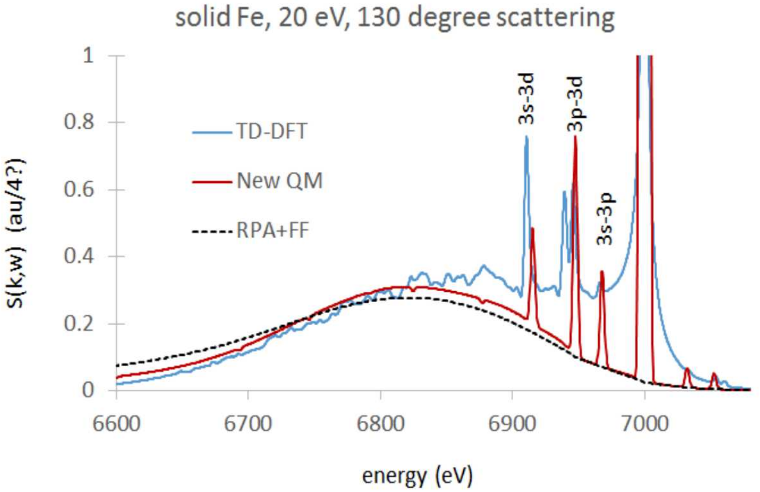
10 eV, 5 g/cc, Z_{free} = 2.6, $Z_{E>0}$ = 2.9 10 eV, 8 g/cc, Z_{free} = 3.2, $Z_{E>0}$ = 8.0



$$S(k,\omega) = \underbrace{|f_I(k) + q(k)|^2 S_{ii}(k,\omega)}_{\text{elastic}} + \underbrace{\bar{Z} S_{ee}(k,\omega)}_{\text{free-free}} + \underbrace{S_{bf}(k,\omega)}_{\text{bound-free}}$$

$+ S_{bb}\ (k,\omega)$ (bound-bound)

Most components of the scattering signal are calculated using fully self-consistent quantities[1,2] (free-free uses RPA)



We find good agreement of the self-consistent average-atom model with time-dependent density functional theory – A. Baczewski *et al.*, PRL 116, 115004 (2016).

1. W.R. Johnson *et al*, *PRE* **86**, 036410 (2012) 2. D. Souza, C. Starrett et al., *PRE* **89**, 023108 (2014)

Electrons: Quantum mechanical average atom

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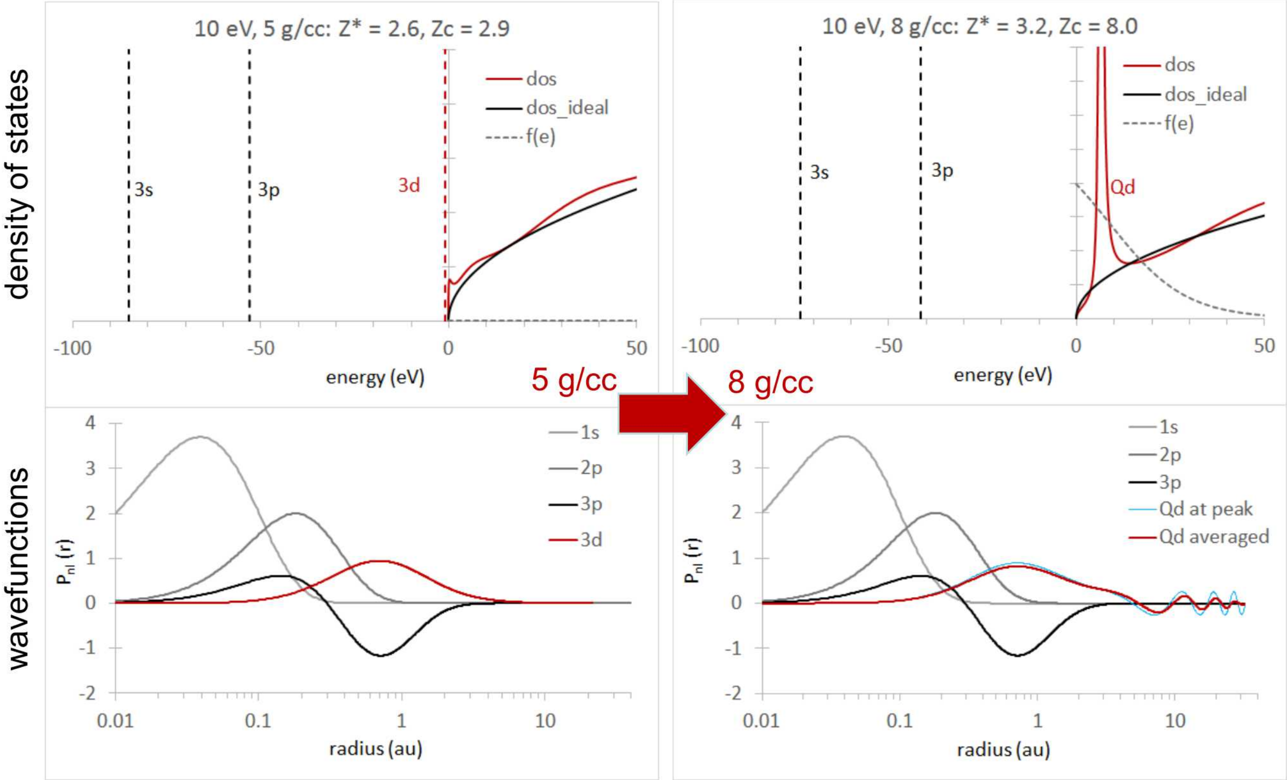
All-electron, fully quantum-mechanical* semi-relativistic self-consistent field solver with flexible exchange



