Simulating EUV Production - an Overview of the Underpinnings

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Outline

- Introduction – what can we expect to get from simulations?
- Physical processes important for EUV generation
- Microphysics simulations
- Macrophysics simulations
- Current EUV simulation efforts
- Summary – where do we go from here?

The goal is to gain an appreciation of what simulations can offer to the EUVL community

What should we simulate (and why)?

*for EUV production

- Explaining the basic behavior of the EUV-producing system requires
  - Identifying the underlying microphysical processes
  - Evaluating each process (and their interactions) under representative conditions
- A basic understanding is sufficient for:
  - Estimating conversion efficiency (CE) vs. density / temperature / timescale
  - Providing guidance towards optimum conditions
- More details, i.e. simulations, are necessary for:
  - Tracking time evolution of conditions and outputs
- High-quality simulations are required for:
  - Optimizing laser pulse shape
  - Minimizing (initial) target mass
  - Evaluating effects from asymmetries and shot-to-shot variations

"The purpose of simulation is insight, not numbers"- R.W. Hamming

How reliable are the results?

- Optimizing a system requires predicting the behavior of the system as it evolves through a range of conditions

- Confidence in predictions will be high when
  - Verified by experiment under full range of conditions

    – or –
  - Simulations of microphysical processes and their interactions have been verified
  - Assumptions / approximations remain valid

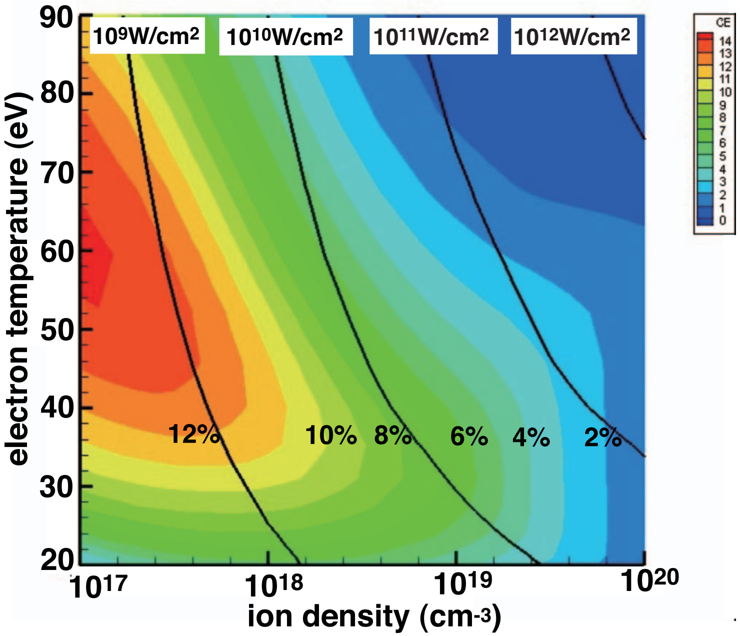
- Getting all the details right is very difficult, but rarely necessary

- Getting the basic descriptions and interactions of the microphysical processes right is critical

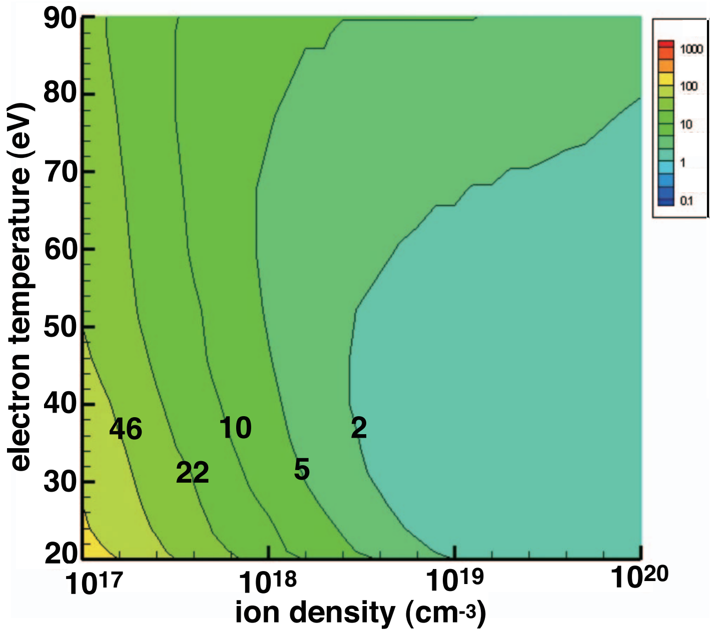
Predicting trends does not depend on details, but does depend on valid assumptions and approximations

