Enhancing spectral and temporal beam diagnostics at European XFEL

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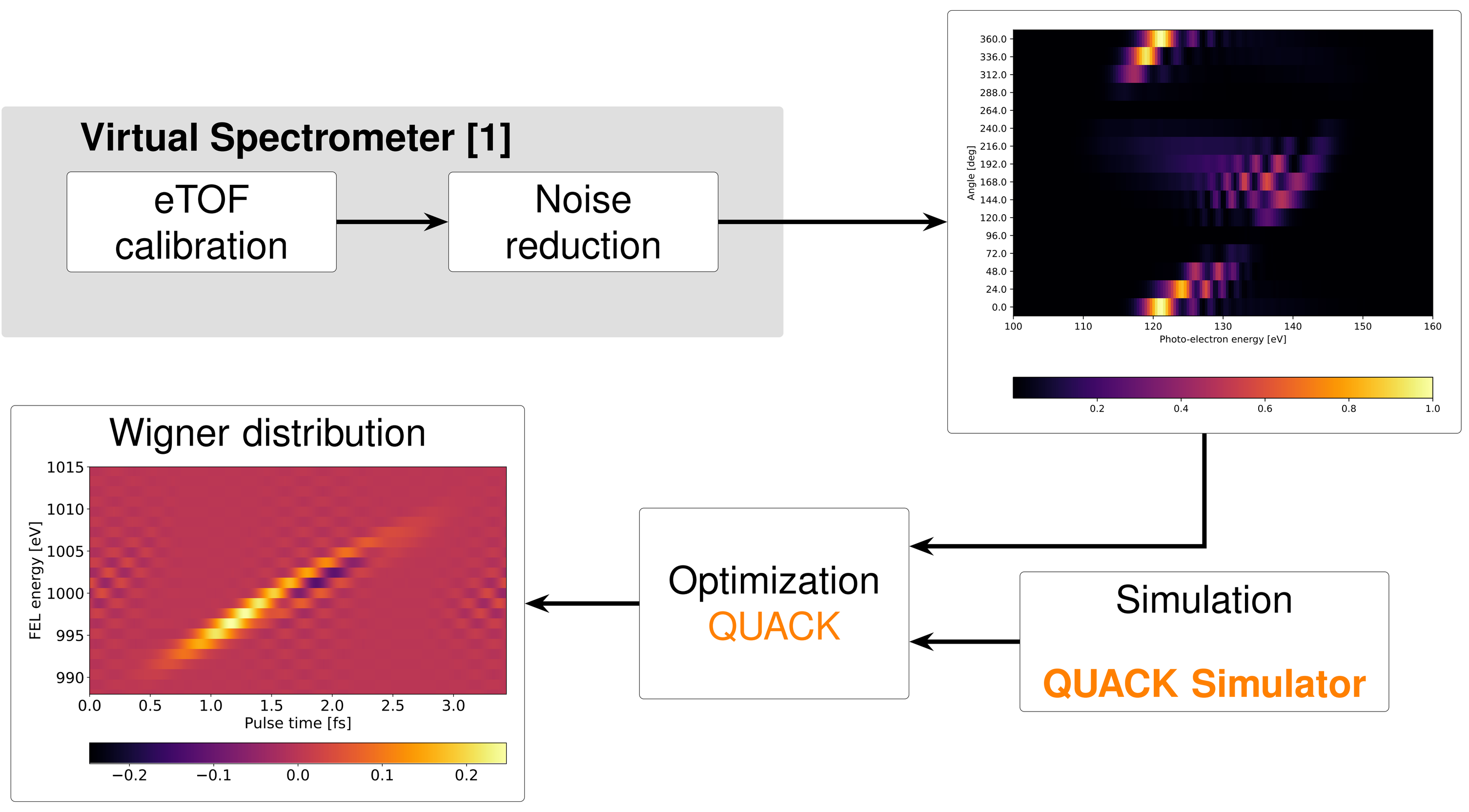
[1]European X-Ray Free Electron Laser

Temporal diagnostics

- High-quality temporal and spectral beam information is essential for several experiments.
- Angular streaking experiments:
  - Beam ionizes gas and produces photo-electrons.
  - Circularly polarized optical laser streaks photo-electrons.
  - *Encodes time spectrum information in energy and angular distribution of photo-electrons.*
- Improve and automate analysis:
  - *Virtual Spectrometer* automates and enhances from angle-resolved TOF spectrometers.
  - QUantum-based Angular streaking ReConstruction Kode reconstructs spectrum.

