ELI-ALPS Research Institute
TOWARDS THE SHARP END OF ATTO SCIENCE

Macroscopic quantum simulation of high-order harmonic generation in a gas jet, using upgraded 1D atomic model potentials

Krisztina Sallai, Szilárd Majorosi, Szabolcs Hack, Attila Czirják

ELI ALPS, Theory and Simulations Group & University of Szeged, Dept. of Theoretical Physics, Szeged, Hungary

GPU Day 2026,
HUN-REN Centre, Budapest, May 29, 2026.

SZÉCHENYI 2020
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Krisztina Sallai, PhD student

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Outline

- ELI ALPS, HHG, attosecond pulses
- MMA-HHG code structure
- 3D vs 1D simulations in strong-field physics
- Upgraded 1D soft-core Coulomb potential (GSC)
- Preliminary numerical results from Komondor
- Conclusions and outlook

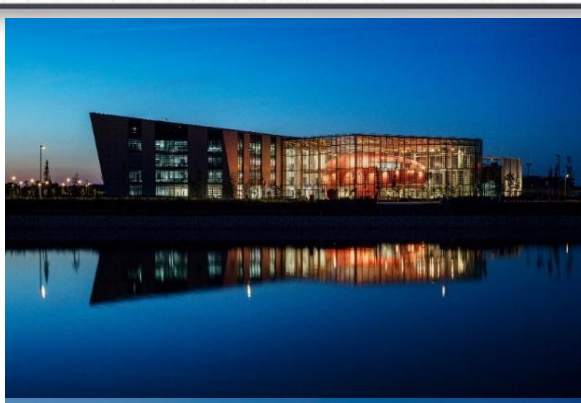
ELI: Extreme Light Infrastructure

International user facility for researchers of various disciplines.

ELI is a **distributed research infrastructure**

- Hungary (ELI-ALPS)
- Czech Republic (ELI Beamlines)
- Romania (ELI-NP)

ELI ALPS is concluding the Implementation Phase (co-financed by European Regional Development Fund), which is managed by ELI-Hu Nonprofit Ltd.



ELI ERIC

To provide access for European and international researchers to the ELI Facilities in the Czech Republic and Hungary. Integrating the ELI facilities, and move to the Operational Phase

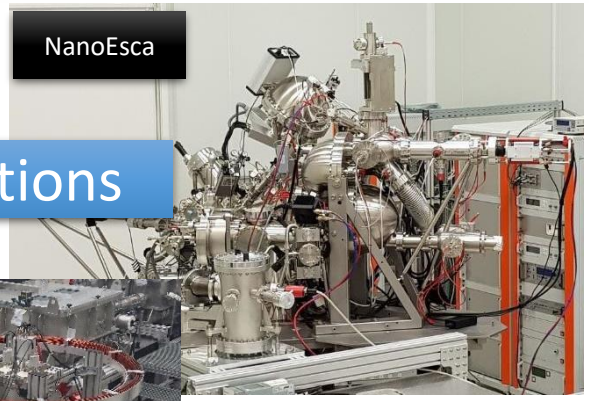
ALPS: Attosecond Light Pulse Source, Szeged

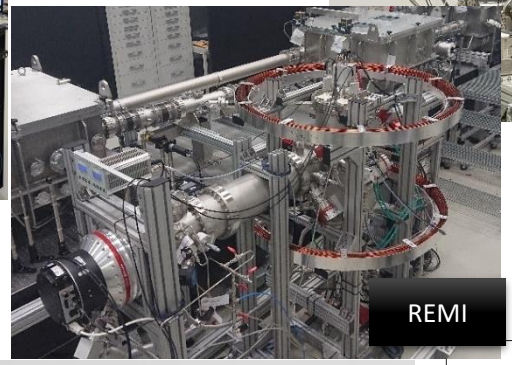
To generate femtosecond and attosecond pulses, for temporal investigations of electron dynamics in atoms, molecules, plasmas and solids.

ELI ALPS Portfolio of research opportunities
Capacity, Capability and Uniqueness

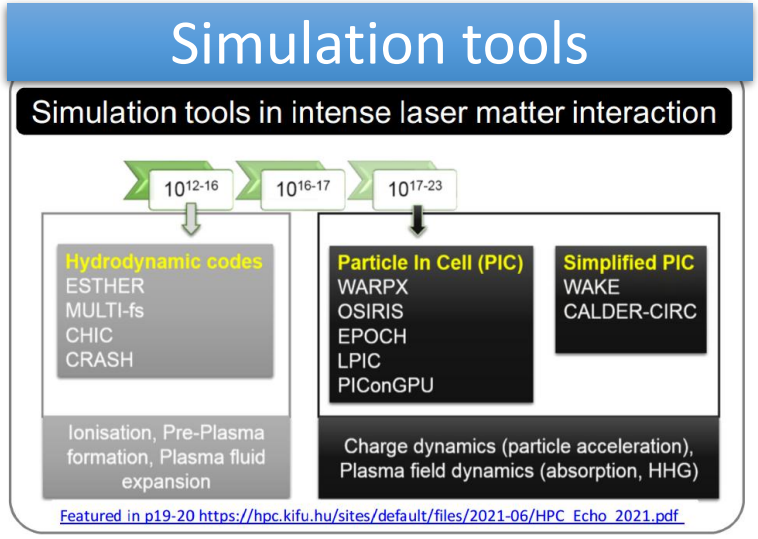
Lasers

Endstations

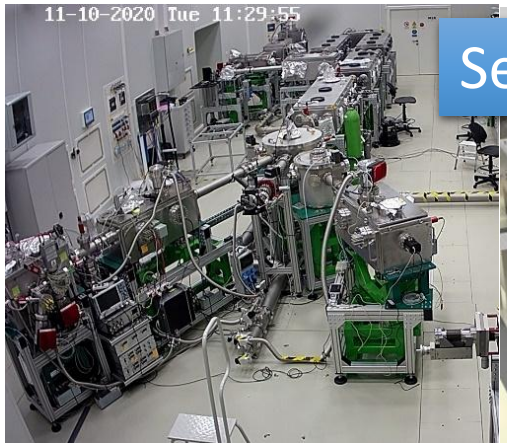




Simulation tools



Featured in p19-20 https://hpc.kifu.hu/sites/default/files/2021-06/HPC_Echo_2021.pdf



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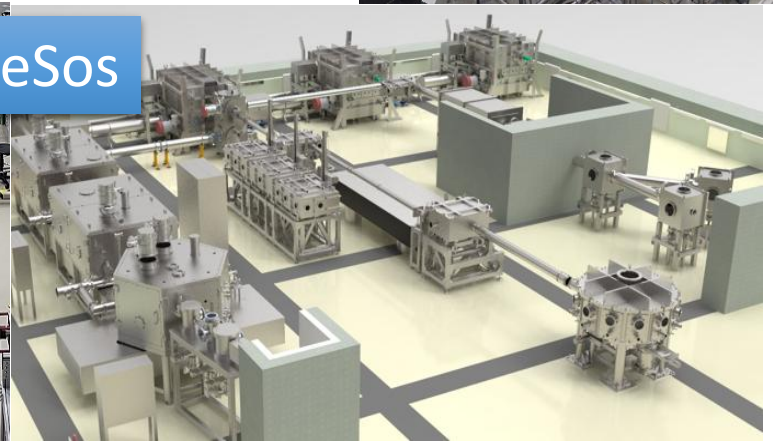
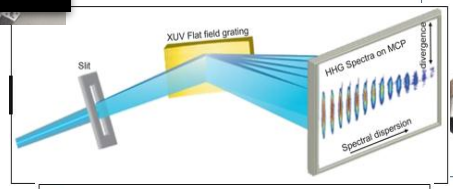
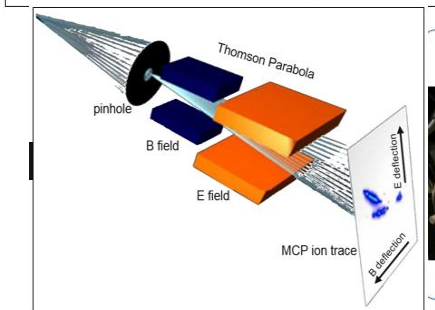
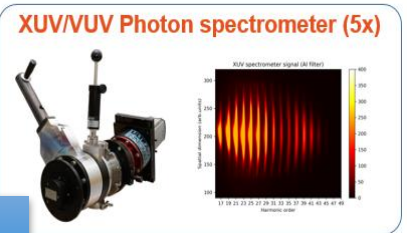
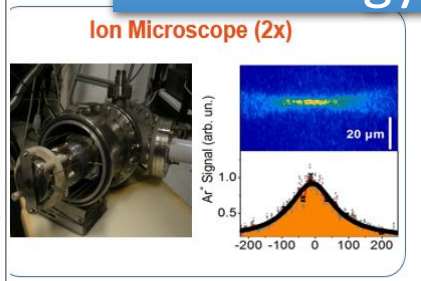


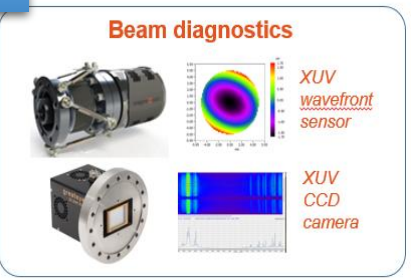
Metrology



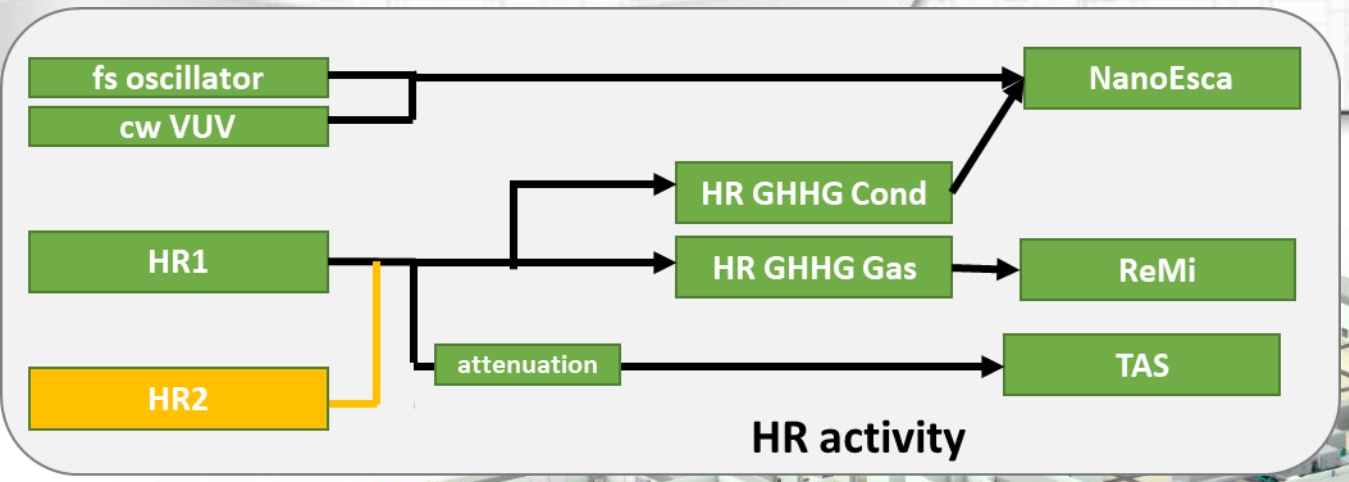








HR GHHG beamlines: attosecond physics



HR2
100 kHz, 7 fs, 5 mJ

- 6 mJ, 76 fs or 9 fs, 3.5 mJ
- problems with beam profile
- CEP stability not addressed
- Development ongoing in Szeged

HR1
100 kHz, 7 fs, 1 mJ

- in user service
- CEP locking @ 600 mrad

HR Condensed + NanoEsca

- beamline commissioned
- monochromatized XUV pulses
- XUV-IR experiments with NanoEsca

HR Gas + ReMi

- ReMi installed
- XUV-IR experiments

HR Alignment
1 kHz, 7 fs, 1 mJ, CEP

- installation

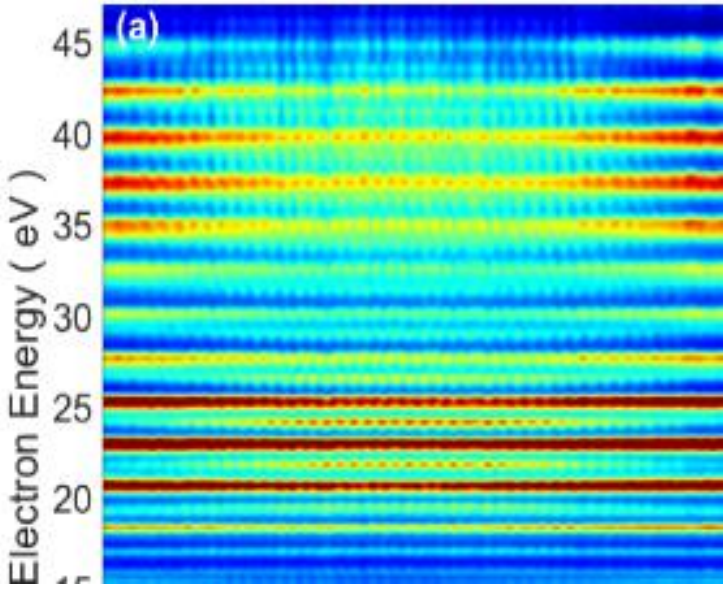
TAS

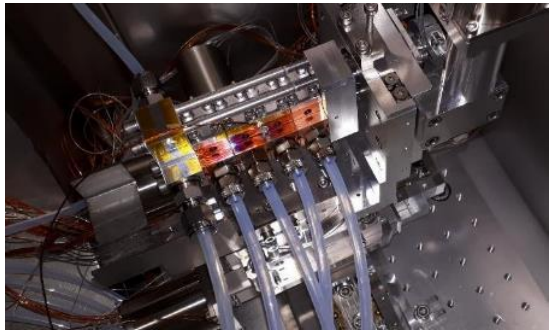
- commissioned

HR GHHG beamlines: attosecond physics

- **XUV-IR pump-probe** studies on **gaseous and condensed targets** at **100 kHz**
- diagnostics for the temporal, spectral and spatial characterization of the XUV pulses
- **flexible reconfiguration** according to user needs
- specially designed, cooled static HHG cell

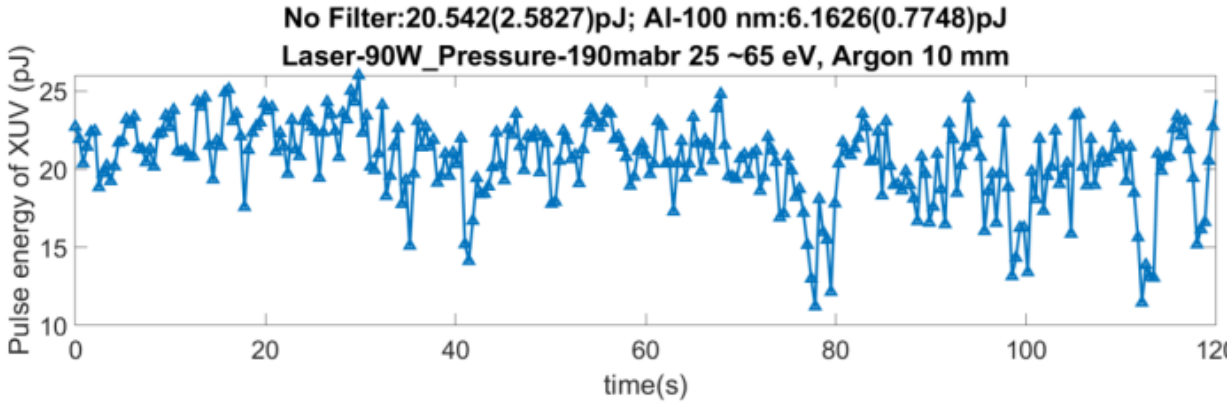
Designed by: CNR IFN Istituto di Fotonica e Nanotecnologie