Near-solid iron at T = 10 eV

Key ansatz:
Quasi-bound states are averaged over resonance features in the DOS and treated *just like* bound states

This ensures smooth variation of constitutive & observable properties under pressure ionization – and collapses multiple definitions of Z* into a single value [*cf.* Murillo *et al.*, *PRE* **87**, 063113 (2013)]:

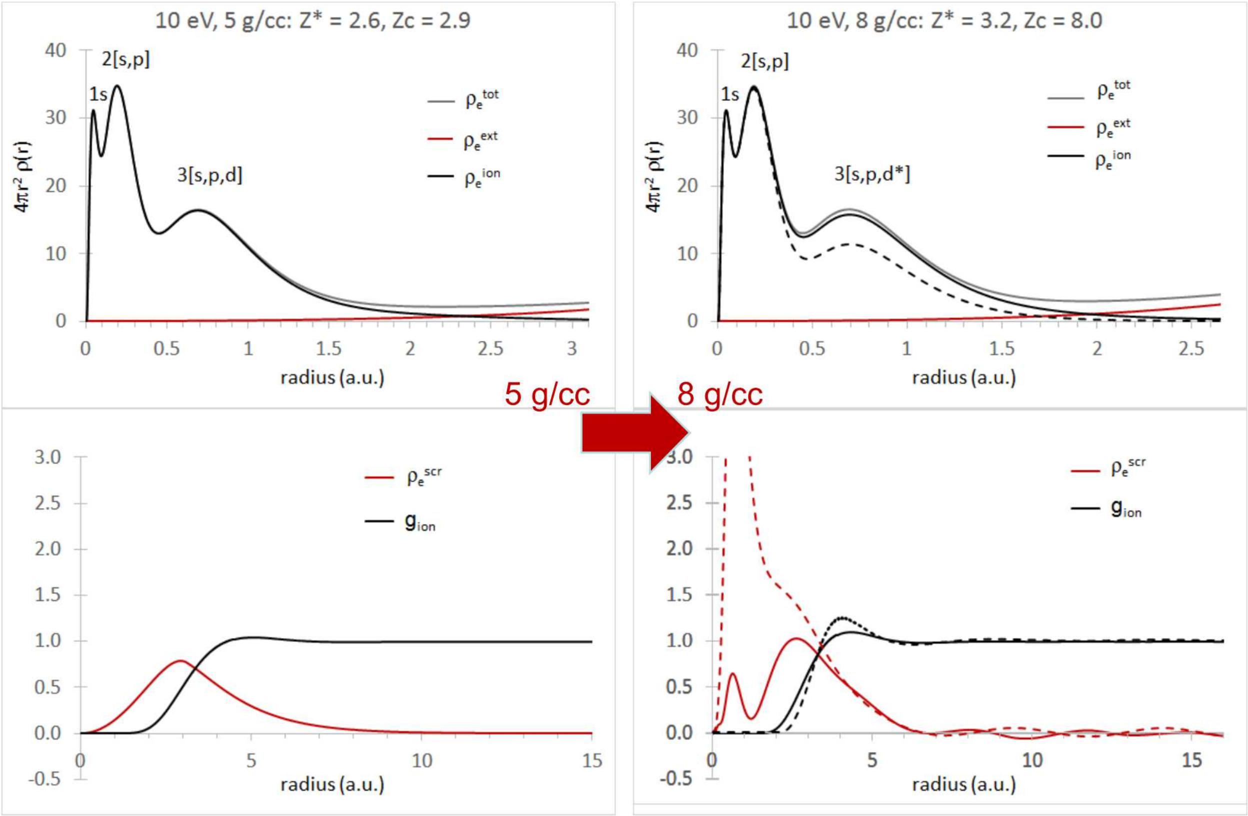
$$
\begin{aligned}
Z^* &= \int d\varepsilon\, f(\mu,\varepsilon)\mathrm{DOS}_{ideal} && (Z_{free})\\
&= \int \rho_{scr}\, dr = \tilde{V}_{ie}(k=0) && (Z_{scr})\\
&= \int d\varepsilon\, f(\mu,\varepsilon)(1 - f(\mu,\varepsilon))\varepsilon^{3/2} && (Z_{Boltz})\\
&= \tfrac{1}{3}(R^3_{WS}/R^2_{max})\rho(R_{max}) && (Z_{asymp})\\
&\approx \tfrac{1}{3} R_{WS}\,\rho(R_{WS}) && (Z_{WS})\\
&\neq \int d\varepsilon\, f(\mu,\varepsilon)\, \mathrm{DOS} = Z_n - Z_b && (Z_{\varepsilon>0})
\end{aligned}
$$

*D. A. Liberman, *Phys. Rev. B* **20**, 4981 (1979), B.G. Wilson *et al*, *JQSRT* **99**, 658 (2006)

Ions: Quantum Ornstein-Zernike

Sandia National Laboratories

Self-consistent V_{ii} & g_{ii} obtained by finding electron density with (ρ^{tot}) and without (ρ^{ext}) central charge*



$\rho^{PA} = \rho^{tot} - \rho^{ext}$
$\rho^{scr} = \rho^{PA} - \rho^{ion}$

Like Z*, ρ^{ion} is not uniquely defined

New ansatz (solid): $\rho^{ion} = \rho^{b} + \rho^{q\text{-}b}$
Standard (dashed): $\rho^{ion} \approx \rho^{b}$

The new ansatz leads to smaller changes in screening under pressure ionization and softer g(r)

Combined with smooth changes in Z*, this leads to smooth variations in model predictions for both constitutive properties and experimental observables

*C. Dharma-Wardana & F. Perrot, *Phys. Rev. E* **26**, 2096 (1982), C. Starrett & D. Saumon, *HEDP* **10**, 35 (2014)