Efficient algorithms for multi-level ionization of high-atomic-number gases and applications

Speaker: Aiqi Cheng[1]

Co-authors: Roman Samulyak[1], Rotem Kupfer[2], Navid Vafaei-Najafabadi[1]

AAC 2022

1. Stony Brook University
2. Lawrence Berkeley National Laboratory

Acknowledgement:
This work is supported by U.S. Department of Energy, Office of Science under Award No. DE-SC-0014043.

Motivations

- Ionization effects of gases, especially produced by higher power lasers, play a major role in laser wakefield accelerations.
- Improve known multi-level ionization algorithms
- Implement multi-ionization feature in electromagnetic code SPACE and enable simulations of ionization injection using high-Z gas target
- CO_2 laser at BNL allows exploration in long-wavelength scale.
- Ionization for high-atomic-number gases presents more complex numerical challenges than ionization of hydrogen.
  - Challenges -->next page

Ionization dynamics

- Step-wise process.

$$\frac{dn_0}{dt} = -W_1\, n_0$$ ← Hydrogen

$$\frac{dn^+}{dt} = W_0\, n_0 - W_1 n^+$$

....

$$\frac{dn^{(Z-1)+}}{dt} = W_{Z-2} n^{(Z-2)+} - W_{Z-1} n^{(Z-1)+}$$

$$\frac{dn^{Z+}}{dt} = W_{Z-1} n^{(Z-1)+}$$

$$n_{e^-} = \sum_{k=1}^{Z} k\, n^{k+}$$

- Challenges of this model:
  - W depends on the ion species and the charge state
  - Different time scales between ionization evolution and the code timestep
  - Dramatically increased memory allocation from multiple ion levels

- Assumption:
  - ignore recombination (much larger time scale)

Tunneling ionization rate

- ADK ionization model, in an alternating electric field
  - In explicit PIC code where $dt \ll \tau_0$

$$W = \omega_\alpha \frac{Z^2}{2{n^*}^2}\left(\frac{2e}{n^*}\right)^{2n^*} \exp\left[-\frac{2E_a}{3E_L}\left(\frac{Z}{n^*}\right)^3\right] \times \frac{(2l+1)(l+|m|)!}{2\pi n^* 2^{|m|}(|m|)!(l-|m|)!}\left(2\frac{E_a Z^3}{E_L {n^*}^3}\right)^{2n^*-|m|-1}$$

→ ion species and charge state dependent variables

Effective principle quantum number $n^* = Z\sqrt{\xi_H / \xi_{ion}}$

Ion charge after ionization Z

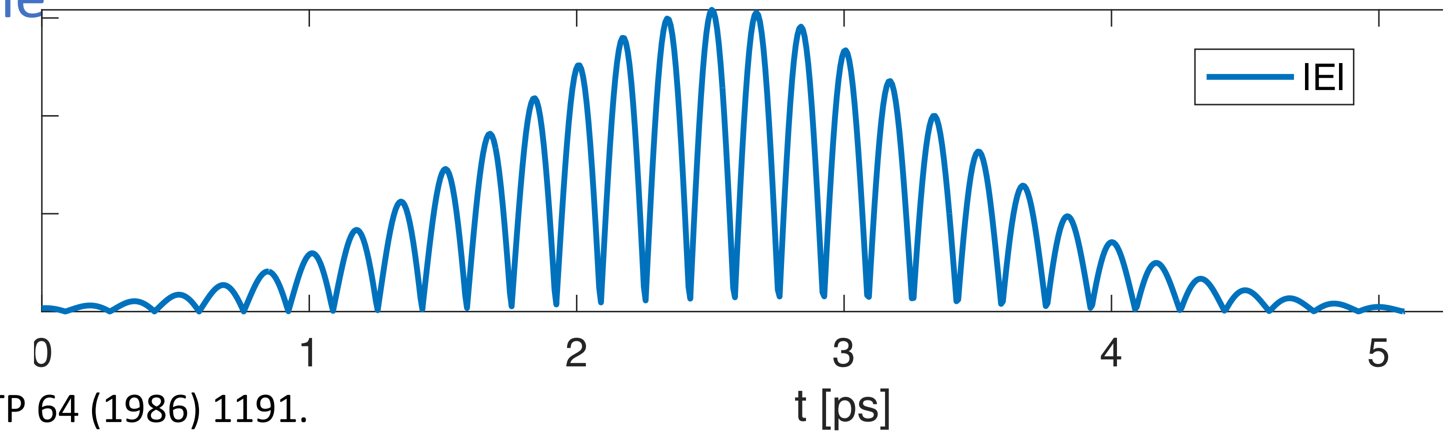
Orbital quantum number l , projection of orbital quantum number m