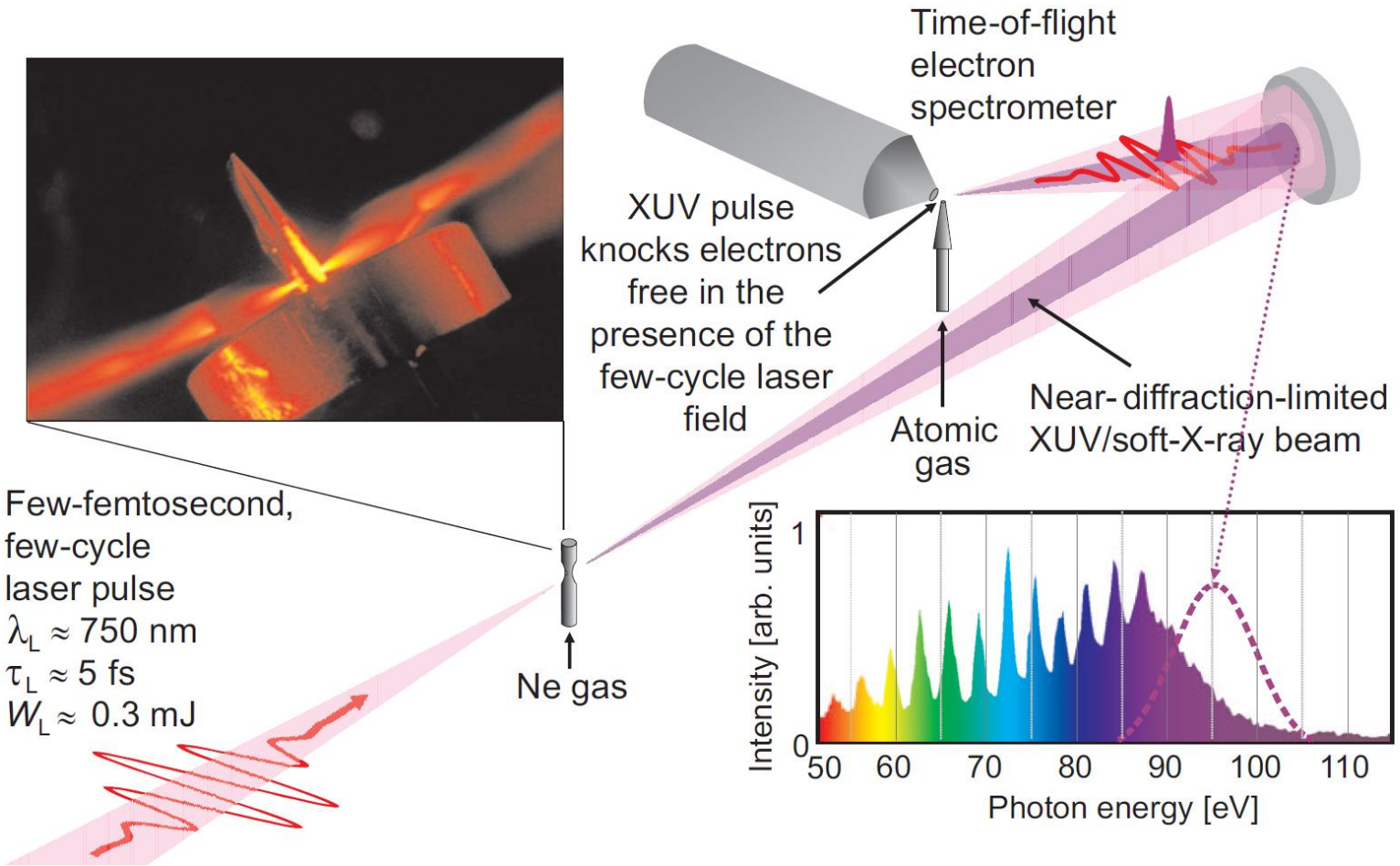
~166 as,
~250 pJ generated,
~50 pJ on target @ 100 kHz

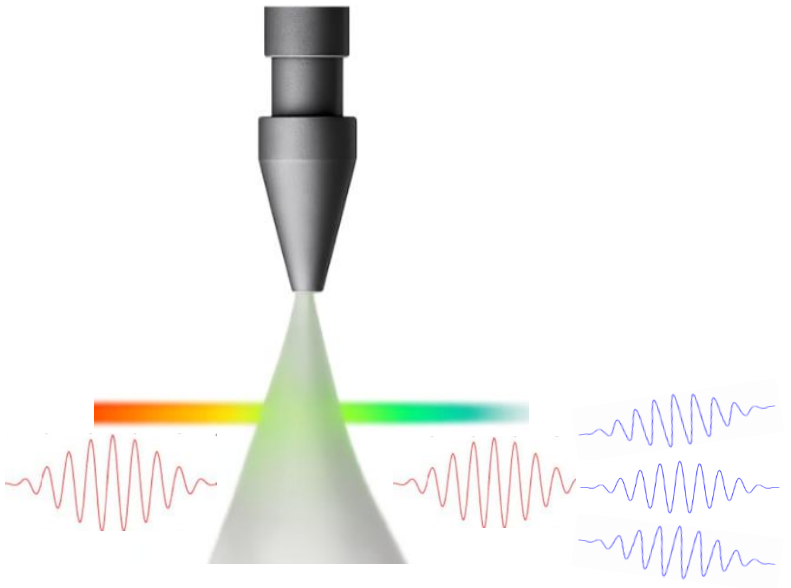
Highest flux attosecond pump-probe beamline @ 100 kHz



Peng Ye *et al., J. Phys. B: At. Mol. Opt. Phys.* **53** 154004 (2020)
Peng Ye *et al.*, *Ultrafast Science* 2022, 9823783 (2022)

Our simulation goal: HHG in a gas jet





F. Krausz and M. Ivanov. Attosecond physics. Reviews of Modern Physics, 81, 2009.

Structure of the MMA-HHG code

Jan Vábek, Tadeás Nemec, Stefan Skupin, Fabrice Catoire

CUPRAD

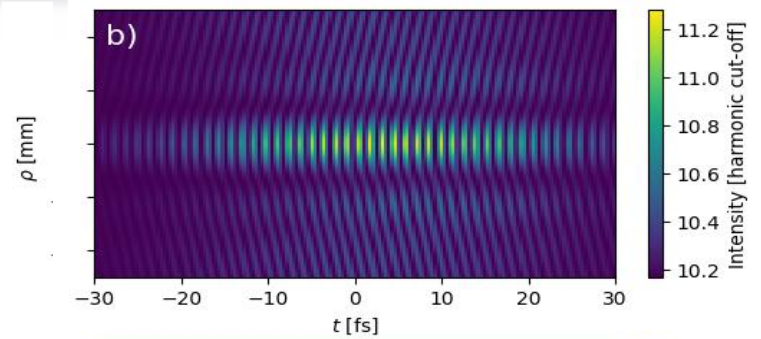
- Parallel Radially Symmetric Unidirectional Solver
- Non-linear laser propagation

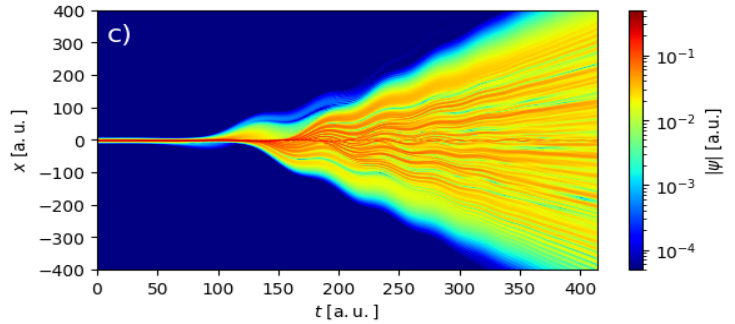
TDSE

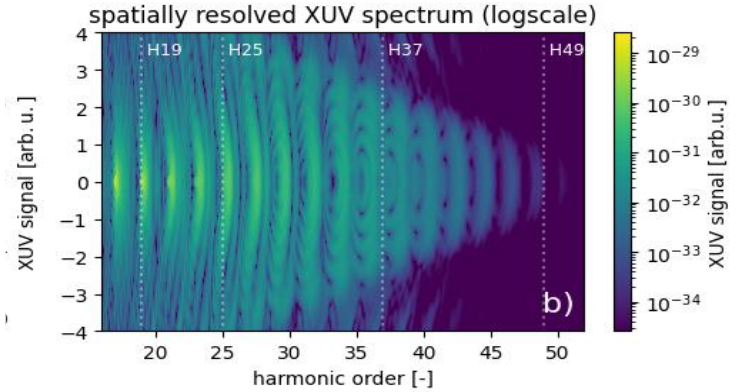
- 1D-TSDE Implementation
- Microscopic response, using SC atomic model pot.

HANKEL

- Linear XUV Propagator
- XUV propagation



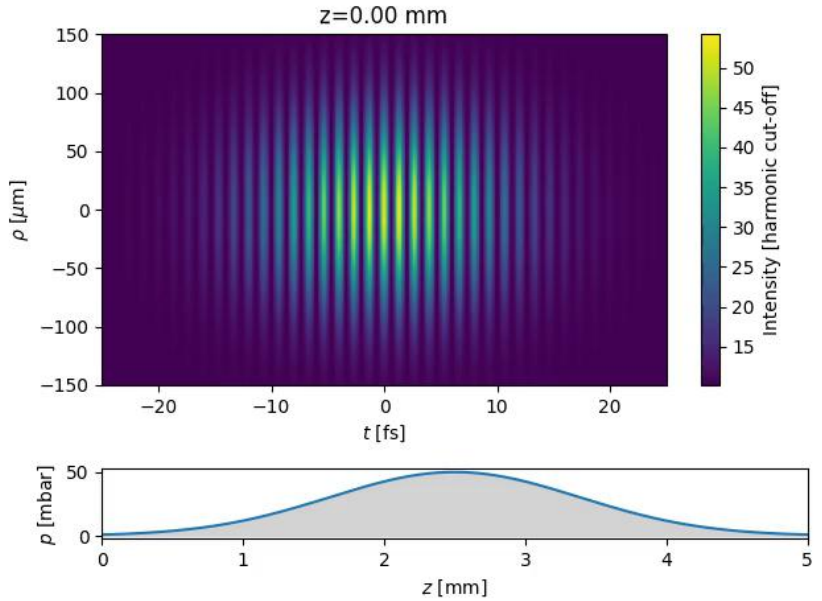




Structure of the MMA-HHG code

CUPRAD – Non-linear Laser Pulse Propagation

- Simulates macroscopic laser propagation
- Linear polarisation
- Cylindrical symmetry
- SVEA approximation
- Split-step scheme
- Includes Kerr response



An illustration of the non-linear propagation of a laser pulse in an argon jet (Gaussian profile bottom panel)

TDSE – Microscopic response

- Solves time-dependent Schrödinger equation
- 1D single-active-electron model (SC)
- Driven by local electric field $E(t)$
- Outputs dipole acceleration
- Parallel over spatial grid points
- Crank-Nicolson scheme

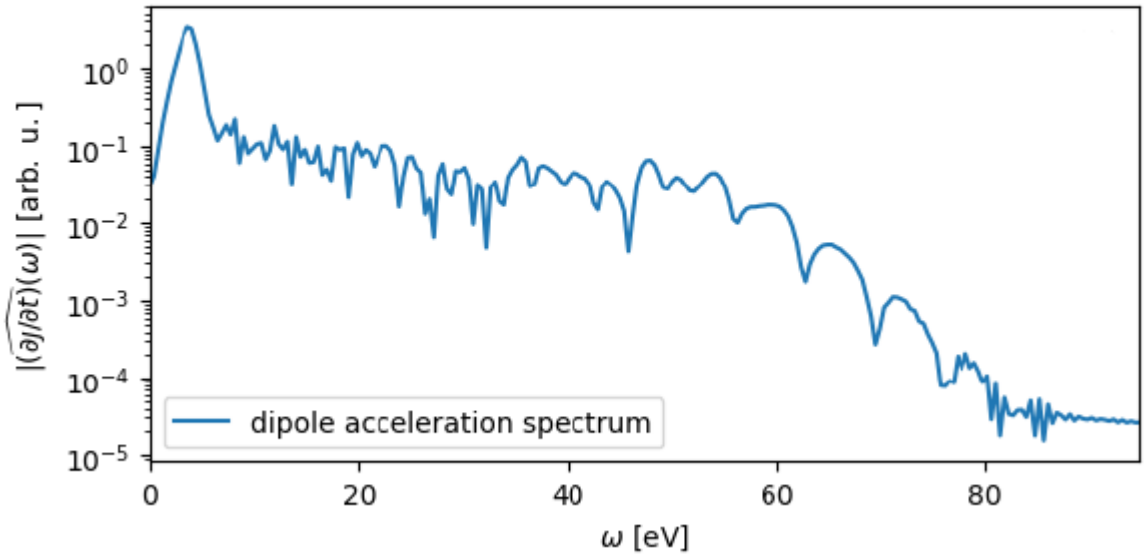
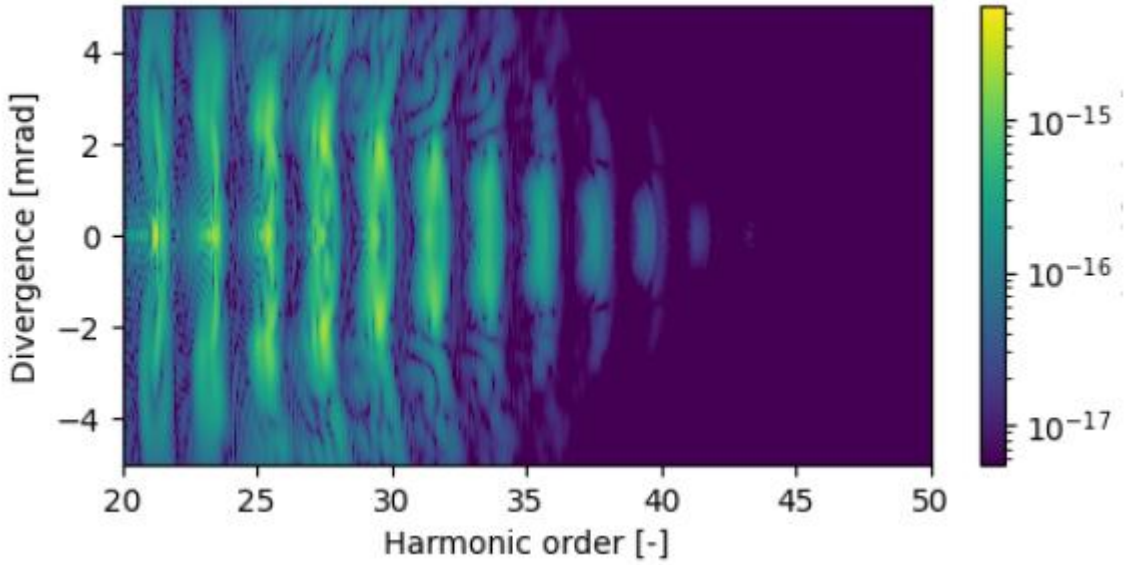