Very basic "simulations" have provided extremely valuable guidance

- Steady-state power balance → conversion efficiency (CE)
  laser absorption / atomic kinetics / hydrodynamics / radiative emission
- Low densities → prepulse + longer wavelength laser (CO_2 , λ = 10.6 µm)



Optimum CE, absorbed laser power (λ = 1.06 µm)

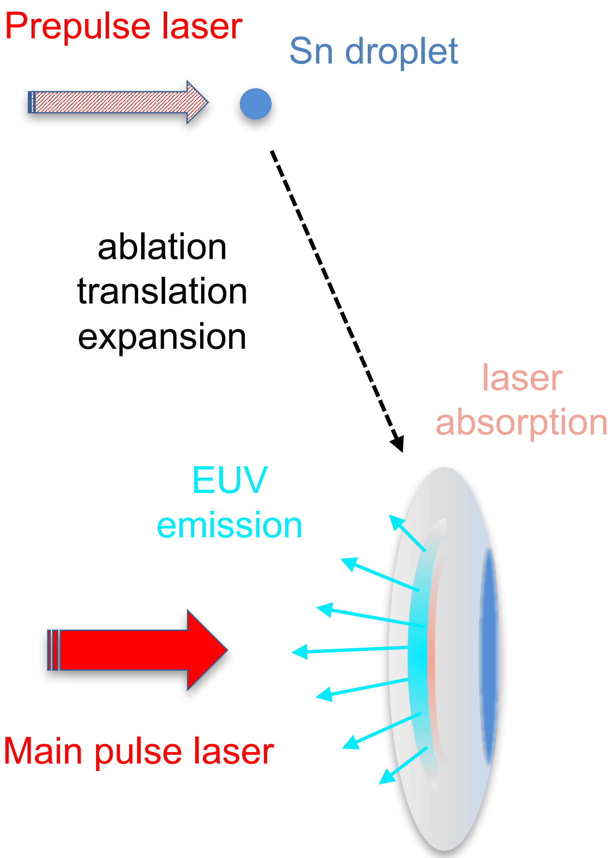


Optimum pulse duration (in ns)

Nishihara, *et al*, Physics of Plasmas **15**, 056708 (2008)

Physical processes important for EUV generation

- Laser absorption
  - 1 µm (Nd:YAG) or 10 µm (CO_2)
- Mass transport
  - particles or hydrodynamics
- Energy transport via radiation, conduction, advection
- Non-LTE atomic kinetics
- EUV (+ other) radiation production
- Radiation transport



These processes are all interdependent

Basic description at the microphysical scale - “first principles”

- Laser absorption / radiation transport
  - Maxwell’s equations + plasma physics
- Transport of particles and energy
  - Kinetic equations → Boltzmann / Vlasov equations + moments + transport coefficients
- Atomic physics
  - Schroedinger / Dirac equation for multi-electron atoms

Simulation at this level is difficult and time-consuming

Simulation at a macroscopic level requires numerous approximations and compromises

- Basic descriptions are replaced by derived models
  - Analytical models, tabulated data, “averaged” equations
  - e.g. Laser absorption modeled with ray tracing + inverse bremsstrahlung
  - e.g. High collisionality limit → Hydrodynamics for mass transport
- Operator splitting
  - Each physical process is calculated separately
  - Splitting methods must respect the physical coupling between processes and obey relevant conservation laws
- Discretization methods with finite resolution
  - Discretized solutions should converge to the continuous solution at high resolution
  - Implicit time discretizations avoid resolving very small timescales

How do these approximations affect our interpretations of (and insights from) the simulation results?