→ E_L Local electric field at certain time

→Atomic unit conversion

ω_α 1 a.u. Frequency

E_a 1 a.u. electric field

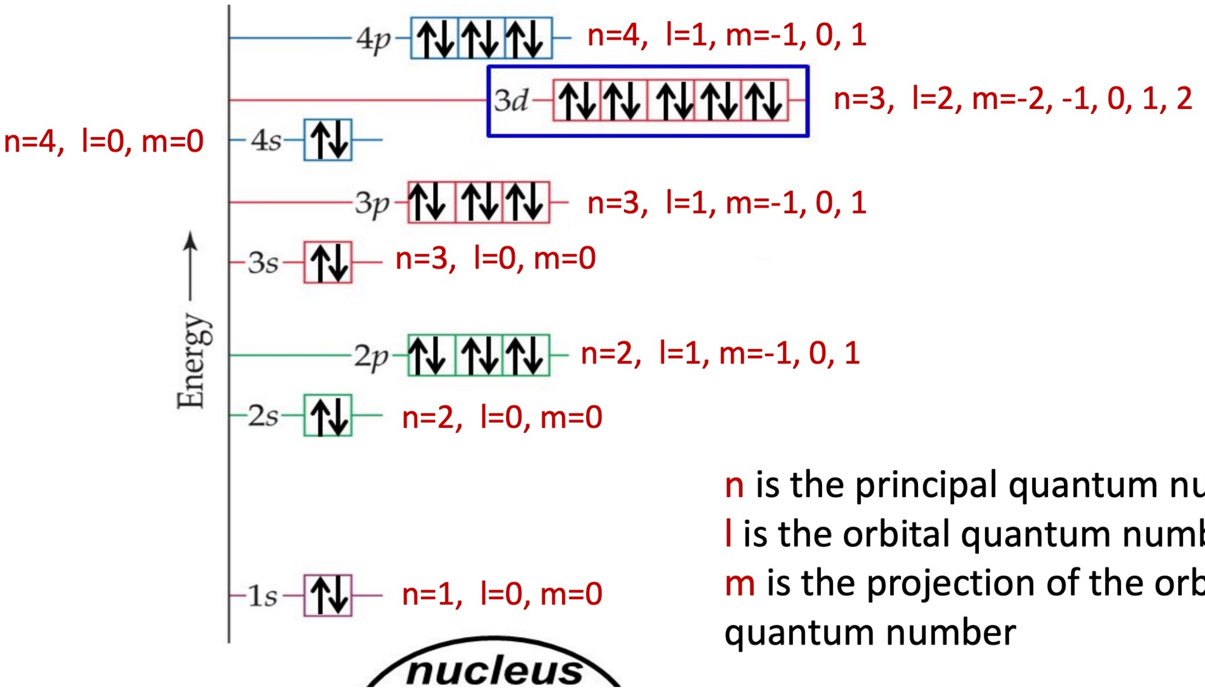


[1] M.V. Ammosov, N.B. Delone, V.P. Krainov, Sov. Phys. JETP 64 (1986) 1191.
[2] M.Chen, Numerical modeling of laser tunneling ionization in explicit particle-in-cell codes Journal of Computational Physics, 2013.