Illustration of a 1D dipole acceleration spectrum

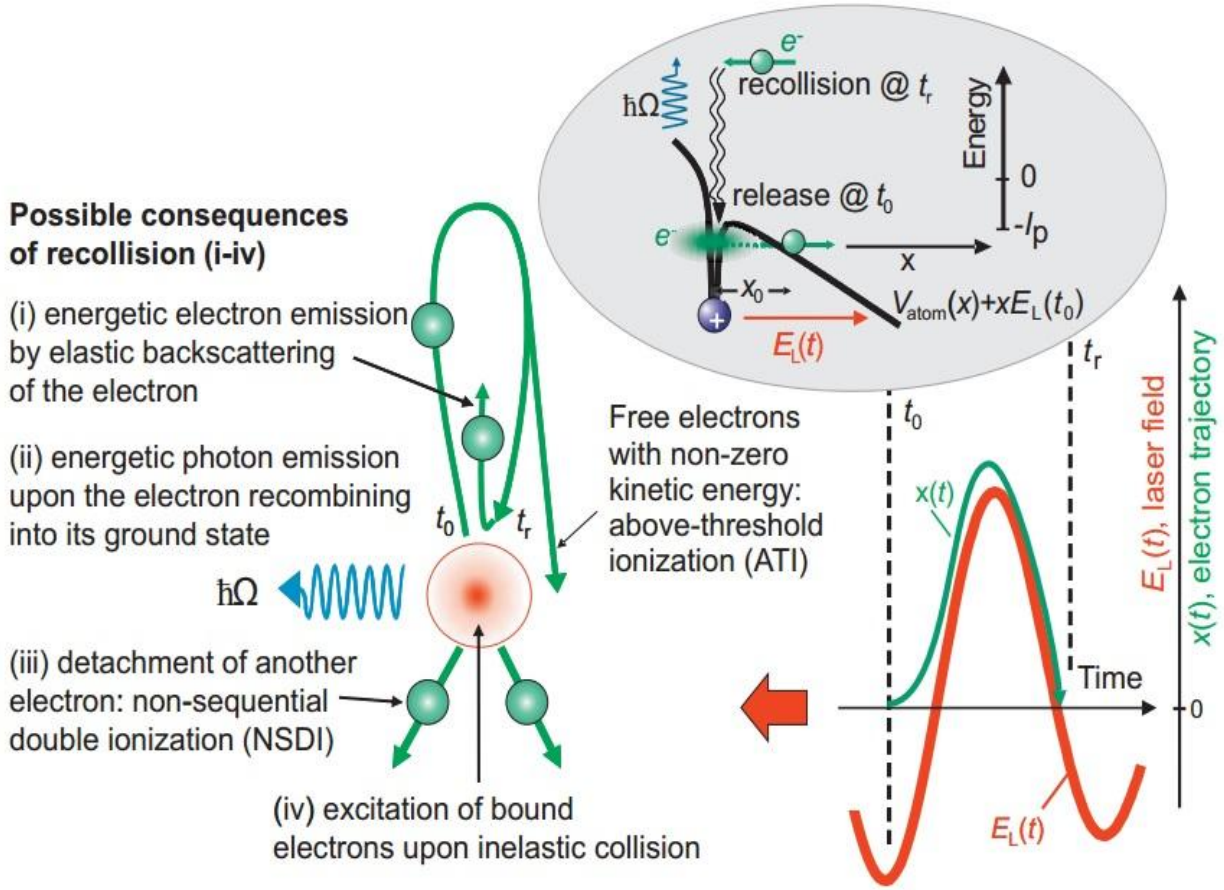
Hankel – XUV far-field propagation

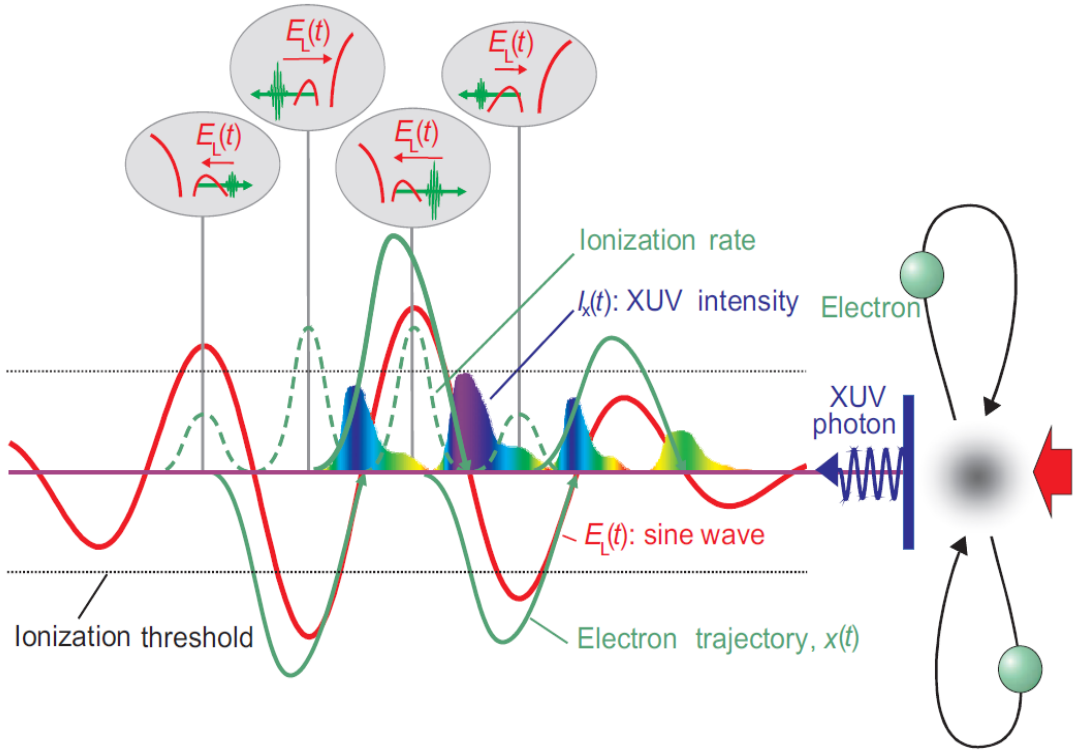
- Linear propagation of XUV radiation
- Diffraction integral
- Hankel transform (cylindrical symmetry)
- Includes phase matching and absorption
- Outputs far-field spectrum and spatial profile



An illustration of spatially resolved far-field harmonic spectra

Theory of strong-field ionization





F. Krausz and M. Ivanov. Attosecond physics. Reviews of Modern Physics, 81, 2009.

Theoretical framework
SAE atom, dipole approximation

Few-cycle laser pulse:

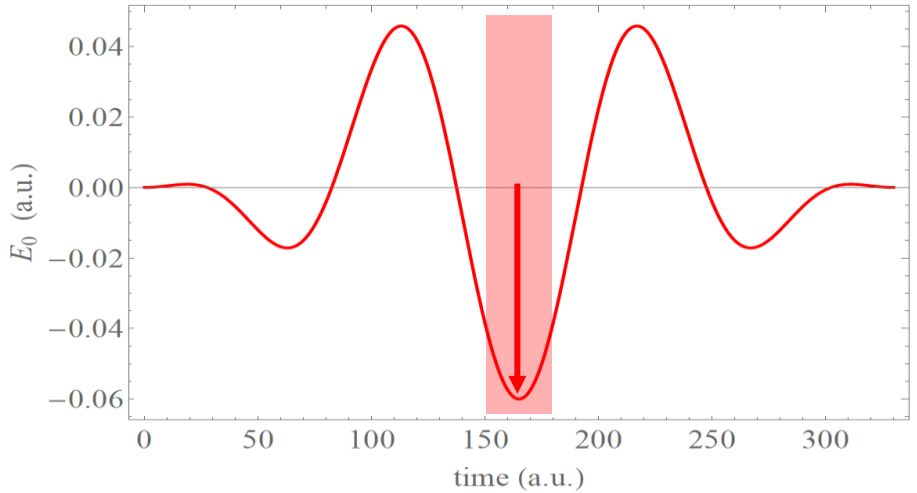
$$\mathcal{E}_z(t) = F \cdot \sin^2\left(\frac{\pi t}{NT}\right)\cos\left(\frac{2\pi t}{T} + \phi\right)$$

Usual parameters:

$$F = 0.06,\ N = 3,\ T = 110,\ \phi = 0$$

$$I \sim 100\,\mathrm{TW/cm^2},\ \lambda \approx 800\,\mathrm{nm}$$

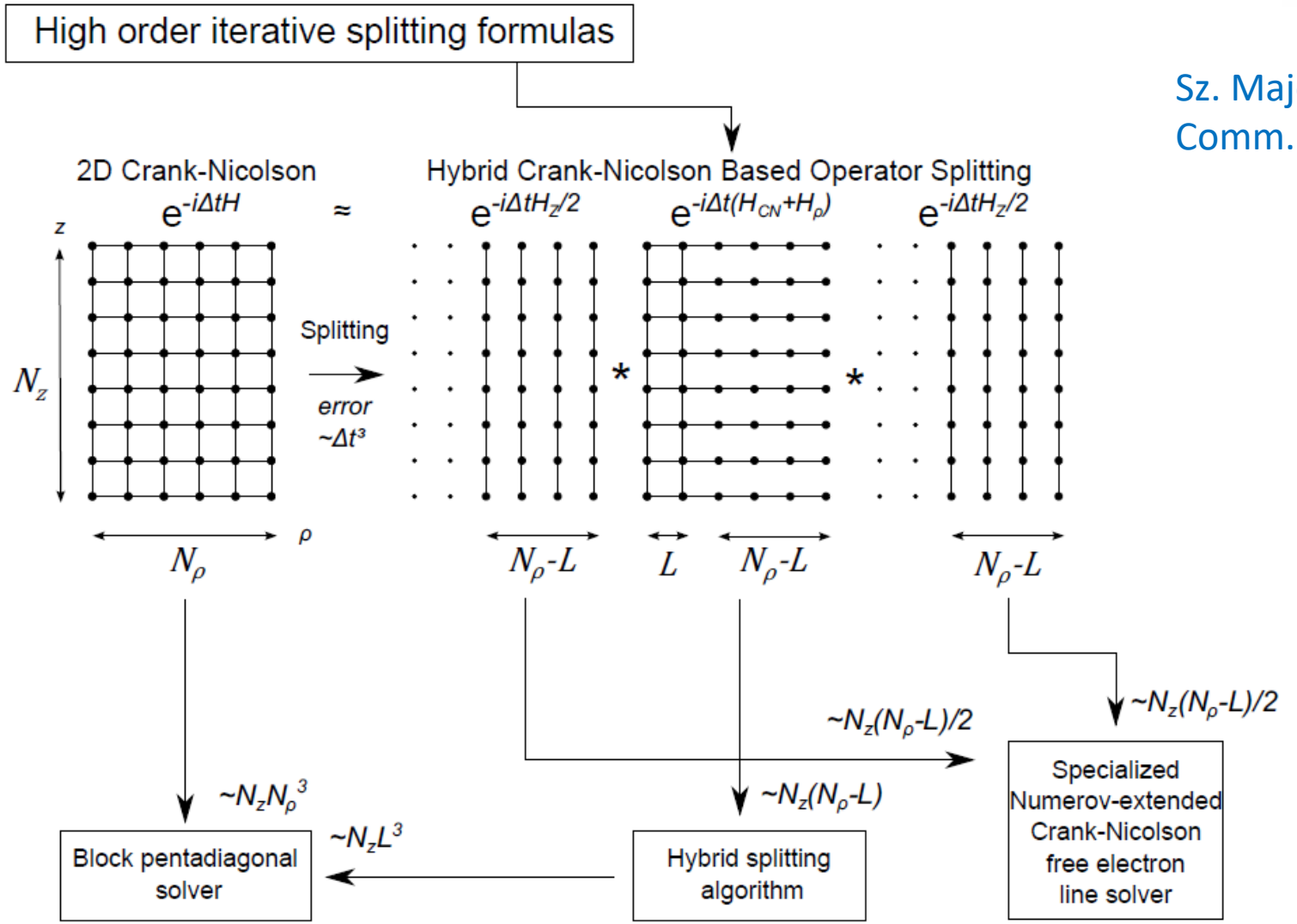
Keldysh parameter: $\gamma \sim 1$



3D Schrödinger equation in cylidrical coordinates and in length gauge:

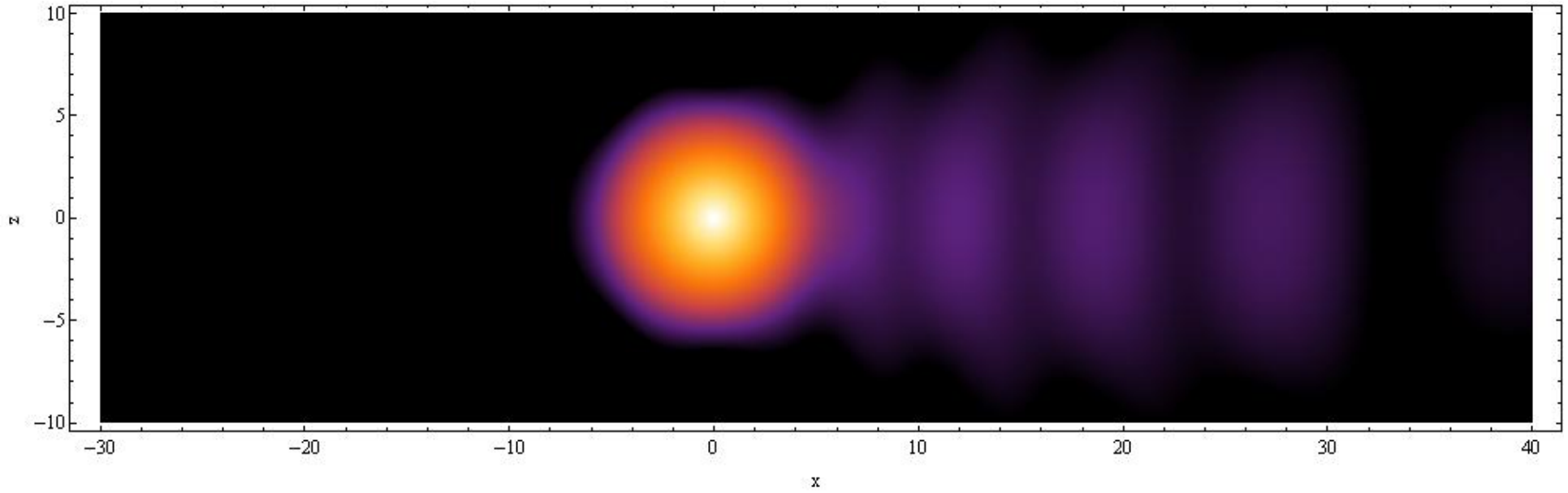
$$i\frac{\partial}{\partial t}\Psi(z,\rho,t) = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial^2 z} + \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho}\right) - \frac{1}{\sqrt{z^2+\rho^2}} + \mathcal{E}_z(t)\cdot z\right]\Psi(z,\rho,t)$$

Accurate and effective numerical algorithm for 3D H-atom driven by a strong lin. pol. laser pulse