Laser absorption (macroscopic)

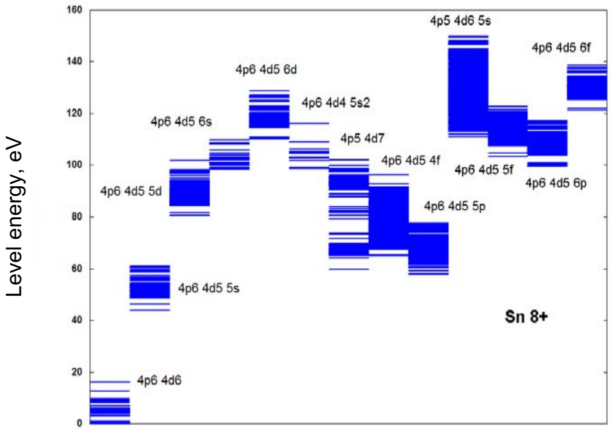
- Absorption of low intensity laser light in a low density ideal plasma is well-described by
  - Geometrical optics ray tracing in a refractive medium
  - Inverse bremsstrahlung absorption (including refractive effects)
- Low level of non-linearities, plasma instabilities, scattering
- Non-ideal plasma effects on absorption / refraction are usually small for long wavelengths
- Main challenges are
  - Absorption in solid / liquid tin
    wave characteristics, small spatial scales
    production of energetic particles
  - refractive raytracing in 2D / 3D expanding geometries

Low intensity: $I \lambda_{\mu}^{2} < 10^{15}$ W cm^{-2}

This approach has been verified with (ideal) microscopic simulations and is in widespread use

Atomic physics of EUV-producing Sn

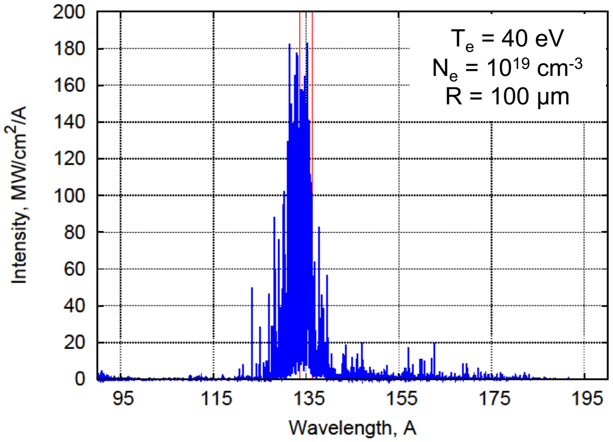
- Transitions producing 13.5 nm radiation:
  4f-4d, 4d-4p, 5d-4p in $Sn^{+8\text{-}13}$
- Data must cover all charge states up to > +28
- Atomic levels sufficient to converge populations
  → very large # of levels (>10^3 per charge state)
  → very high resolution needed for spectrum



Koshelev, *et al*, 2006 Source Workshop

Possible approximations:

- Limited accuracy QM calculations
- Omit / average levels and transitions
- Less resolution inspectrum



Zakharov, *et al*, SPIE 7969, 2001

Atomic physics + NLTE kinetics

- NLTE: Non-Local Thermodynamic Equilibrium
  → excited state populations not in Saha-Boltzmann distribution

- Evaluation of populations:
  Atomic data (energy levels, transition cross-sections)
  - + Electron and photon distributions
    → atomic populations (time evolution)
  - + radiative cross-sections
    → radiative emission / absorption
  - + radiation transport
    → $T_e + T_i$ + photon distribution