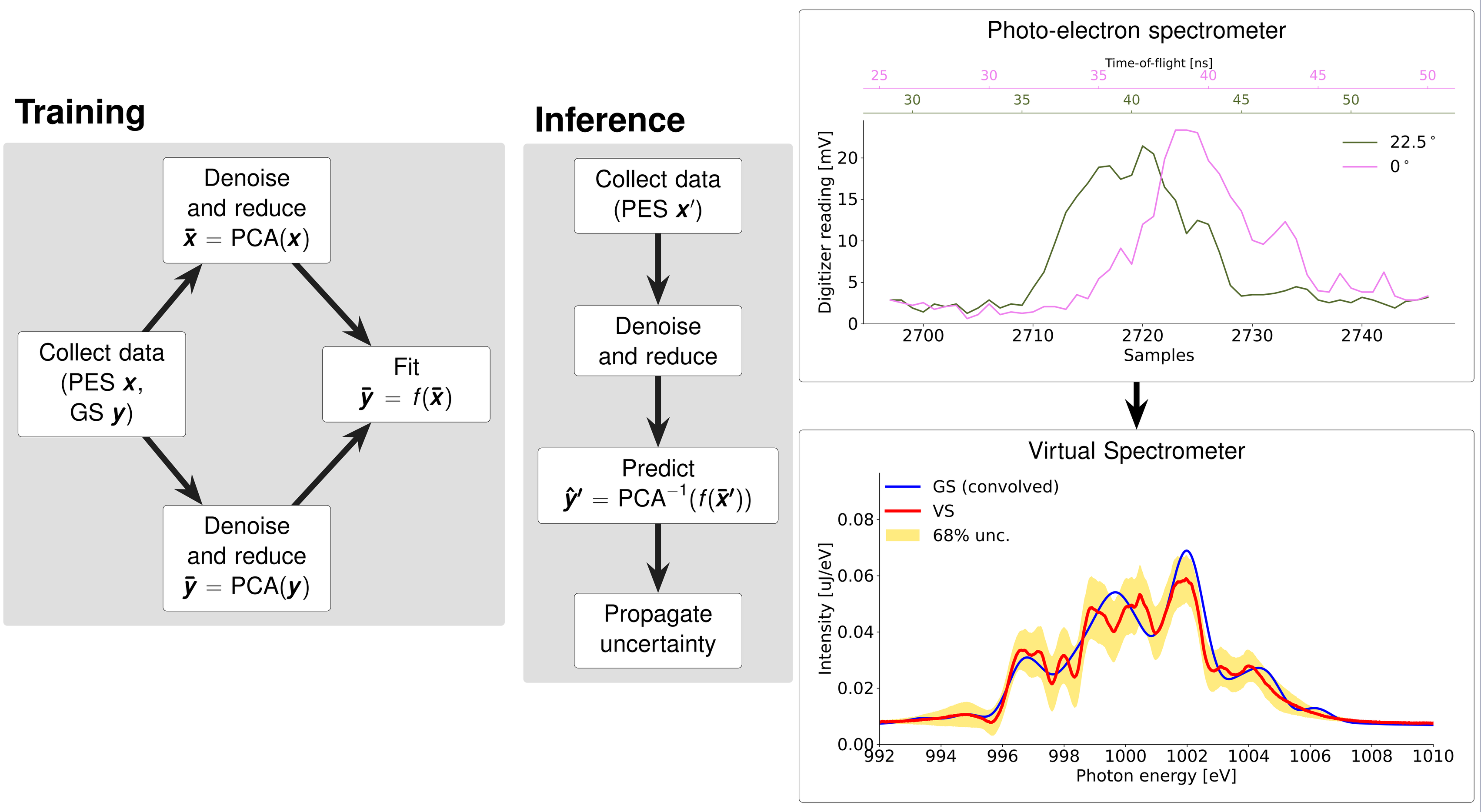


Virtual Spectrometer

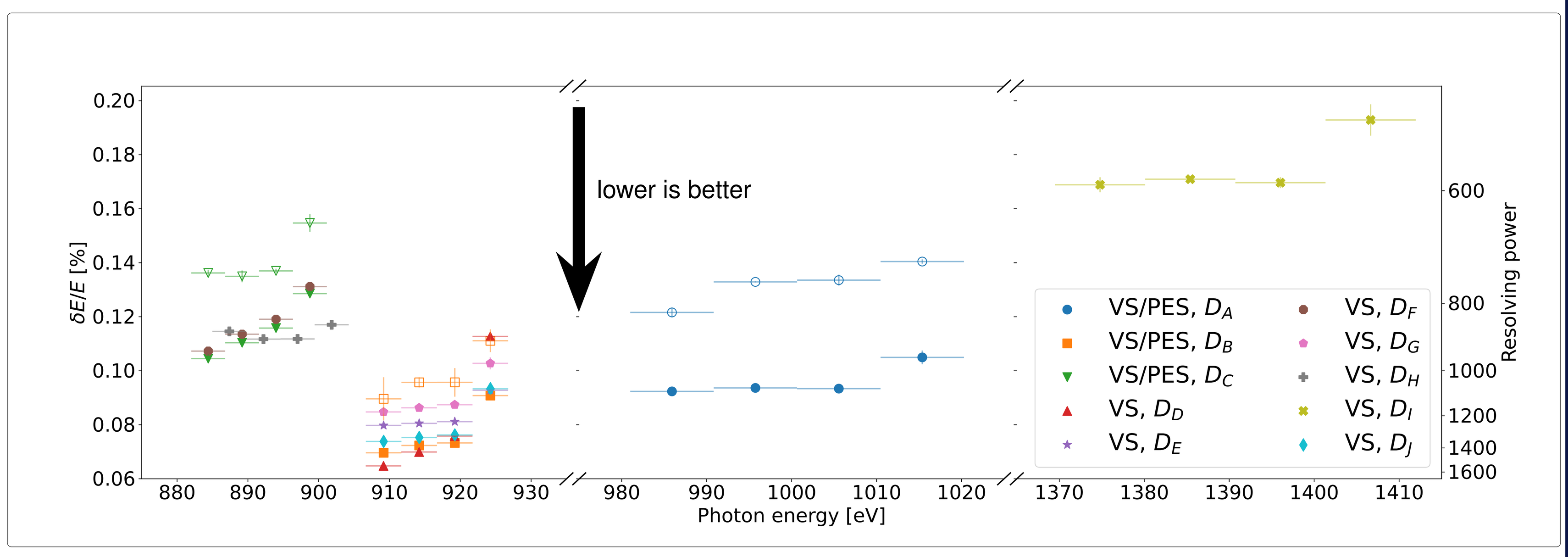
Spectral diagnostics devices available in SASE3:

Grating Spectrometer (GS)	*Photo-Electron Spectrometer (PES)*
High resolution.	Low resolution.
Simple calibration	Complex calibration.
Invasive.	Non-invasive.
Train-resolved.	Pulse-resolved.