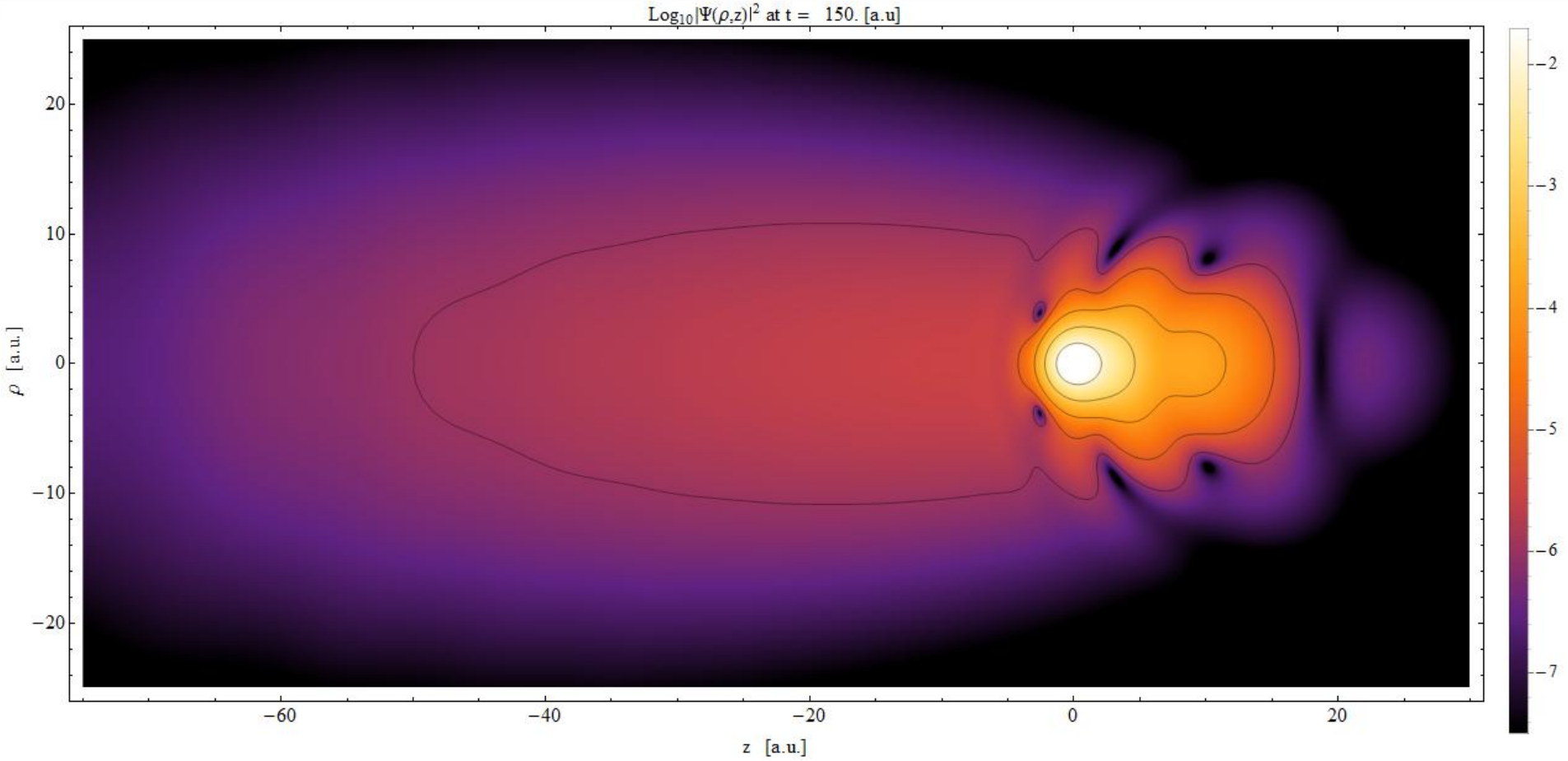
Sz. Majorosi and A. Czirják, Comp. Phys. Comm. **208**, 9-28, (2016)

Typical numerical results in 3D: Strong-field ionization of atomic H, lin. pol. NIR fs pulse



S. Majorosi, A. Czirják / Computer Physics Communications **208** (2016) 9–28

Typical numerical results in 3D: Strong-field ionization of atomic H, lin. pol. NIR fs pulse



S. Majorosi, A. Czirják / Computer Physics Communications **208** (2016) 9–28

3D vs 1D simulations in strong-field physics

3D, cylindrical coordinates:

$$i\frac{\partial}{\partial t}\Psi^{3\mathrm{D}}(z,\rho,t) = \left[H_0^{3\mathrm{D}} + V_{\mathrm{ext}}(z,t)\right]\Psi^{3\mathrm{D}}(z,\rho,t)$$

$$H_0^{3\mathrm{D}} = T_z + T_\rho - \frac{Z}{\sqrt{\rho^2+z^2}} \qquad V_{\mathrm{ext}}(z,t) = z\cdot\mathcal{E}_z(t)$$

1D, along z-axis, parallel with laser polarization:

$$i\frac{\partial}{\partial t}\Psi^{1\mathrm{D}}(z,t) = \left[H_0^{1\mathrm{D}} + V_{\mathrm{ext}}(z,t)\right]\Psi^{1\mathrm{D}}(z,t)$$

$$H_0^{1\mathrm{D}} = T_z + V_0^{1\mathrm{D}}(z) \qquad V_{\mathrm{ext}}(z,t) = z\cdot\mathcal{E}_z(t)$$

Good 1D model: **good match** of 1D and 3D physical quantities, using the **same laser field**

Majorosi, Benedict and Czirják, Phys. Rev. A, **98** (2018) 023401

Construction of the density-based 1D model potential

3D ground state:
(Z: effective ion-core charge)

$$H_0^{3D}\psi_{100}(z,\rho) = E_0\psi_{100}(z,\rho) \qquad E_0 = -\frac{\mu Z^2}{2}, \qquad \psi_{100}(z,\rho) = \mathcal{N}\, e^{-\mu Z\sqrt{\rho^2+z^2}}$$

Reduced ground state density:

$$\varrho_z^{100}(z) = 2\pi\int_0^\infty |\psi_{100}(z,\rho)|^2\rho \mathrm{d}\rho = \frac{\mu Z}{2}\left(2Z\mu|z|+1\right)e^{-2Z\mu|z|}$$

Idea: Let 1D ground state density be identical to reduced ground state density!

1D ground state wave function:

$$\psi_0(z) = \sqrt{\frac{\mu Z}{2}}\sqrt{2\mu Z|z|+1}e^{-\mu Z|z|}$$

Substitute the ground state into 1D Schrödinger eq. and solve for the potential:

$$V_{0,\mathrm{M}}^{1D}(z) = E_{0,\mathrm{M}} + \frac{1}{\psi_0(z)}\frac{1}{2\mu}\frac{\partial^2}{\partial z^2}\psi_0(z) \qquad \lim_{|z|\to\infty} V_{0,\mathrm{M}}^{1D}(z) = 0$$

Majorosi, Benedict and Czirják, Phys. Rev. A, **98** (2018) 023401

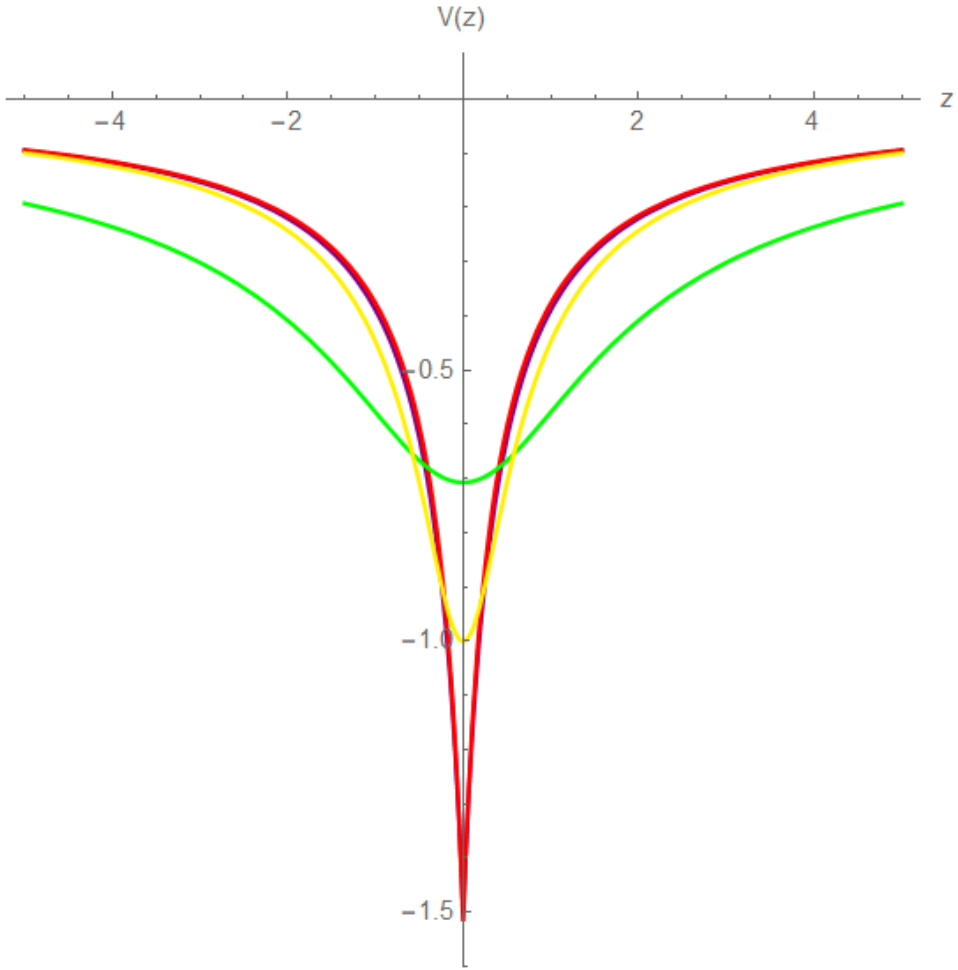
Improved 1D model potentials for H and simulation results

The density-based 1D model potential (red curve):

$$V_{0,\mathrm{M}}^{1\mathrm{D}}(z) = -\frac{1}{2\mu}\frac{1}{2^2\left(|z| + \frac{1}{2\mu Z}\right)^2} - \frac{\frac{1}{2}Z}{|z| + \frac{1}{2\mu Z}}$$

Improved soft-core Coulomb potential (MSC potential, yellow curve):

$$V_{0,\mathrm{M,Sc}}^{1\mathrm{D}}(z) = -\frac{\frac{1}{2}Z}{\sqrt{z^2 + \frac{1}{4Z^2}}}$$



Majorosi, Benedict and Czirják, Phys. Rev. A, **98** (2018) 023401

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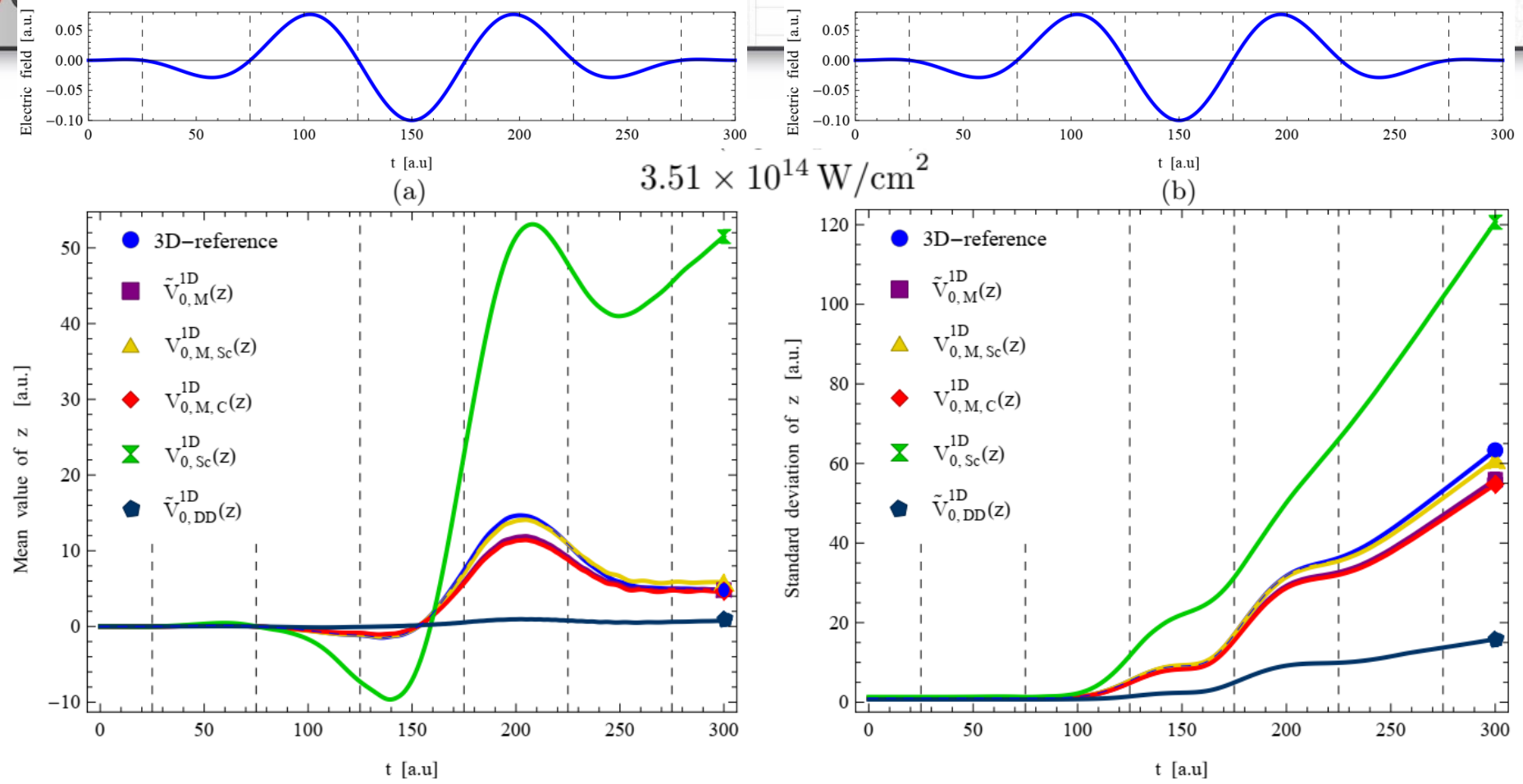


Figure 2. Time-dependence of the mean values $\langle z \rangle (t)$ (a) and the standard deviations $\sigma_z(t)$ (b) using different 1D model potentials, under the influence of the same external field with $F = 0.1$, $N_{\mathrm{Cycle}} = 3$ and $T = 100$. Results of the corresponding 3D simulation are plotted in blue.