iterative procedure

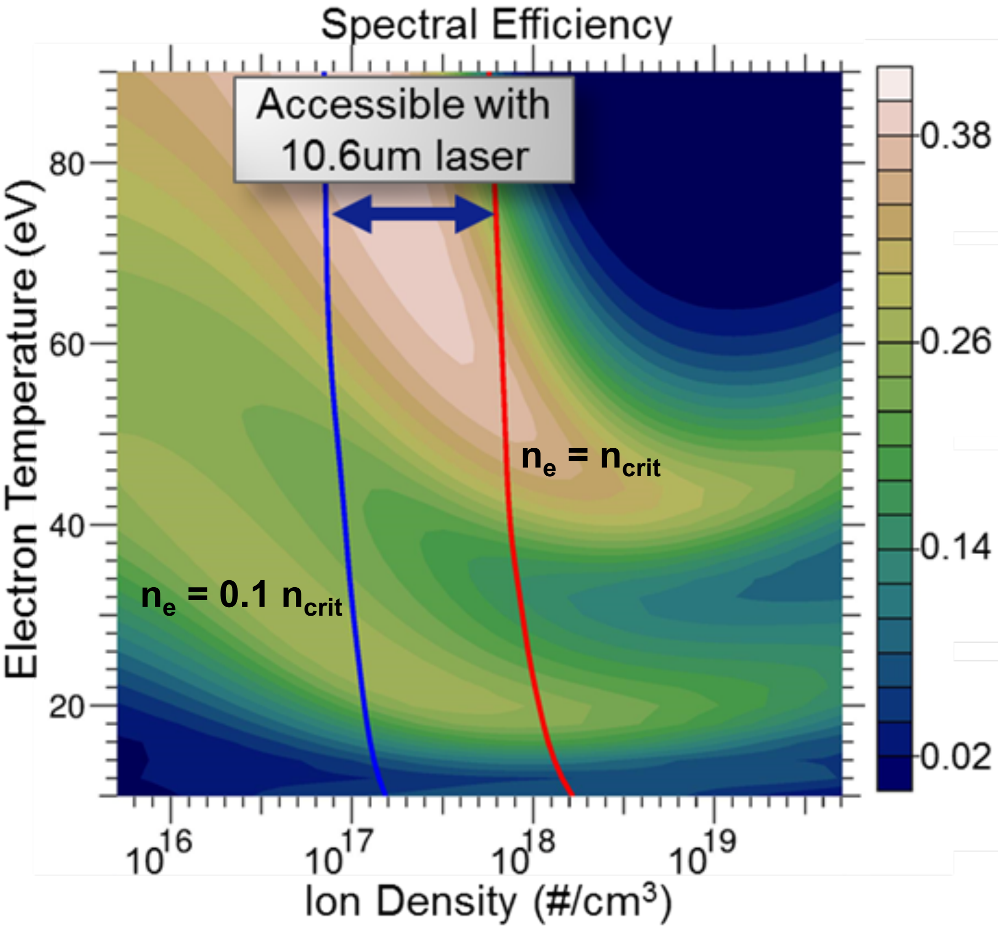
- Populations and radiation are tightly coupled

Atomic physics provides the EUV-producing transitions
NLTE kinetics drives the radiative emission

NLTE kinetics of EUV production

- Spectral efficiency:
  fractional emission in bandpass
- Bandpass emission comes from material with $n_e \sim 0.1\ n_{crit}$
- Calculated with highly-averaged atomic data
- Assumes steady-state, no radiation field
- Timescales for low n_e, high T_e exceed laser pulse timescale

→ Minimal benefit to pursuing lower densities

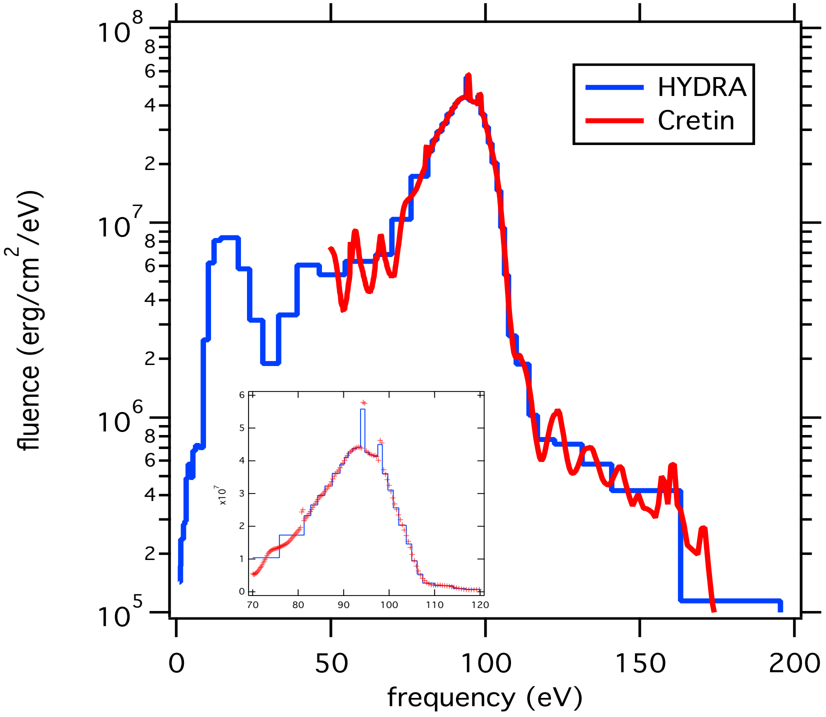


Incorporating NLTE atomic kinetics into rad-hydro

- Tabulated methods allow inexpensive use of complete atomic data
  - Assumptions / approximations are built into the table
    - NLTE equations solved in steady-state
    - Radiation field specified by assumed conditions
  - Coupling to other physics is severely limited