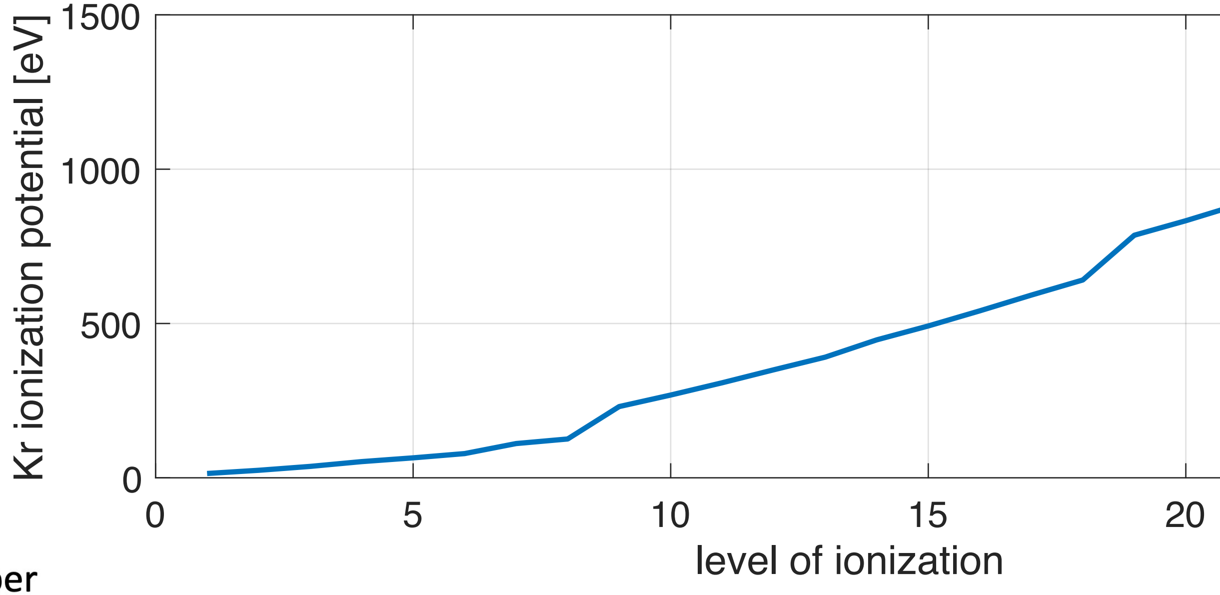
Dependence on l and m

- The ionization rate also depends on the orbital quantum numbers l and their projections m_l

Krypton electronic configuration: 1s2 2s2 2p6 3s2 3p6 4s2 3d10 4p6



n is the principal quantum number
l is the orbital quantum number
m is the projection of the orbital quantum number



Analytical solution

$$\begin{bmatrix} \dot{n_0} \\ \dot{n}^{+} \\ \dot{n}^{2+} \\ \cdots \\ \dot{n}^{(Z-1)+} \\ \dot{n}^{Z+} \end{bmatrix} = \begin{bmatrix} -W_0 & 0 & 0 & \cdots & 0 & 0 \\ W_0 & -W_1 & 0 & \cdots & 0 & 0 \\ 0 & W_1 & -W_2 & \cdots & 0 & 0 \\ \vdots & \cdots & \cdots & \ddots & \vdots & \vdots \\ \vdots & \cdots & \cdots & W_{Z-2} & -W_{Z-1} & 0 \\ 0 & \cdots & \cdots & 0 & W_{Z-1} & 0 \end{bmatrix} \begin{bmatrix} n_0 \\ n^{+} \\ n^{2+} \\ \cdots \\ n^{(Z-1)+} \\ n^{Z+} \end{bmatrix}$$

- at t=0, $[n_0 \quad n^{+} \quad \cdots \quad n^{Z+}]^T = [n_0 \quad 0 \quad \cdots \quad 0]^T$
- calculate $W_j(E, j)$ at each time step, assume the values are constant during dt
- the general solution of this ODE system: $$n^{i+}(t+dt) = \sum_{j=0}^{Z} C_j \vec{V}_j(i) e^{-W_j(t)dt}$$

  $\overrightarrow{V_j}$: eigenvector of the bidiagonal matrix of $[W_j]$

  C_j: coefficient for particular solution, solved using $\overrightarrow{V_j}$ and [n(t)] as initial condition at the beginning of each time step