Majorosi, Benedict and Czirják, Phys. Rev. A, **98** (2018) 023401

Improved 1D atomic model potentials for HHG and simulation results

HHG spectra of H: scaling of the power spectrum needed

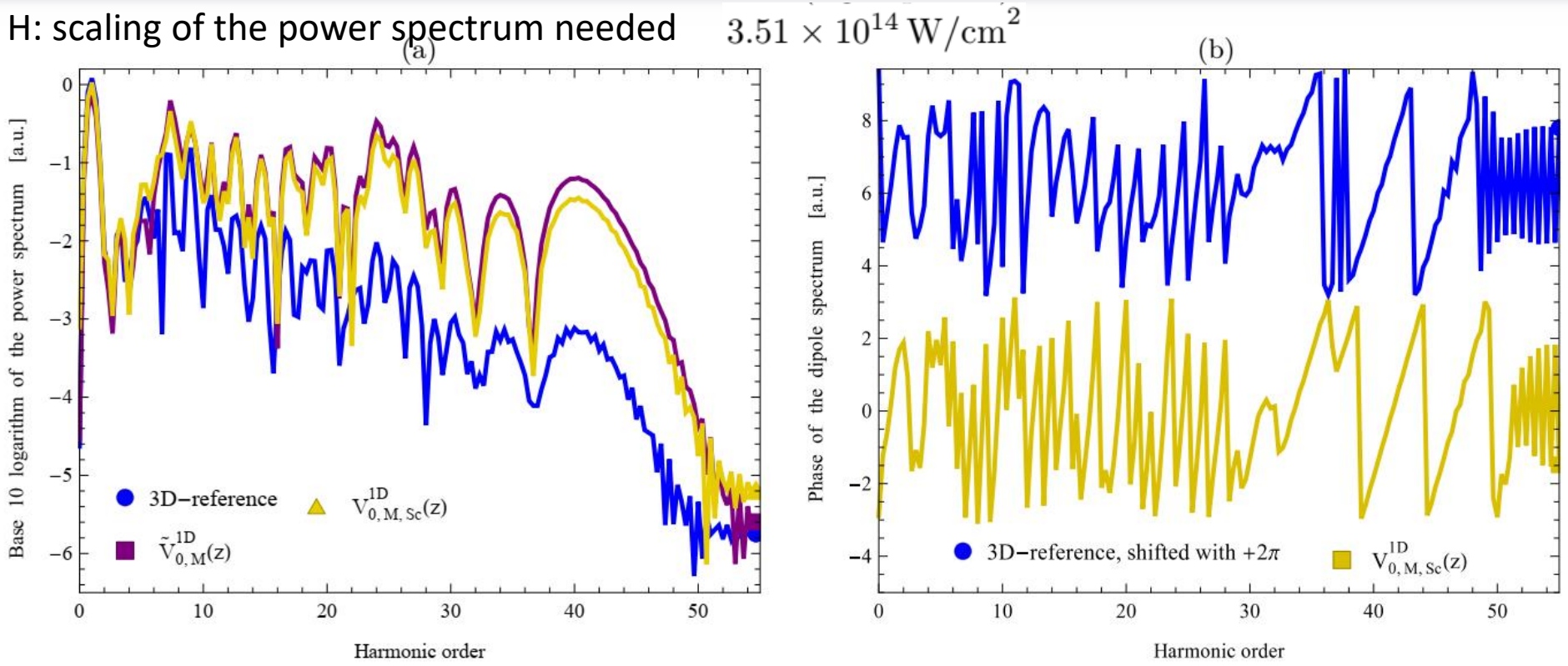
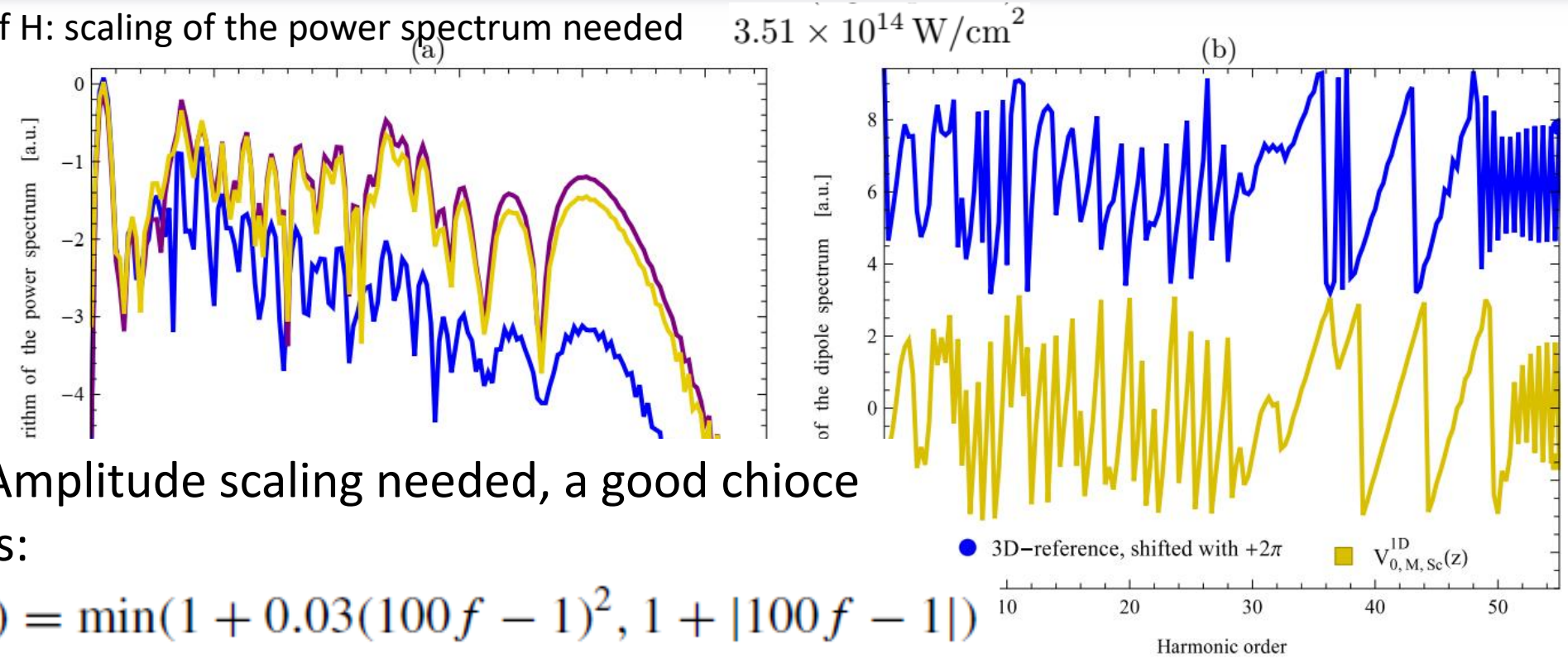


Figure 6. Panel (a): Logarithmic plot of the power spectra vs. the harmonic order, i.e. $p(nf_1)$ (where $f_1 = 1/T = 0.01$ a.u. is the fundamental frequency). Panel (b): Phase of the dipole acceleration spectra vs. the harmonic order (up shifted by 2π for the 3D case). We plot the results for the density-based 1D model potential (purple) and for the improved soft-core Coulomb potential (gold) in comparison with the 3D reference (blue). The parameters $F = 0.1$, $N_{\mathrm{Cycle}} = 3$, $T = 100$ and $Z = 1$ are the same as for Figs. 2 and 3.

Majorosi, Benedict and Czirják, Phys. Rev. A, **98** (2018) 023401

Improved 1D atomic model potentials for HHG and simulation results

HHG spectra of H: scaling of the power spectrum needed



Amplitude scaling needed, a good chioce is:

$$s(f) = \min(1 + 0.03(100f - 1)^2, 1 + |100f - 1|)$$

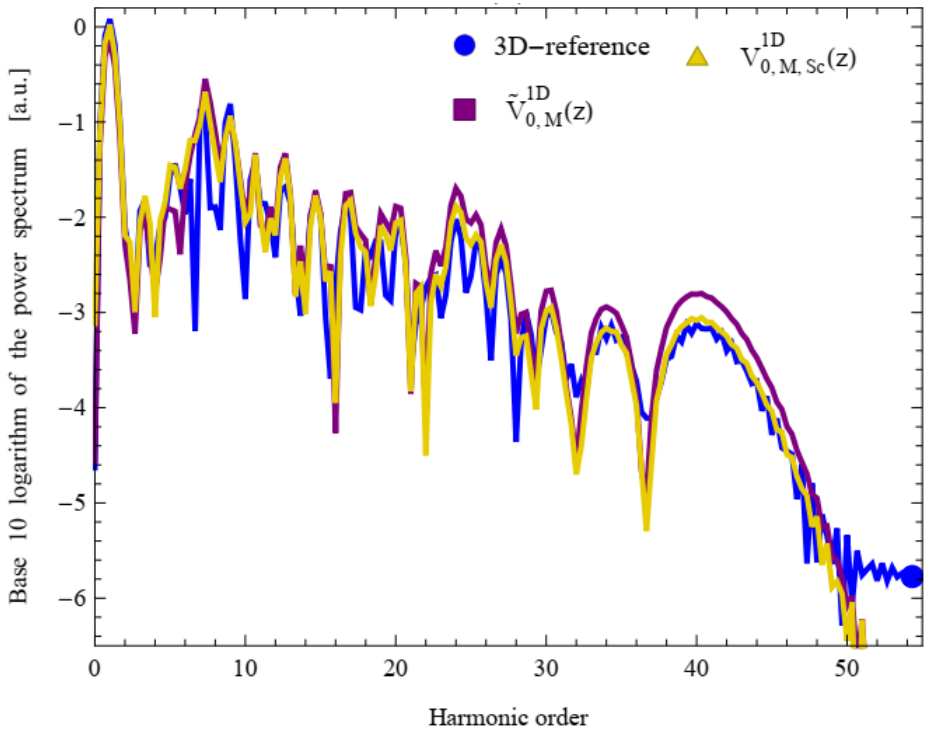
Figure 6. Panel (a): Logarithmic plot of the power spectra vs. the harmonic order, i.e. $p(nf_1)$ (where $f_1 = 1/T = 0.01$ a.u. is the fundamental frequency). Panel (b): Phase of the dipole acceleration spectra vs. the harmonic order (up shifted by 2π for the 3D case). We plot the results for the density-based 1D model potential (purple) and for the improved soft-core Coulomb potential (gold) in comparison with the 3D reference (blue). The parameters $F = 0.1$, $N_{\mathrm{Cycle}} = 3$, $T = 100$ and $Z = 1$ are the same as for Figs. 2 and 3.

Majorosi, Benedict and Czirják, Phys. Rev. A, **98** (2018) 023401

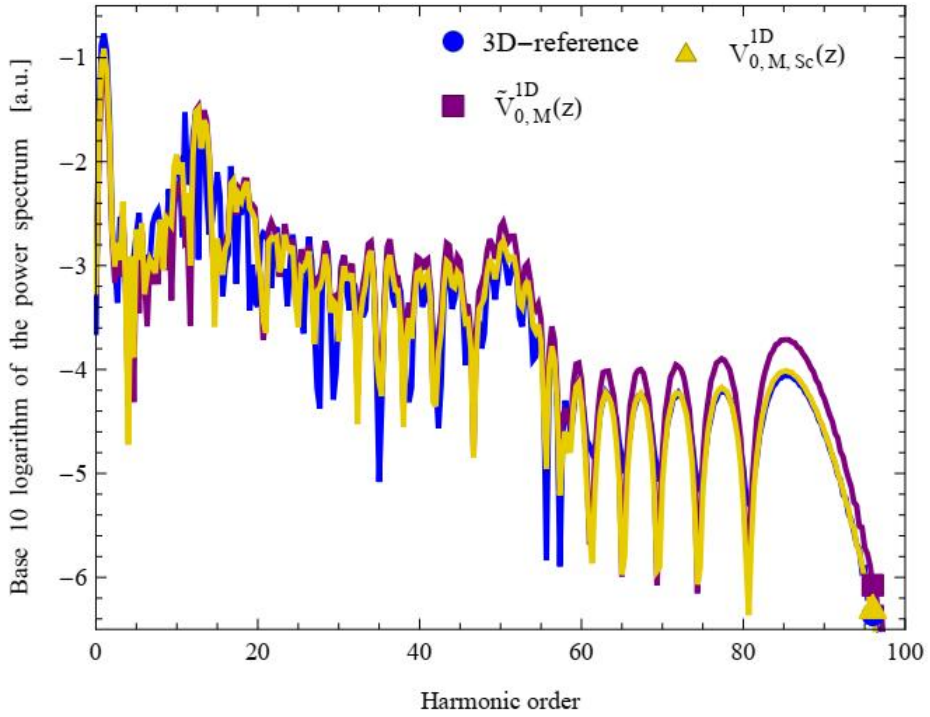
Improved 1D atomic model potentials for HHG and simulation results

HHG spectra:

H, $3.51 \times 10^{14}\,\mathrm{W/cm^2}$



Ne (SAE), $7.89 \times 10^{14}\,\mathrm{W/cm^2}$

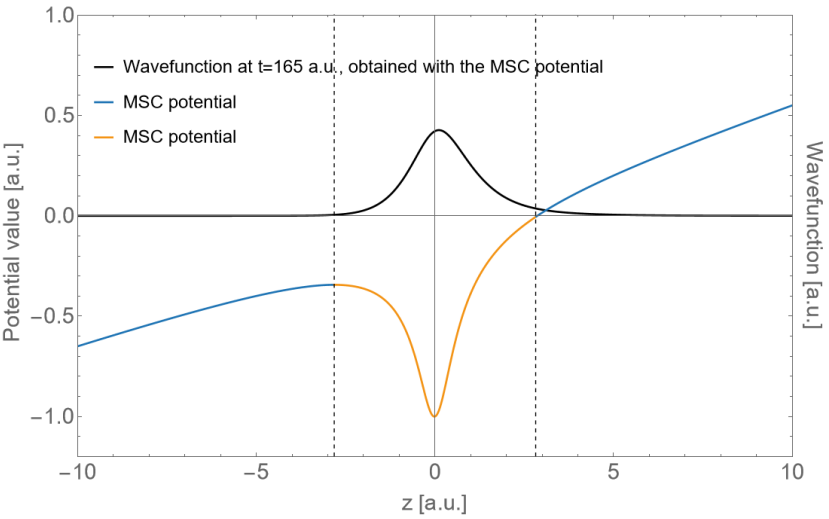


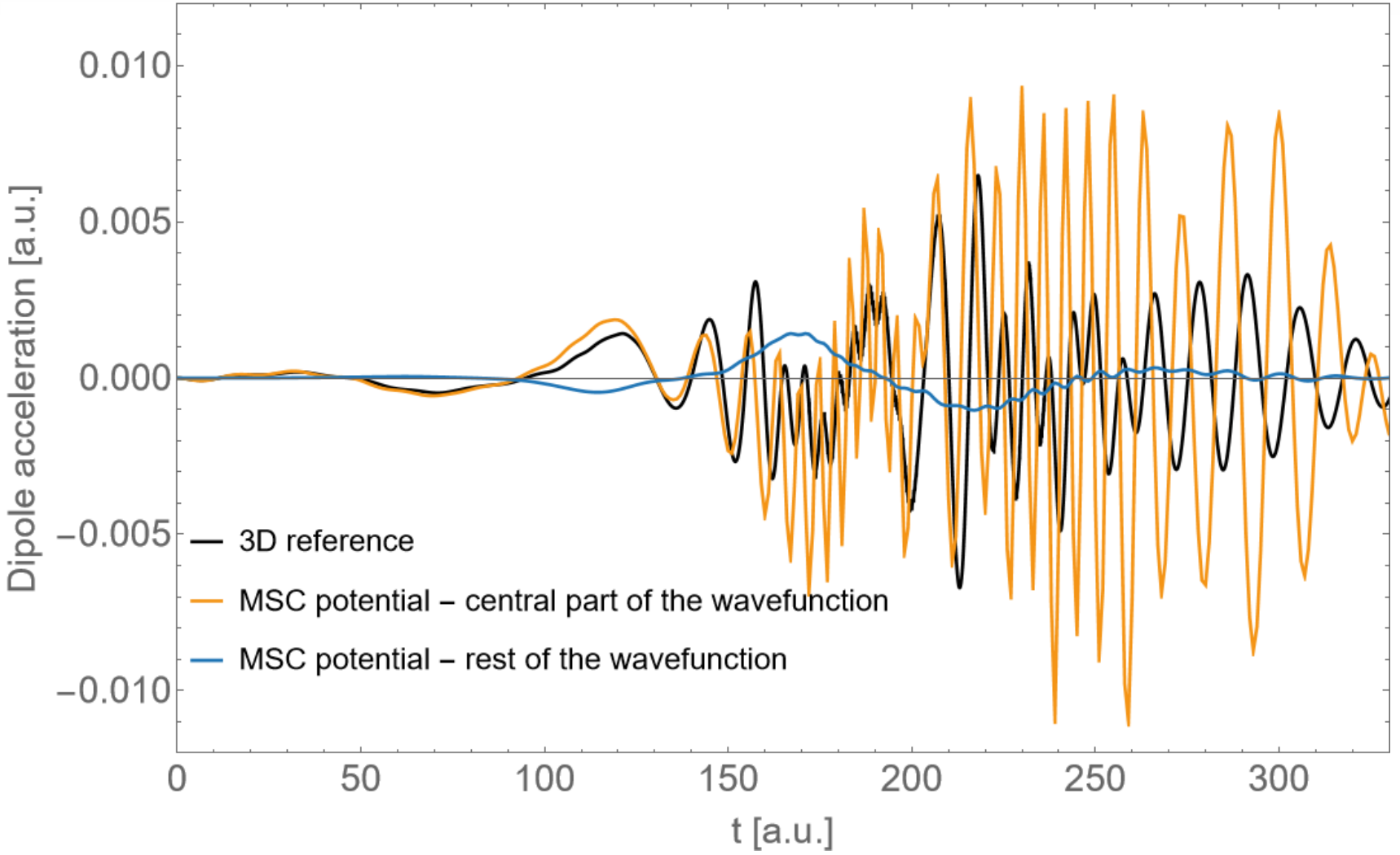
Same simple scaling for power spectrum works for different SAE atoms and in a reasonable range of pulse intensities.