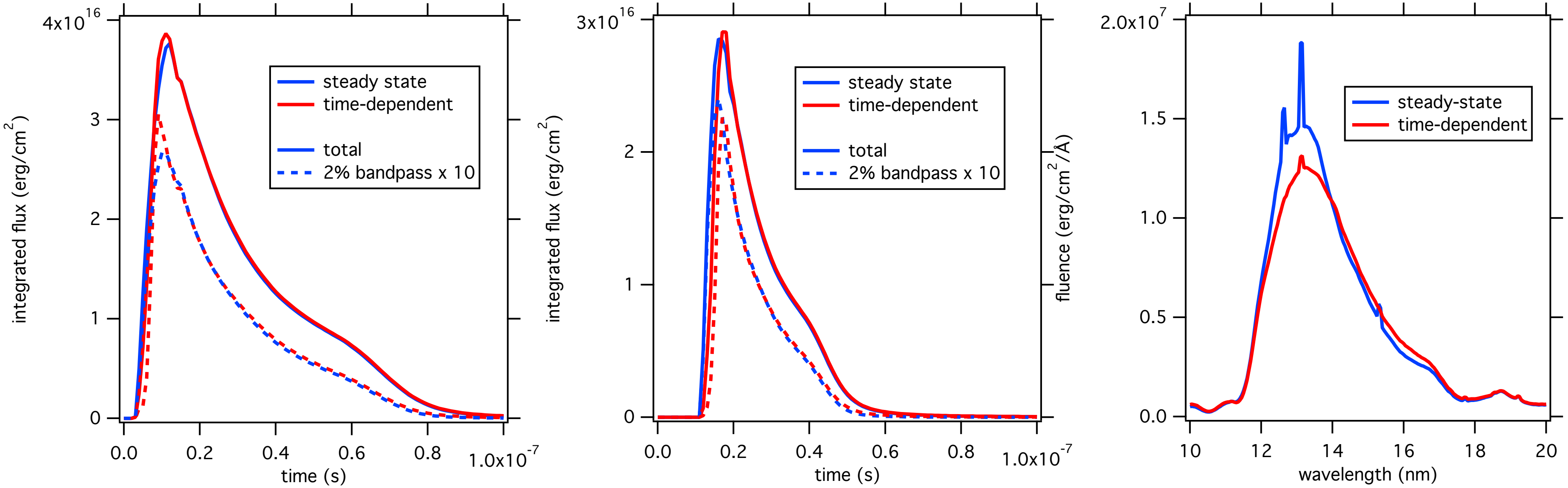
- Inline methods allow full coupling
  - Complete atomic data is prohibitive in CPU time and memory usage
  - Use averaged atomic data
  - Frequency resolution sufficient for energy balance
  - Higher frequency resolution can be restored by postprocessing
  - Approximations can be relaxed by using less averaging

1D rad-hydro + postprocessing



Time-dependent or steady-state kinetics?

- Inline kinetics are run in a time-dependent mode
- Postprocessing can use either time-dependent or steady-state mode
- Validity of steady-state kinetics is necessary for a tabular approach



100 ns pulse, ~10 ns risetime

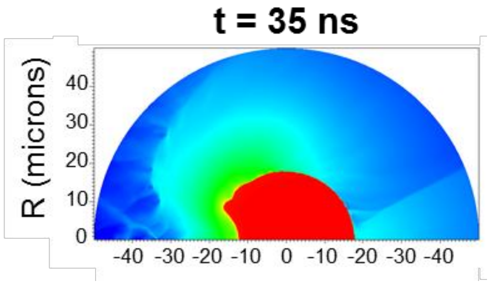
½ x timescale, 2x intensity

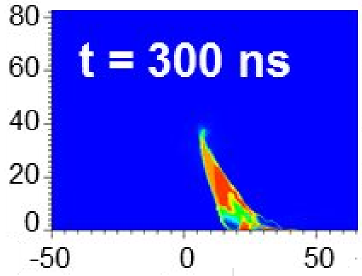
A fast-rising pulse requires a time-dependent treatment