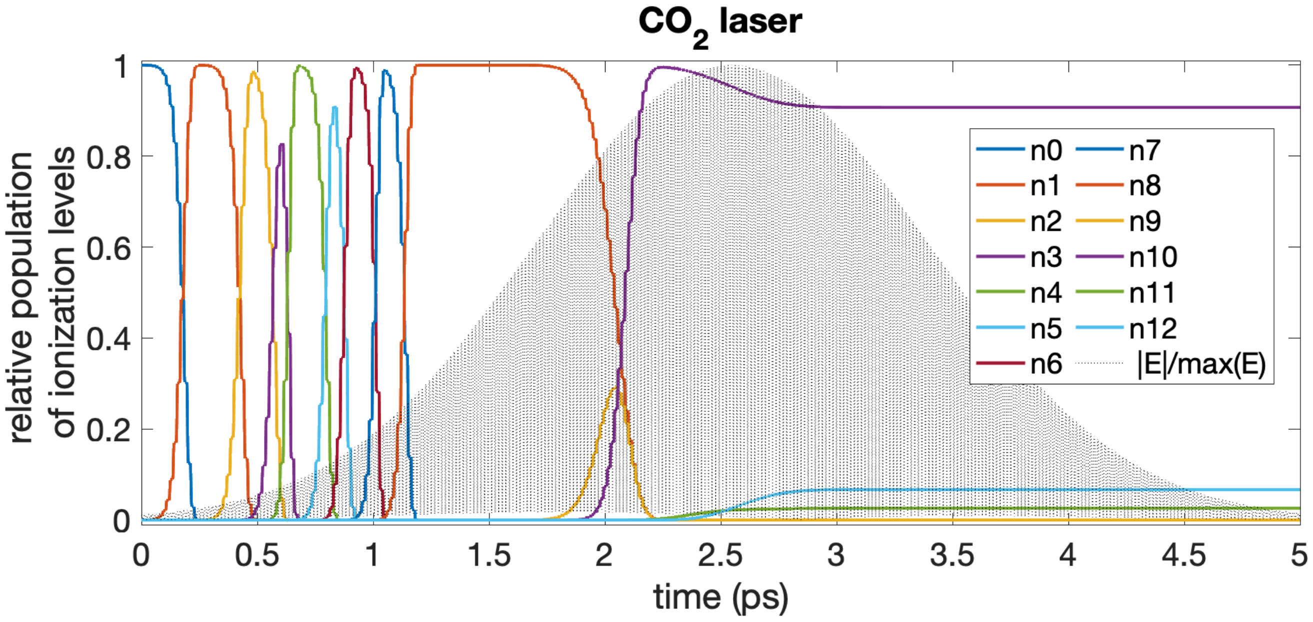
$$\begin{bmatrix} \vec{V}_0 & | & \vec{V}_1 & \cdots & | & \vec{V}_Z \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ \vdots \\ C_Z \end{bmatrix} = \begin{bmatrix} n_0(t) \\ n_1(t) \\ \vdots \\ n_Z(t) \end{bmatrix}$$

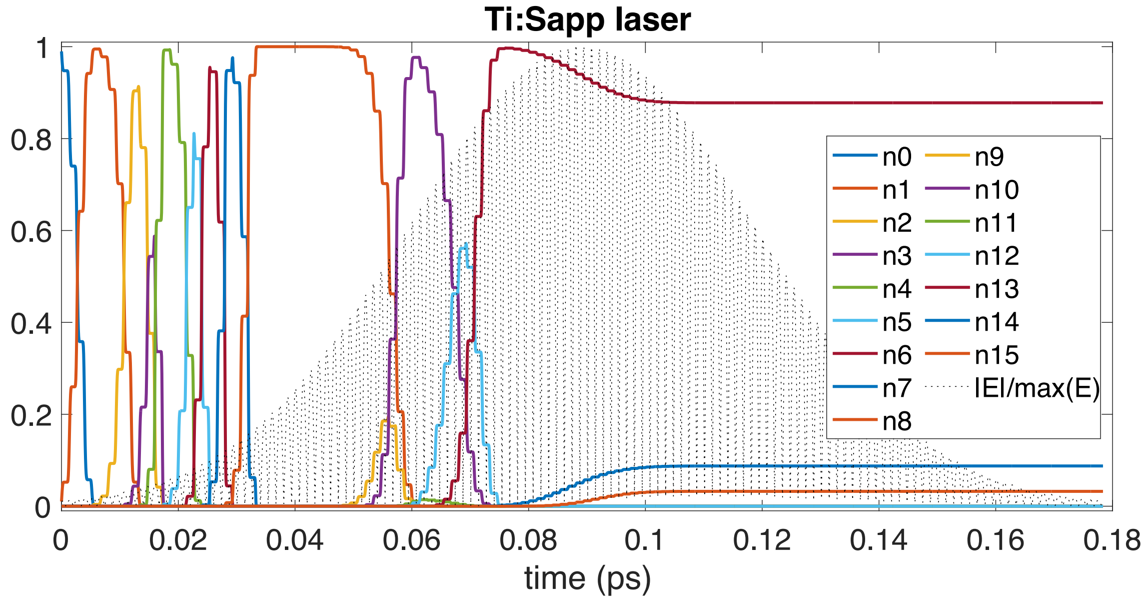
- correct selection of W + solve as analytical solution

  ➔ <u>overcome time discrepancy between ionization process and PIC time step</u>

Evolution of ionization

- Example: ionization evolution of Kr, near the focusing location of the laser.