Majorosi, Benedict and Czirják, Phys. Rev. A, **98** (2018) 023401

Majorosi, Benedict, Bogár, Paragi and Czirják, Phys. Rev. A, **101** (2020) 023405

Upgraded 1D atomic model potentials for HHG and simulation results



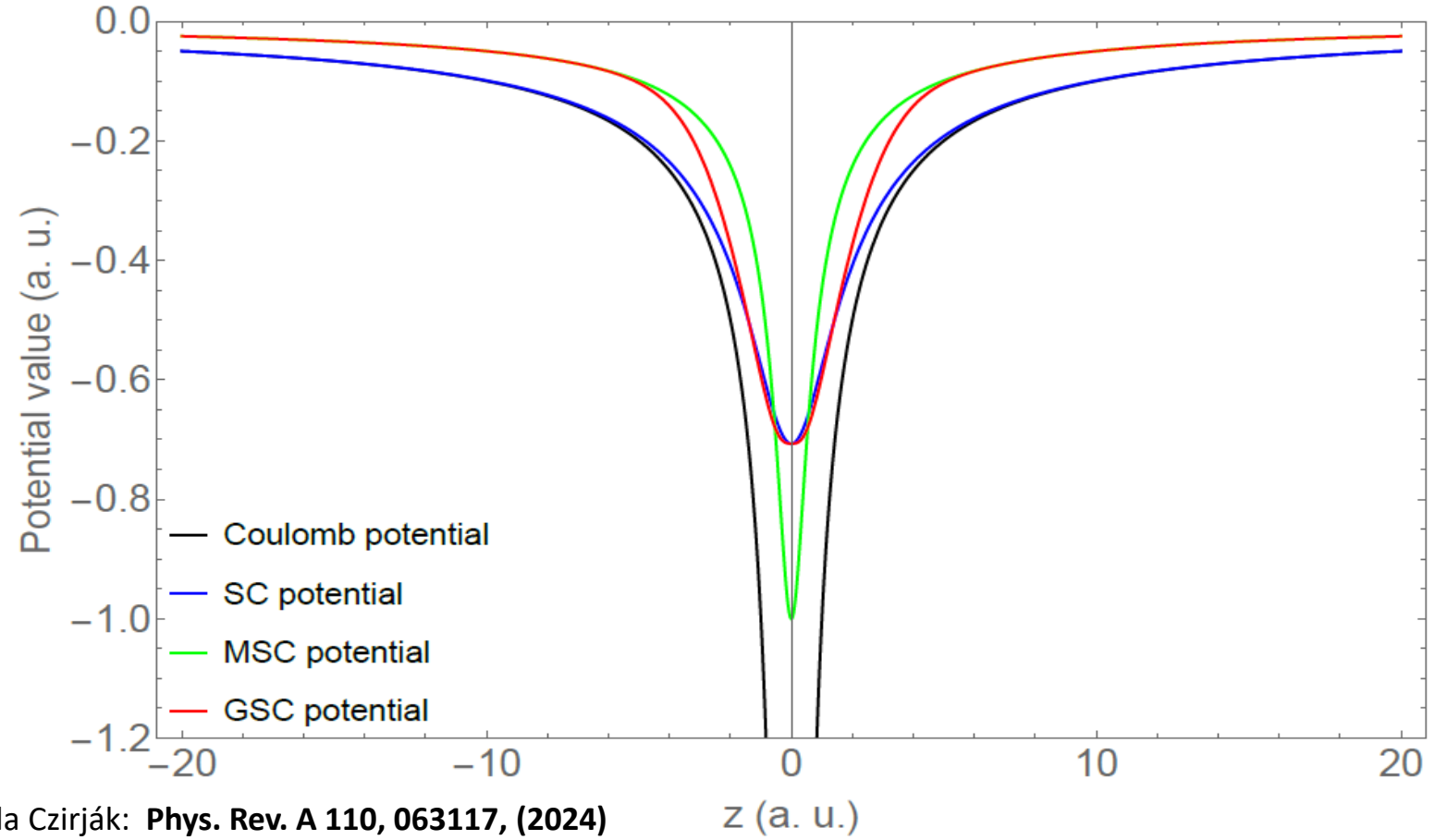


Krisztina Sallai, Szabolcs Hack, Szilárd Majorosi and Attila Czirják: **Phys. Rev. A 110, 063117, (2024)**

The Gaussian windowed soft-core Coulomb (GSC) potential

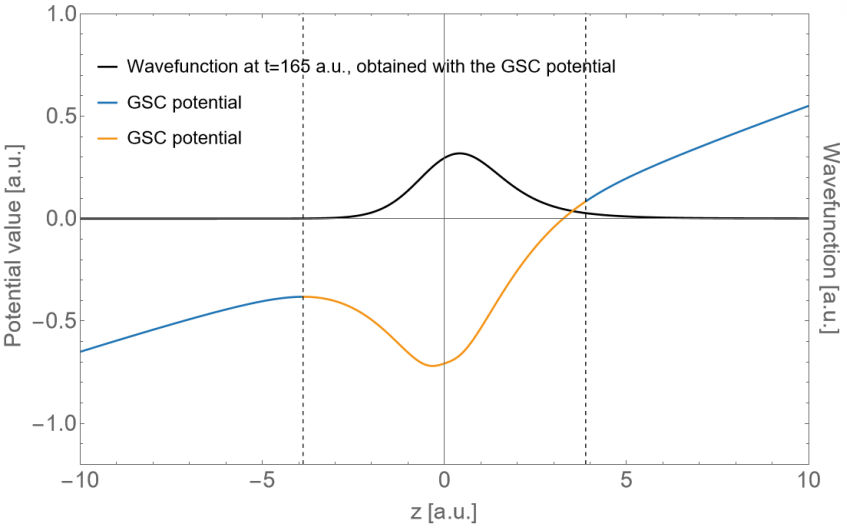
$$V_{GSC}^{1D}(z) = V_{SC}^{1D}(z) \cdot e^{-(z/a)^2} + V_{MSC}^{1D}(z) \cdot \left(1 - e^{-(z/b)^2}\right)$$

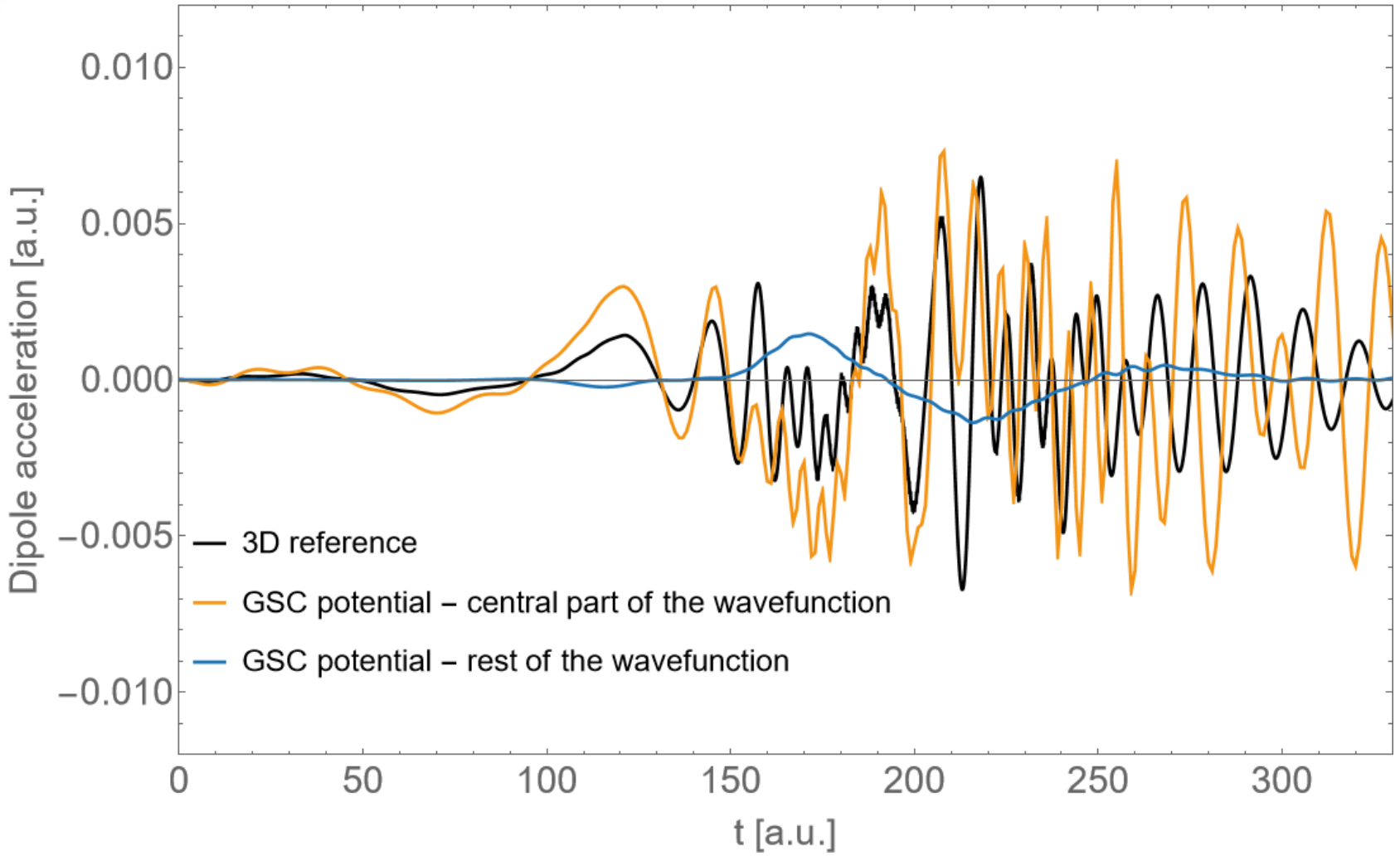
(with $a = 2.551$ and $b = 2.$)



Krisztina Sallai, Szabolcs Hack, Szilárd Majorosi and Attila Czirják: **Phys. Rev. A 110, 063117, (2024)**

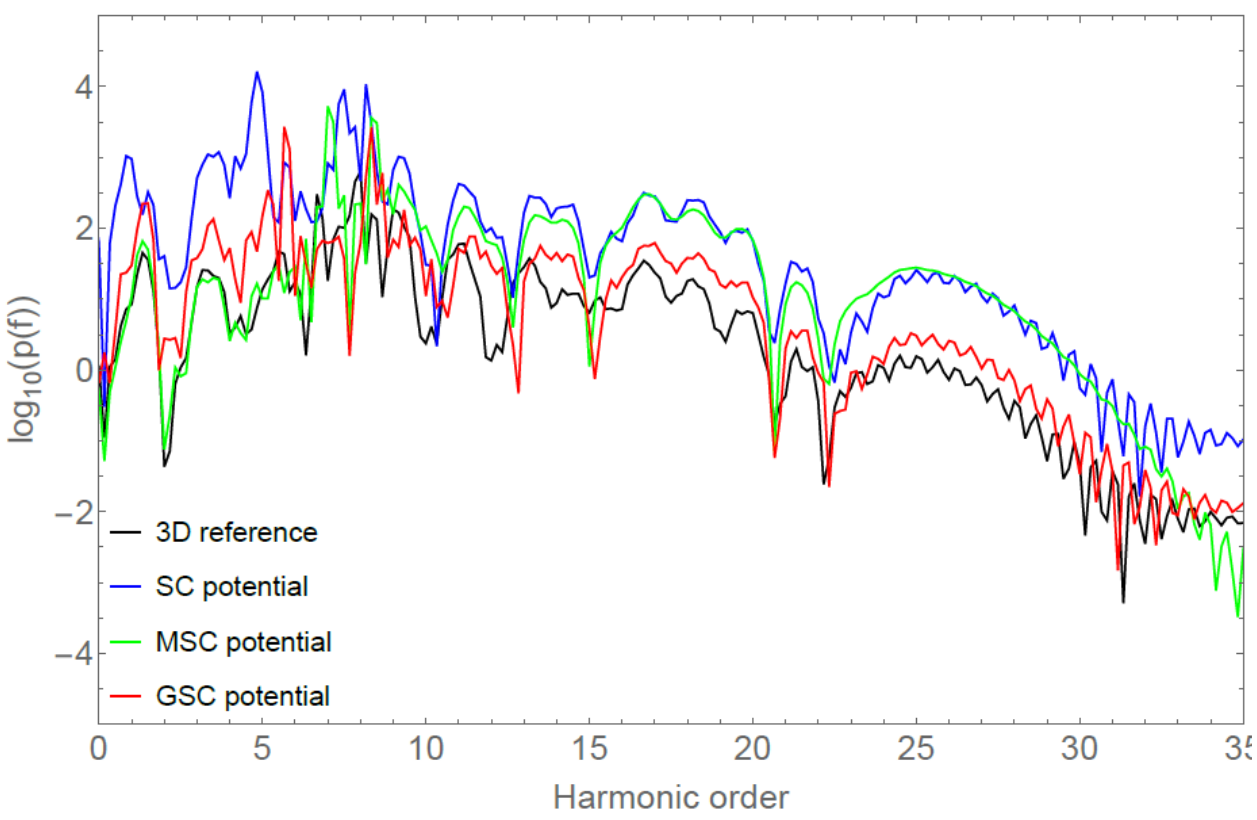
The Gaussian windowed soft-core Coulomb (GSC) potential

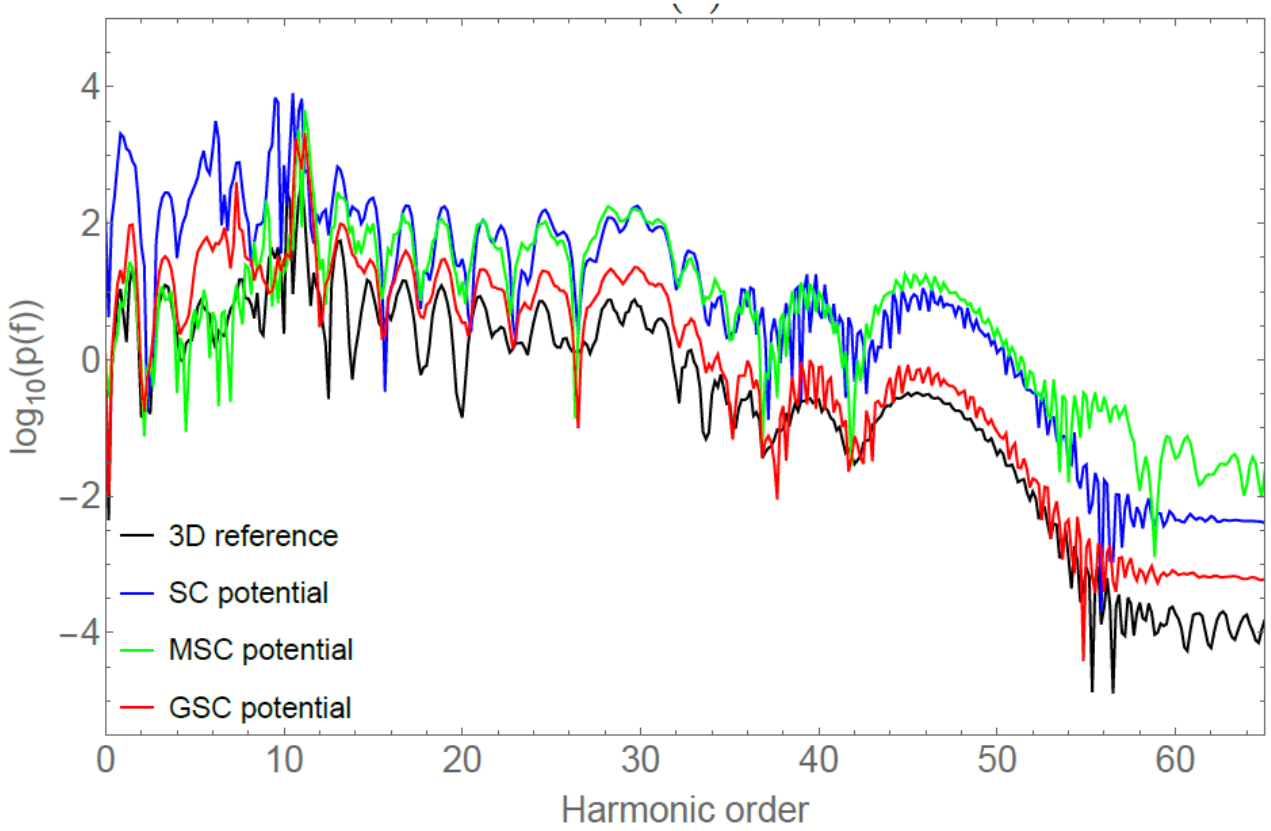




Krisztina Sallai, Szabolcs Hack, Szilárd Majorosi and Attila Czirják: **Phys. Rev. A 110, 063117, (2024)**