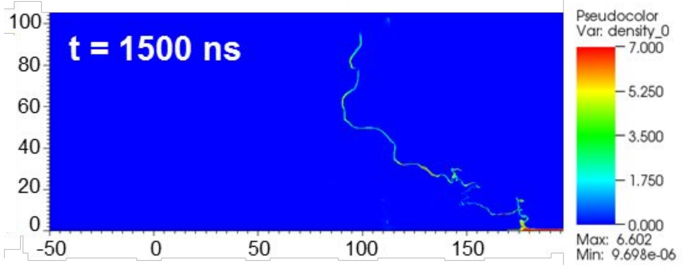
Insights from a pre-pulse simulation

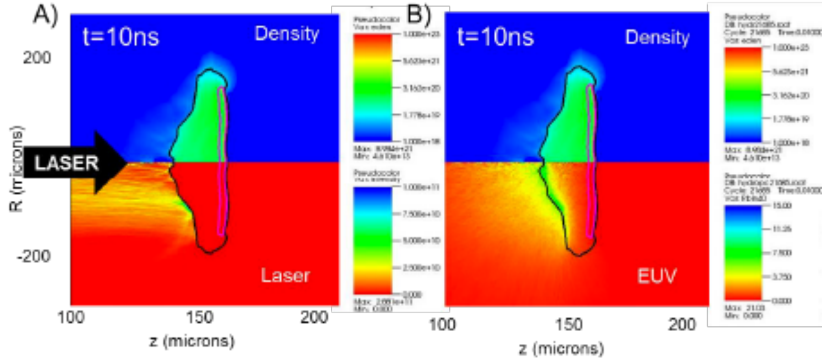
- Pre-pulse turns spherical droplet into a thin strand surrounded by a low-density plasma

- Main pulse is absorbed up to critical surface, well away from the high-density material

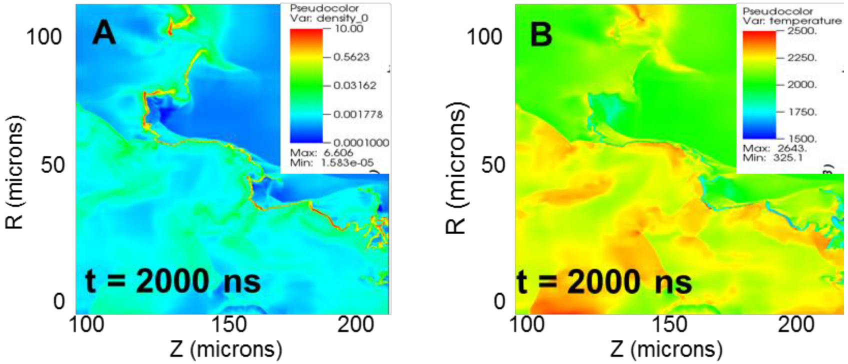








Purvis, et al, SPIE 9776, 2016



Behavior is much like a "mist" target

EUV simulation efforts

- LLNL / UC Berkeley (HYDRA, CRETIN, ALE/AMR, LSP)
  - Fully integrated physics in 3D (massively parallel) + postprocessing
  - Attempts to minimize uncontrolled approximations
  - Aimed at a predictive capability (single shots w/ prepulse)
- ISAN / EPRA / KIAM / Institute of Spectroscopy (Z*, RZLINE, RALEF + OpenFOAM)
  - Partially integrated full physics in 2D + postprocessing, 3D hydrodynamics
  - Models tailored for good results under reasonable conditions
  - Aimed at fast turnaround (but more detailed simulations are available)
  - Now doing system level simulations with multiple laser shots
- JAEA (STAR, …)
  - Integrated plasma hydrodynamics in 2D
  - Developing an integrated capability
- Purdue / ANL (HEIGHTS)
  - Integrated physics in 3D + Monte Carlo ion production

A useful simulation program should operate at all levels

Summary – what is next for EUV simulations?

- Simulation capabilities are improving
  - Macroscopic models based on higher fidelity microscopic models
  - Multiple physical processes with better coupling algorithms
  - Capability to test approximations with more fundamental methods
  - Larger, faster computers allow better models and/or higher resolution
- Confidence requires comparisons to multiple experiments
- Producing a predictive capability will take a dedicated effort

Simulations can provide important guidance for EUV production, but only if the industry is prepared to understand the results

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