Spectroscopic and X-Ray Scattering Models in SPECT3D

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SPECT3D Imaging and Spectral Analysis Package

- SPECT3D is a collisional-radiative spectral analysis package used to compute:
  - Detailed emission and absorption spectra
  - Filtered images (e.g., X-ray framing camera, monochromatic images)
  - XRD signals

- A wide variety of 1-D, 2-D, and 3-D geometries are supported:
  - 1-D planar, cylindrical and spherical
  - 2-D Cartesian X-Y, cylindrical R-Z
  - 3-D Cartesian X-Y-Z

- Atomic level populations (LTE or Non-LTE), spectra, and images are computed for:
  - Plasma distributions from multi-D simulation codes (ALEGRA, CTH, DRACO, HYDRA, LSP, ...)
  - User-defined plasma distributions generated by PlasmaGen code.

- Time-dependent kinetics based on time-dependent hydro properties is supported.

- Radiative transfer along lines-of-sight is computed using an integral transport approach.

- Radiographs can be computed using either continuum or line backlighters.

- SPECT3D is a user-friendly code that provides:
  - Direct comparisons between simulation results and experiment (images, spectra)
  - Tools for obtaining physical insight into the plasma radiative properties and experimental measurements
New Features of SPECT3D

- Various improvements have been made to support post-processing of large-scale multi-dimensional hydrodynamics grids:
  - Significantly reduced memory requirements,
  - The implementation of multi-threading has been improved,
  - Substantial improvements have been made to algorithms used to compute the intersections of the hydro grid with lines-of-sight (LOSs),
  - Volume elements may be grouped into sectors (or sub-domains) for LOS-sector intersections calculations.

Test case, hot radiating spheres:
- 1000 photon energy points,
- ~ 52 million volume elements,
- 14 distinct non-DCA materials,
- 250x250 pixel detector,
- ~50 minutes clock time (multi-threaded, 4 cores).

- Added support for PDB/SILO format (HYDRA).
The x-ray scattering model, based on a formalism developed by G. Gregori, has been added to the multi-dimensional collisional-radiative spectral and imaging package SPECT3D.

- Scattering angle determined by the positions of the volume element, the detector and the source.
- Scattering is added to the local source function in every zone.
- Source and scattered photons are transported as they propagate through the plasma.
X-ray Thomson Scattering (XRTS) Model

Scattering cross-section:
\[
\frac{d^2\sigma}{d\Omega d\omega} = \frac{3}{8\pi} N_i\sigma_T \frac{1 + \cos^2\theta}{2} \left(\frac{\omega_1}{\omega_0}\right)^2 S(k, \omega)
\]

Total dynamic structure factor:
\[
S(k, \omega) = |f_1(k) + g(k)|^2 S_{\text{ii}}(k, \omega) + Z_f S_{\text{ee}}^0(k, \omega) + Z_c \int \tilde{S}_{\text{ee}}(k, \omega - \omega') S_s(k, \omega') d\omega'
\]

- Density correlations of electrons that dynamically follow the ion motion. Includes both core and free electrons.
- Scattering from free electrons that do not follow the ion motion. Includes contributions from truly free and valence electrons.
- Inelastic scattering by core electrons. Rises from bound-free transitions.

Spectrally resolved elastic and inelastic scattering features can be used to determine:
- Electron temperature,
- Electron density,
- Average ionization,
- Structure of matter.
Benchmarks for Single Cell Plasma: $Z_{\text{free}}$ and Angle

Scattering angle = 135°

Calculations were performed for a uniform, single cell carbon plasma:
- $T = 10$ eV,
- $\rho = 0.72$ g/cm³
- Source energy = 4.750 keV.
SPECT3D supports apertures by computing the intersection of lines that connect cell centers and the x-ray source through the aperture.
Isochorically heated beryllium plasmas were probed by observing the forward scattering of the narrow-band chlorine Lyα line with an energy of 2.96 keV.

- $T_e \sim 10 - 15$ eV,
- $N_e \sim 2 - 3 \times 10^{23}$ cm$^{-3}$,
- Scattering angles: $25^\circ < \theta < 55^\circ$.

Foam Scattering Data, Experimental Setup

Spec. A
Source monitor
Viewing laser spot thru foam at 10° from rear Mn surface normal

Spec. B
Captured Scattering
eff. atten. Cu = 0.85 mm

TPX (CH2) 0.23 g/cc
3 mm dia.

50 micron Au 2 mm tall exit aperture
200 um wide Au spatial fiducial 1.14 mm from foam front

Spatial res. direction

Pinhole Camera
Viewing 10° from Mn surface normal

ZBL
2.2 kJ
3e15 W/cm2

5 mm

0.66 mm
45°
137°

5 mm

0.22

0.24
148°

3 mm

Courtesy of Eric Harding
Foam Scattering Data, Space-Resolved Spectra

Mn source plasma viewed through Cu

Foam scattering signal. The dark line is from the Au fiducial

Simulated Spectrum

Laser

Mn plasma plume

Faint tail originates from bound-free scattering

Experimental data from shot 34. Courtesy of Eric Harding
Foam Scattering Data, SPECT3D Analysis

Spatial distribution of experimentally measured and computed scattered signal. The lineout is averaged over FWHM of the Mn He-alpha at 6181 eV.

Comparison of an x-ray scattered spectrum (spectrometer B) The synthetic spectrum utilized the experimentally-measured x-ray source (spectrometer A).
Application: He Emission in a Small Tokamak


SPECT3D simulation: toroidal He plasma configuration, T=57 eV, N_\text{i}=7.2\times10^{12} \text{ cm}^{-3}
Conclusions

- SPECT3D Imaging and Spectral Analysis package was upgraded to support modeling of HEDP experiments in which x-ray scattering is used as a diagnostic to determine plasma conditions.

- Integration with the latest version of the X-ray Thomson Scattering (XRTS) code (ver. 5.0.1), was implemented in a way that will simplify further code development and maintenance.

- SPECT3D calculations show the importance of modeling the x-ray scattering for the full range of angles and volume elements that contribute to the measured x-ray spectrum.

- Preliminary analysis of experimental data indicates the importance of accurate modeling of geometry effects on scattered spectra and its implications in interpreting the experimental results.