Hydrogen single atom HHG spectra simulated using GSC potential





The power spectrum of the dipole acceleration for hydrogen, $N_C = 3$, $F = 0.06$,

Krisztina Sallai, Szabolcs Hack, Szilárd Majorosi and Attila Czirják: **Phys. Rev. A 110, 063117, (2024)**

Argon single atom HHG spectra simulated using GSC potential

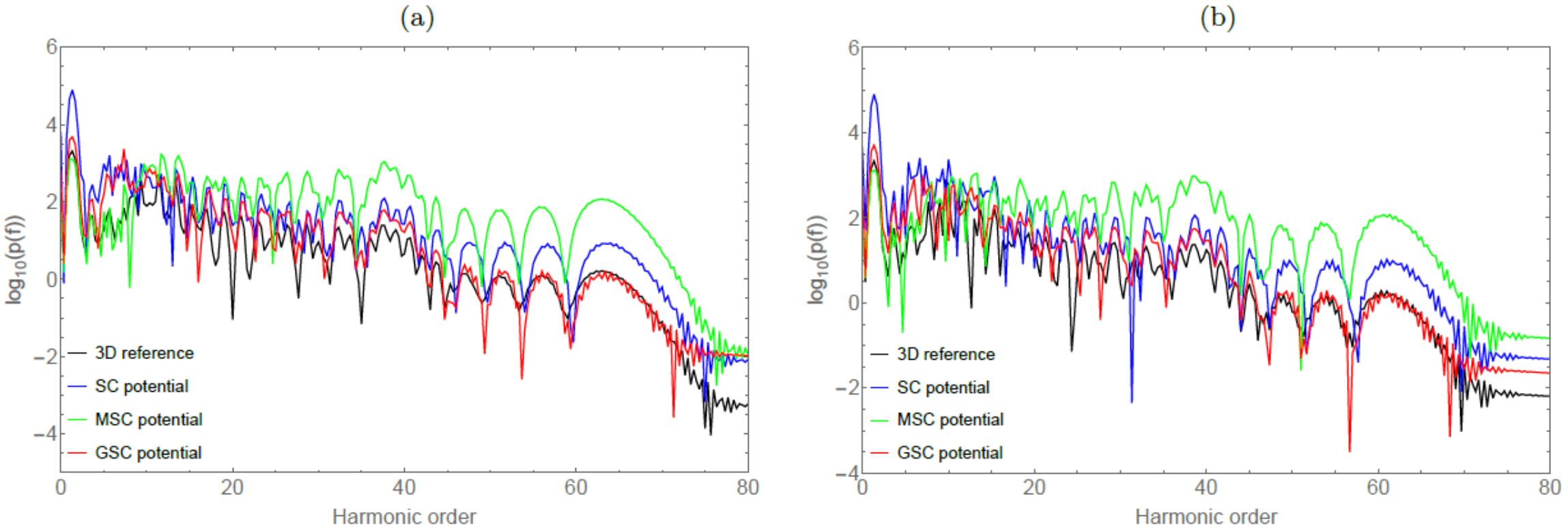


Figure 9. The power spectrum of the dipole acceleration for argon with $T = 117$, $N_C = 11$, $F = 0.1$ with (a) $k = 0$ and (b) $k = 3.88 \cdot 10^{-6}$.

Krisztina Sallai, Szabolcs Hack, Szilárd Majorosi and Attila Czirják: **Phys. Rev. A 110, 063117, (2024)**

MMA-HHG code with GSC atomic model potential, running on Komondor

CUPRAD

- Parallel Radially Symmetric Unidirectional Solver
- Non-linear laser propagation

TDSE

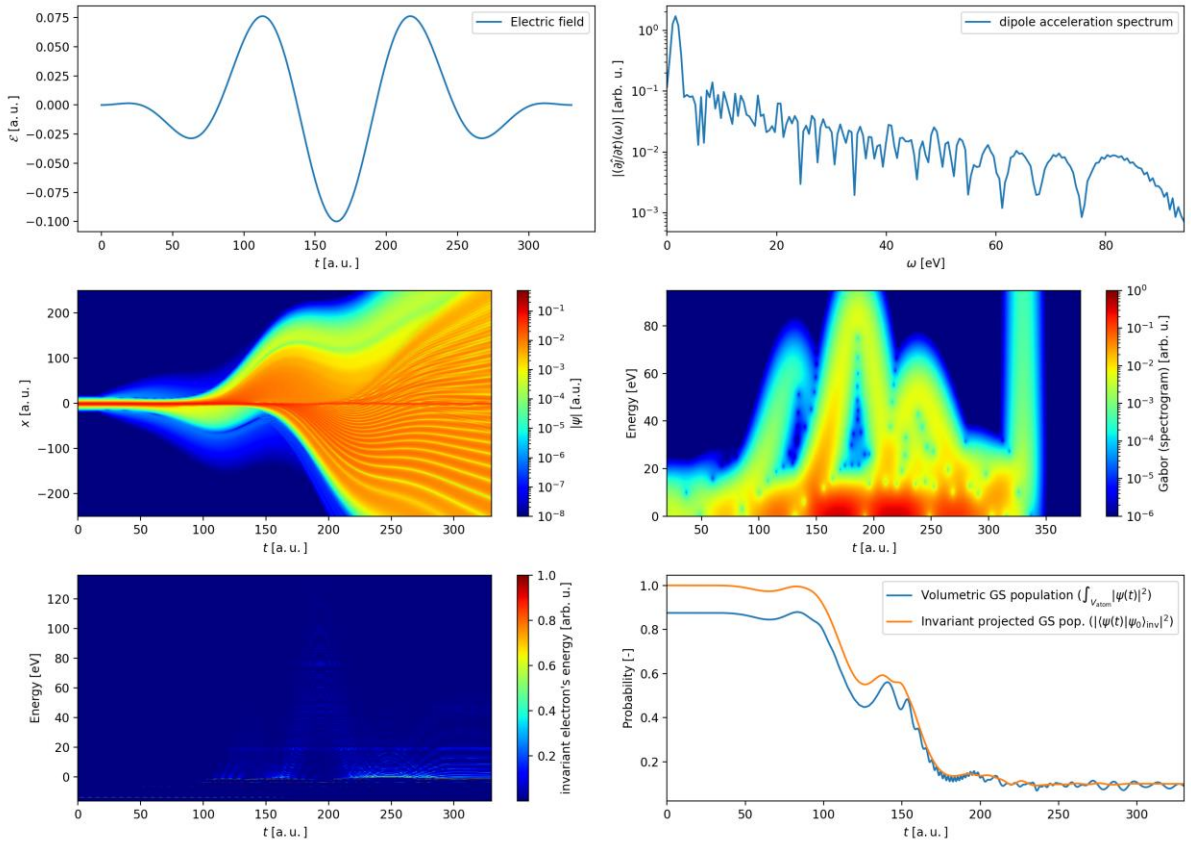
- 1D-TSDE Implementation
- Microscopic response, using GSC atomic model pot.

HANKEL

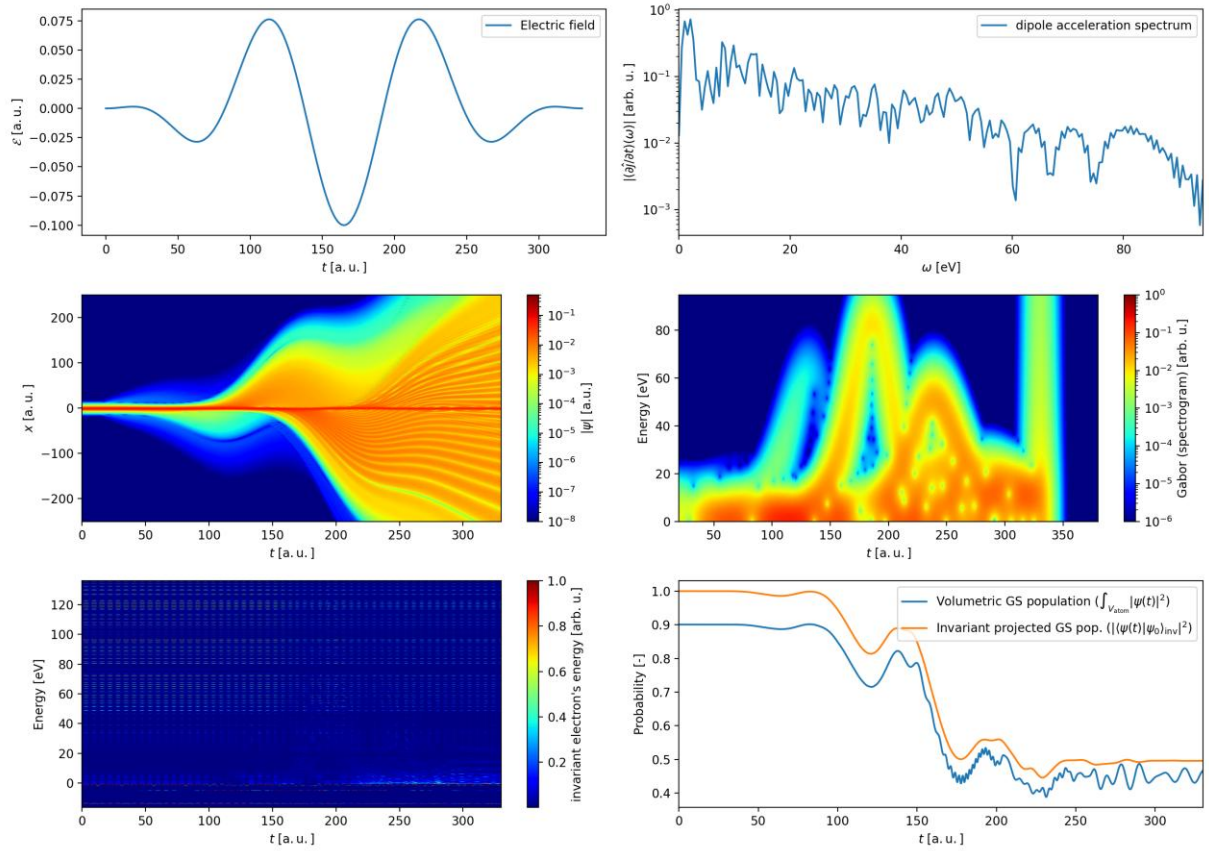
- Linear XUV Propagator
- XUV propagation