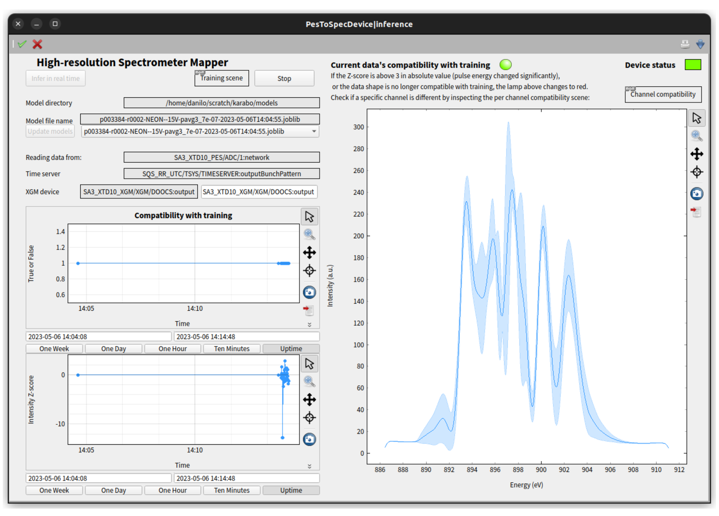
Map PES to GS to get best of both worlds → *Virtual Spectrometer (VS)* [1].



- Systematic resolution studies under several conditions done.
- Comparison with PES show better resolution.



- Software deployed.
- Requires unchanged measurement conditions.
- *Quality control* and *explainability*:
  - Uncertainty informs on results quality.
  - Conditions are monitored and alarmed on.
  - Resolution estimates provided.
  - Interface informs on method and procedure.



Related posters

Electron-photon correlations: towards x-ray pulse diagnostics at MHz repetition rate, F. Bishara
Experiment overview and automated data analysis with DAMNIT, T. Michelat
Interpretable Machine Learning at the EuXFEL, D. Ferreira de Lima

QUACK

QUACK Simulator

- Strong Field Approximation [2] with first order perturbative expansion on FEL-gas interaction.
- Calculate amplitude b for a photo-electron detection with momentum $\boldsymbol{p}$ due to a FEL with photon energy $\hbar\omega$.
- Transition dipole moment $\boldsymbol{d}$ estimated with XATOM [3].

$$b(\boldsymbol{p},\hbar\omega) = \frac{i}{\hbar}\int_0^{t_{\mathrm{detection}}} dt'\,\boldsymbol{E}(t')\cdot\boldsymbol{d}(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}(t'))\exp\left\{-\frac{i}{\hbar}\left[\phi(t_{\mathrm{detection}})-\phi(t')\right]\right\}$$

$$\phi(t) = \int_0^t d\tilde{t}\left[\frac{1}{2m_e}(\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}(\tilde{t}))^2 + I_p\right]$$

QUACK Reconstruction

- Reconstruct observation intensity $\boldsymbol{y}$ from simulated amplitudes $\boldsymbol{b}$.
- Prediction: $\hat{\boldsymbol{y}}$.
- Electric field Fourier coefficients: $\boldsymbol{x}$.
- Non-linear phase retrieval algorithm [4] used to obtain electric field expansion.

$$E_x(t) = \mathrm{Re}\left\{\sum_n x_n e^{i\omega t}\right\} \qquad x_n \in \mathbb{C}$$