Preliminary results by the MMA-HHG code using SC vs. GSC atomic potential

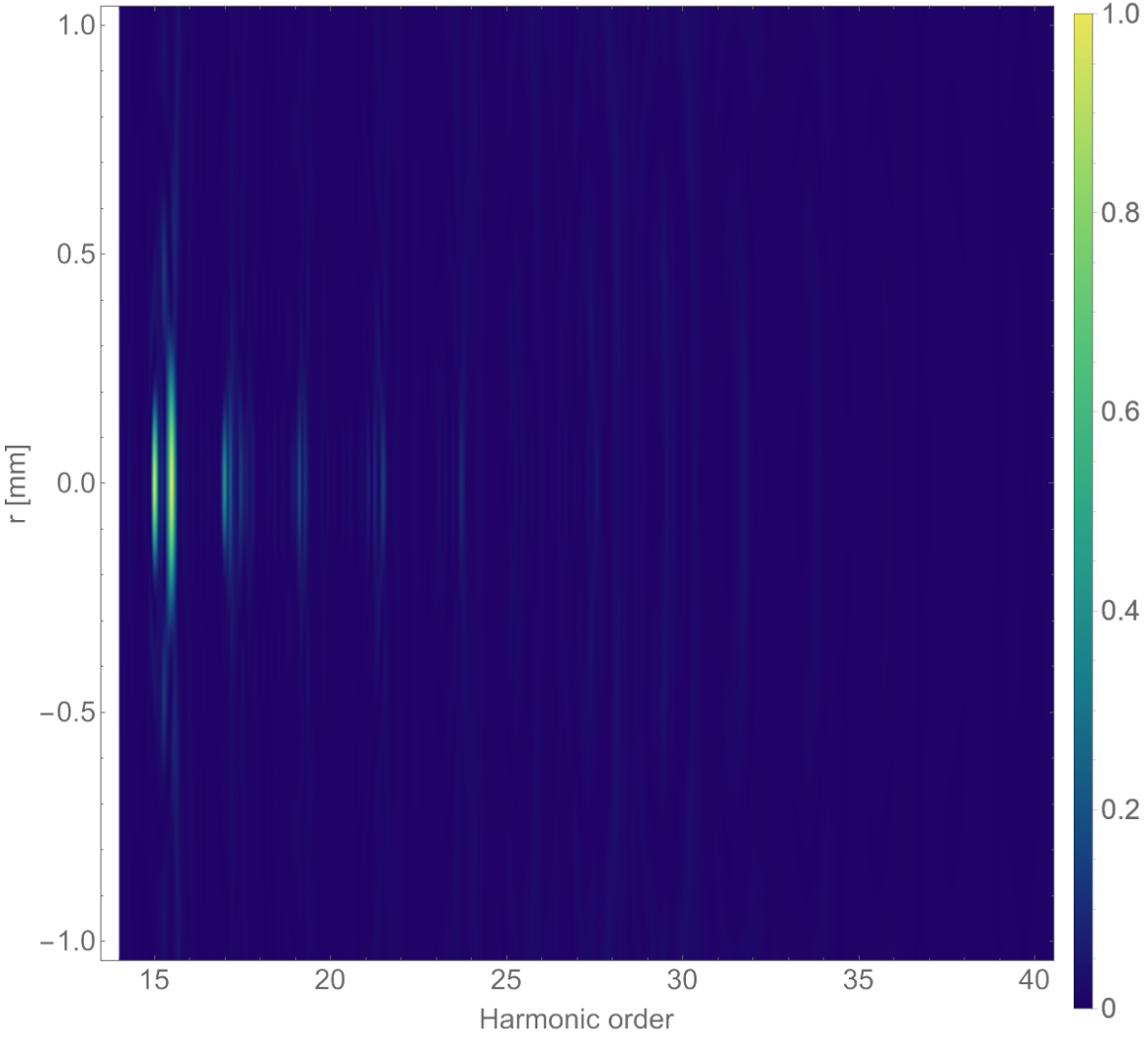
SC

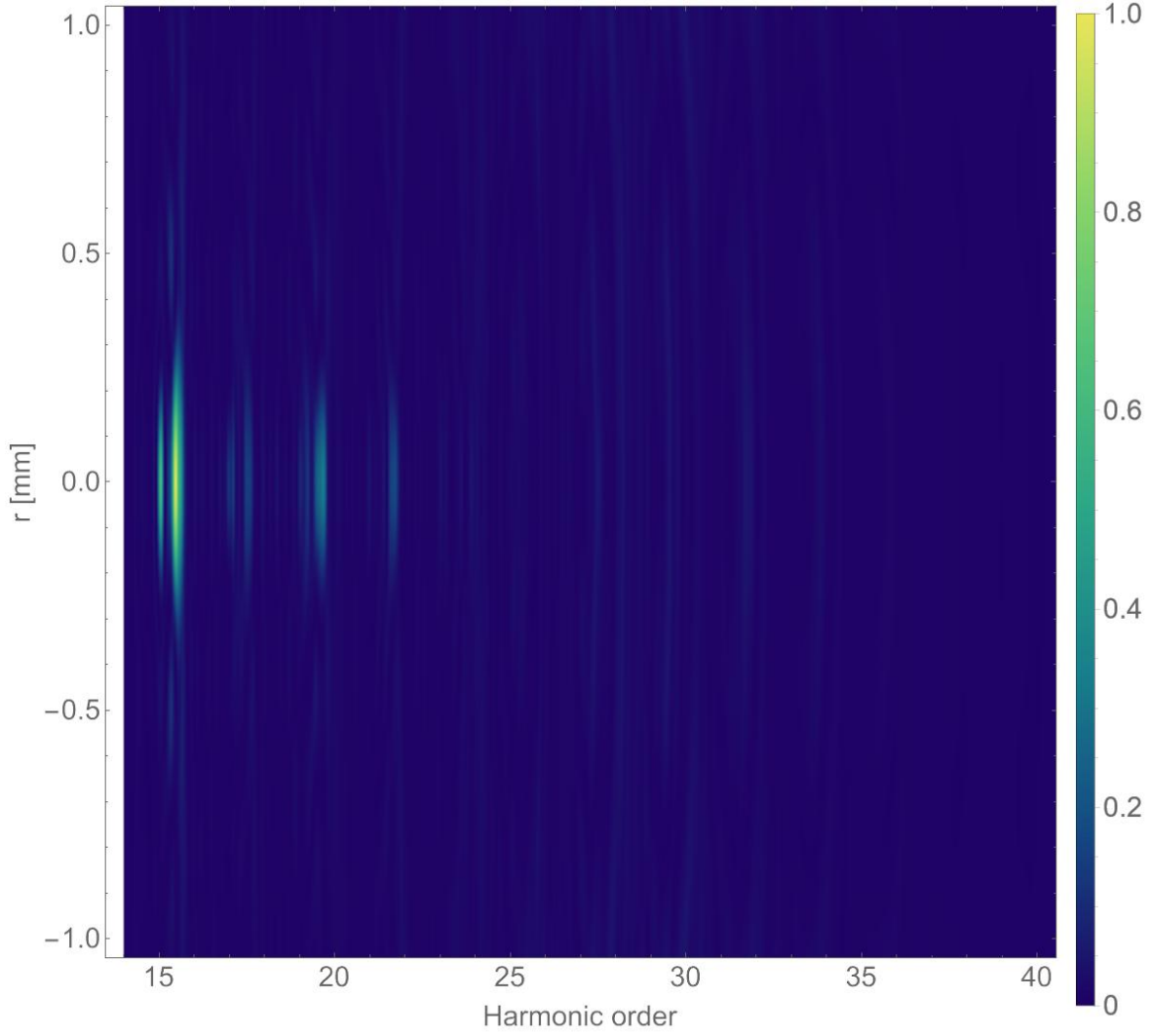


GSC

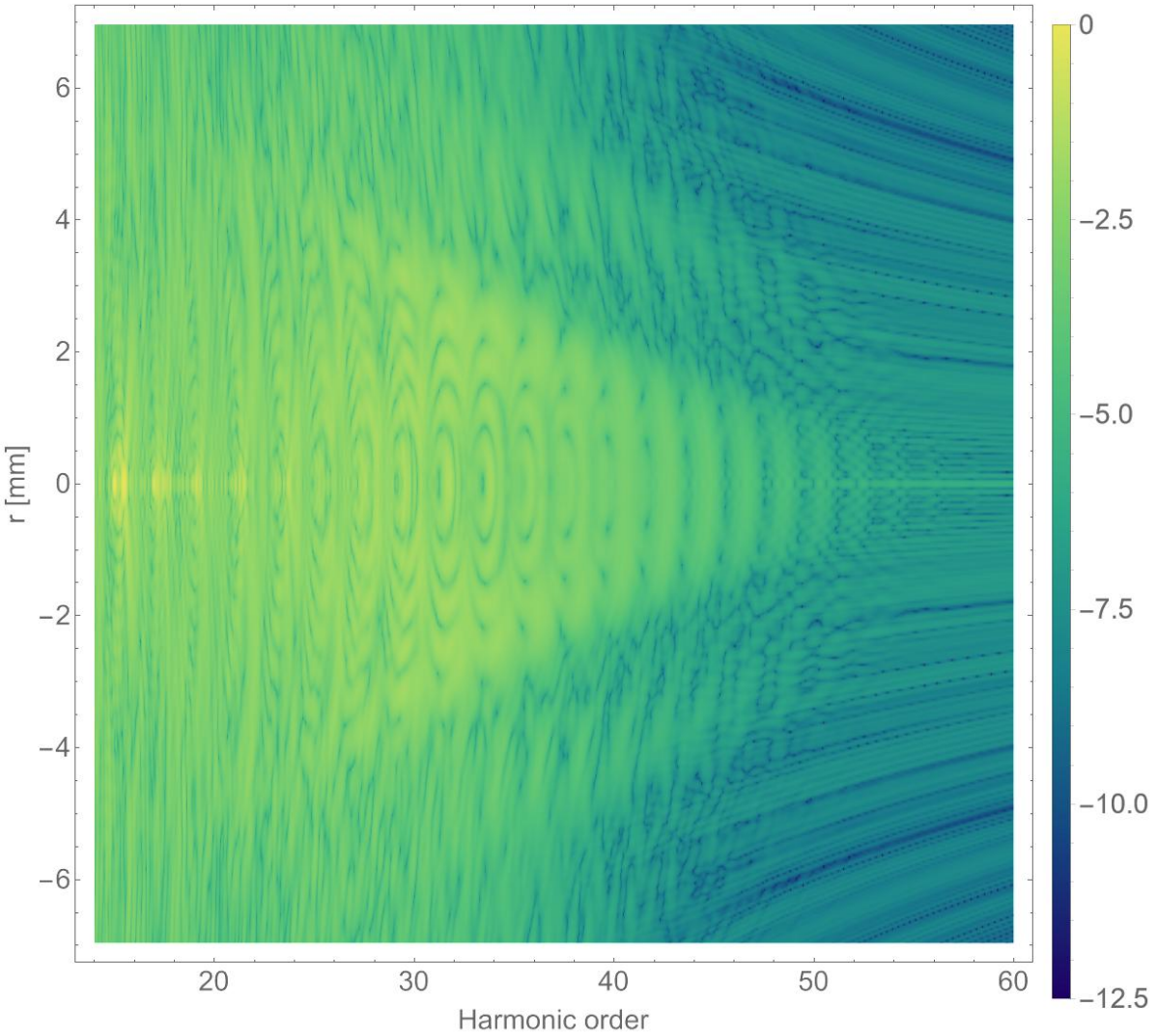


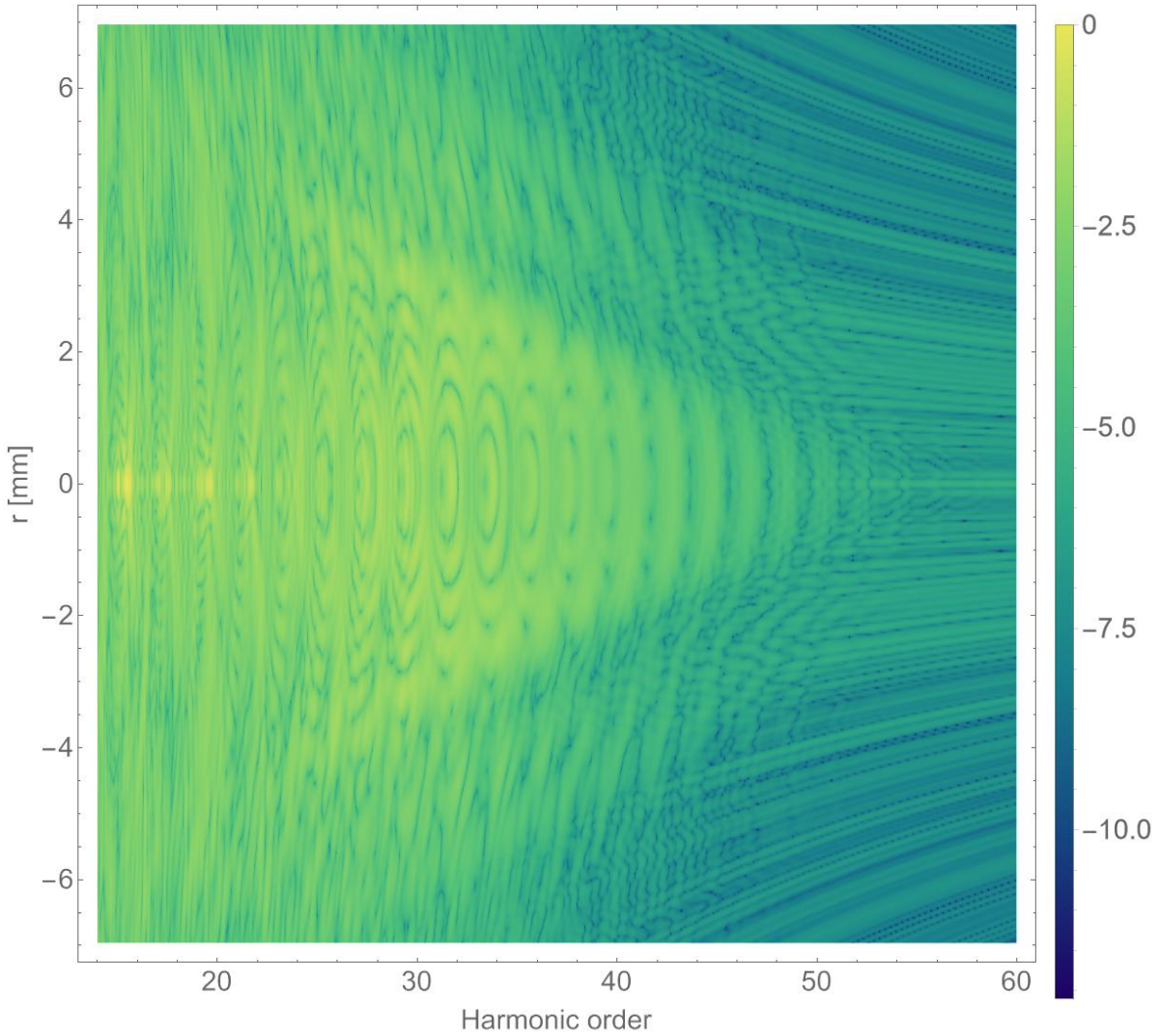
Preliminary results by the MMA-HHG code using SC vs. GSC atomic potential



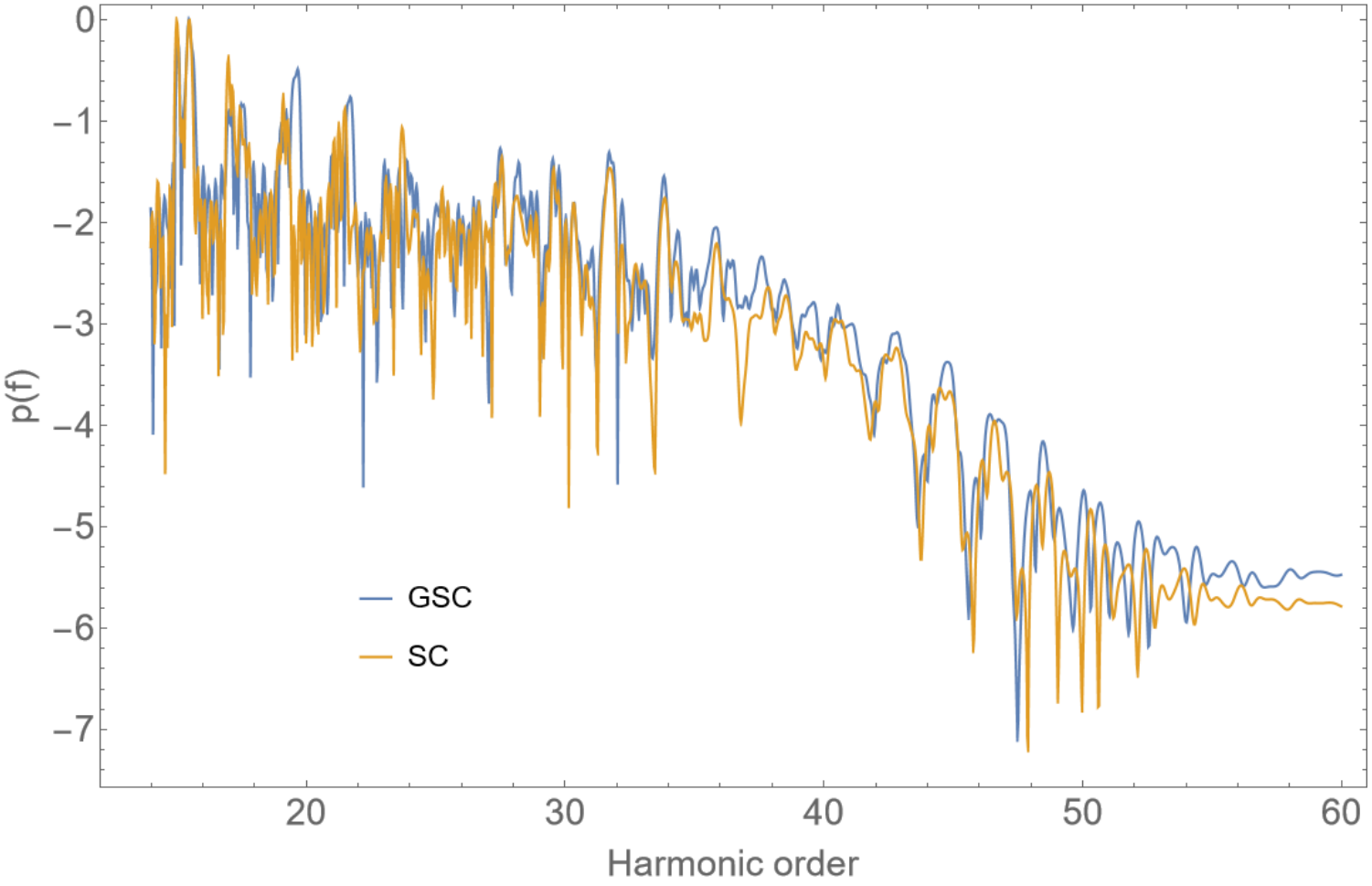


Preliminary results by the MMA-HHG code using SC vs. GSC atomic potential





Preliminary results by the MMA-HHG code using SC vs. GSC atomic potential



- Should enable direct comparison with experimental results
- Supercomputer load: TDSE solver parallel processing up to 1000s of CPU cores should be efficient
- Runtime for a medium with experimental relevance is close to upper limit at Komondor

Summary and Acknowledgements

Upgraded GSC 1D atomic model potentials enable efficient simulation of typical strong-field physics scenarios involving noble gas atoms driven by near- and mid-infrared laser pulses, with impressively increased accuracy compared to SC potentials.

The use of proper 1D atomic model potentials in the MMA-HHG code enables 1D TDSE-based numerical simulations of a macroscopic medium (low pressure gas jet or gas cell) and thus direct comparison of simulations and experiments.

More details: Phys. Rev. A **98** (2018) 023401; Phys. Rev. A **101** (2020) 023405; Phys. Rev. A **110** (2024) 063117;

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We acknowledge the Digital Government Development and Project Management Ltd. for awarding us access to the Komondor HPC facility based in Hungary.

At last but not least,

- PhD students, postdocs are welcome, both at ELI-ALPS and University of Szeged

- We are ready to help (also potential) users of ELI-ALPS with theory and simulation support

- Contact: attila.czirjak@eli-alps.hu

THANK YOU FOR YOUR ATTENTION!

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