$$\hat{\boldsymbol{y}} = |\boldsymbol{b}\,\boldsymbol{x}|^2$$

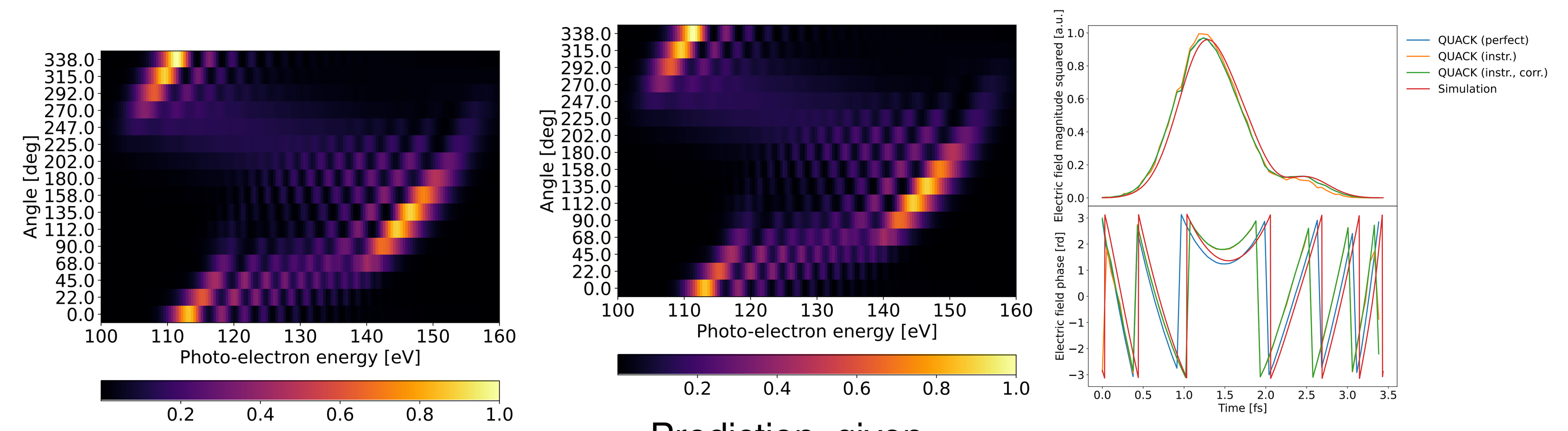
$$\boldsymbol{x} = \mathrm{argmin}_{\boldsymbol{x}}\left[\hat{\boldsymbol{y}}-\boldsymbol{y}\right]^2$$

$$\boldsymbol{x} = \mathrm{argmin}_{\boldsymbol{x}}\left[|\boldsymbol{b}\,\boldsymbol{x}|^2-\boldsymbol{y}\right]^2$$

- QUACK's output is the electric field of the X-ray pulse.
- We use the formalism in Ref. [5] to obtain a Wigner distribution per X-ray pulse.

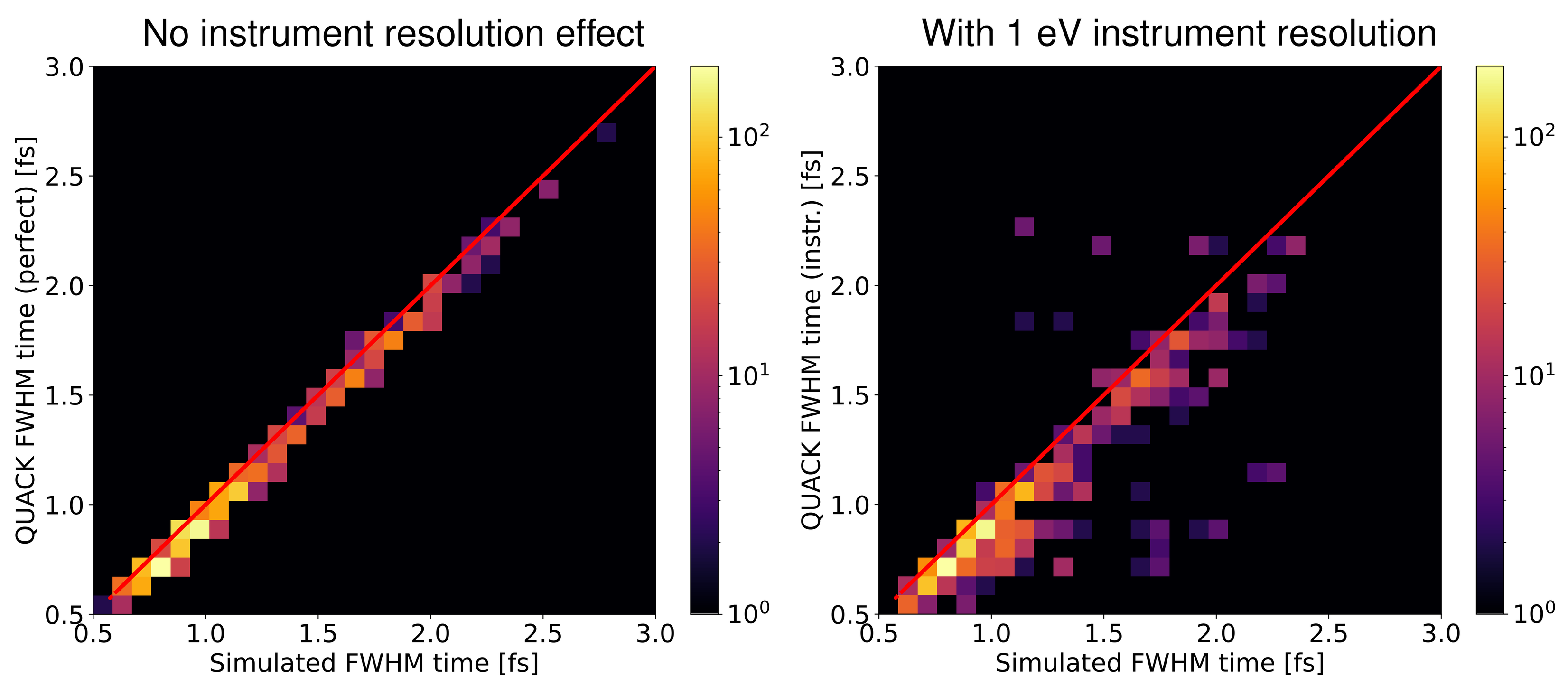
$$\Gamma(t,\Delta t) = E_x(t)\,E_x^*(t+\Delta t)$$
$$\mathcal{W}(t,\omega) = \mathcal{F}_{\Delta t\to\omega}\{\Gamma(t,\Delta t)\}$$

- QUACK can provide the FEL field including phase.
- Example: linear chirp, circular polarization.
- Detector effects in the right-hand-side plot: 1 eV Gaussian resolution.



Simulated observation | Prediction, given reconstructed spectrum | Reconstructed electric field time spectrum

- Width calculated from the intensity time spectrum.
- Without detector effects, QUACK reconstructs the time FWHM very well.
- Detector effects (right-hand-side) include only 1 eV Gaussian resolution.



Summary

- Data science methods can be leveraged to enhance the spectral and temporal diagnostics of X-ray pulses.
- The Virtual Spectrometer combines the advantages of two different spectrometers leveraging machine learning.
- QUACK leverages the Virtual Spectrometer to improve the quality of its output.
- Interpretability, explainability and quality control assets to guide towards adequate solutions.

References

[1] Danilo Enoque Ferreira de Lima et al. "Machine-learning-enhanced automatic spectral characterization of x-ray pulses from a free-electron laser". In: *Communications Physics* 7.1 (Dec. 2024), p. 400. URL: https://doi.org/10.1038/s42005-024-01900-6.

[2] Kasra Amini et al. "Symphony on strong field approximation". In: *Reports on Progress in Physics* 82.11 (Oct. 2019), p. 116001. URL: http://dx.doi.org/10.1088/1361-6633/ab2bb1.

[3] Sang-Kil Son, Linda Young, and Robin Santra. "Impact of hollow-atom formation on coherent x-ray scattering at high intensity". In: *Phys. Rev. A* 83 (3 Mar. 2011), p. 033402. URL: https://link.aps.org/doi/10.1103/PhysRevA.83.033402.

[4] Tuomo Valkonen. "A primal–dual hybrid gradient method for nonlinear operators with applications to MRI". In: *Inverse Problems* 30.5 (May 2014), p. 055012. URL: https://dx.doi.org/10.1088/0266-5611/30/5/055012.

[5] Svitozar Serkez et al. "Wigner distribution of self-amplified spontaneous emission free-electron laser pulses and extracting its autocorrelation". In: *Journal of Synchrotron Radiation* 28 (Dec. 2020), pp. 3–17.