- Highest level of ionization depends on peak intensity of the laser. → though not necessary to record all Z levels of number density, still need 12+ levels
- **Low and intermediate levels are highly transient.**
- **Only 2 to 3 ionization levels are present at an instance of time and location.**

Ionization evolution using reduced ODE system

- Full system of equations → reduced-order system with only 3 or 4 ionization levels
- Initialize number densities for each cell with only 4 levels
- This greatly improves efficiency of the algorithm for finely meshed 3D problems.

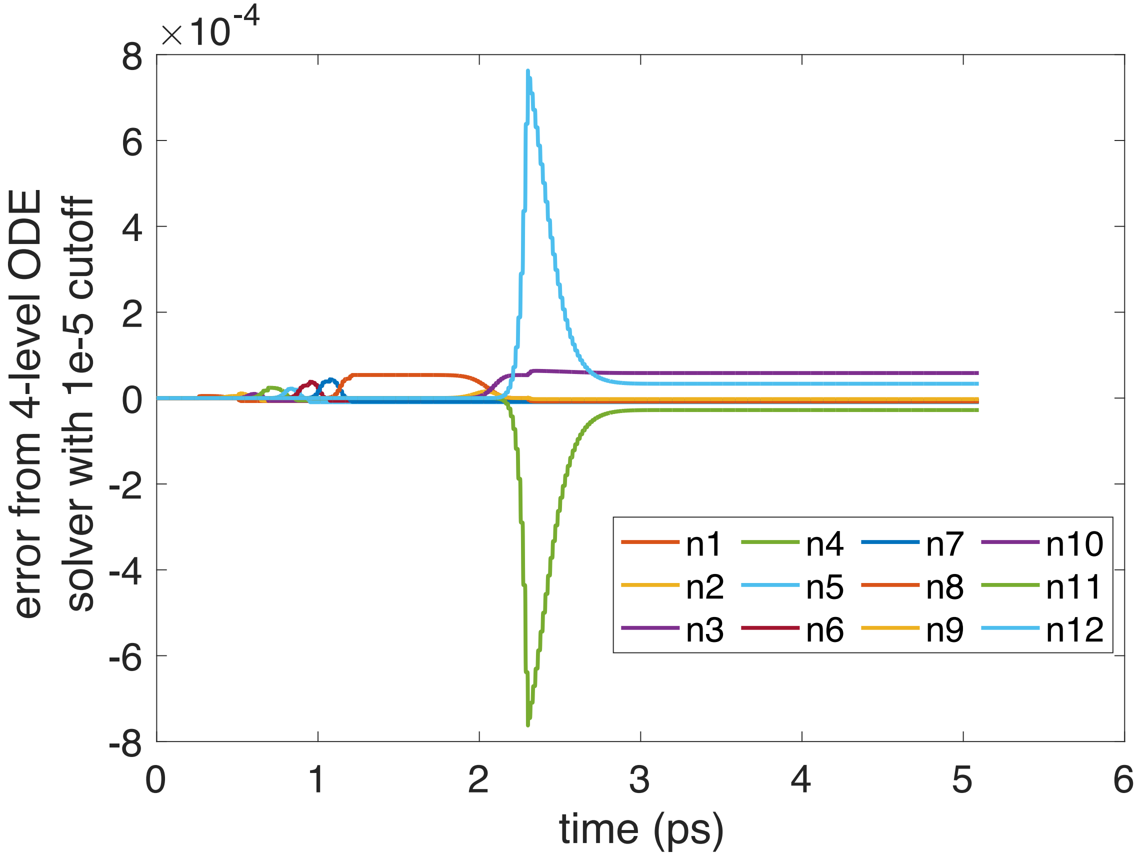
$$\begin{bmatrix} \dot{n}^{p+} \\ \dot{n}^{(p+1)+} \\ \dot{n}^{(p+2)+} \\ \dot{n}^{(p+3)+} \end{bmatrix} = \begin{bmatrix} -W_p & 0 & 0 & 0 \\ W_p & -W_{p+1} & 0 & 0 \\ 0 & W_{p+1} & -W_{p+2} & 0 \\ 0 & 0 & -W_{p+2} & W_{p+3} \end{bmatrix} \begin{bmatrix} n^{p+} \\ n^{(p+1)+} \\ n^{(p+2)+} \\ n^{(p+3)+} \end{bmatrix}$$

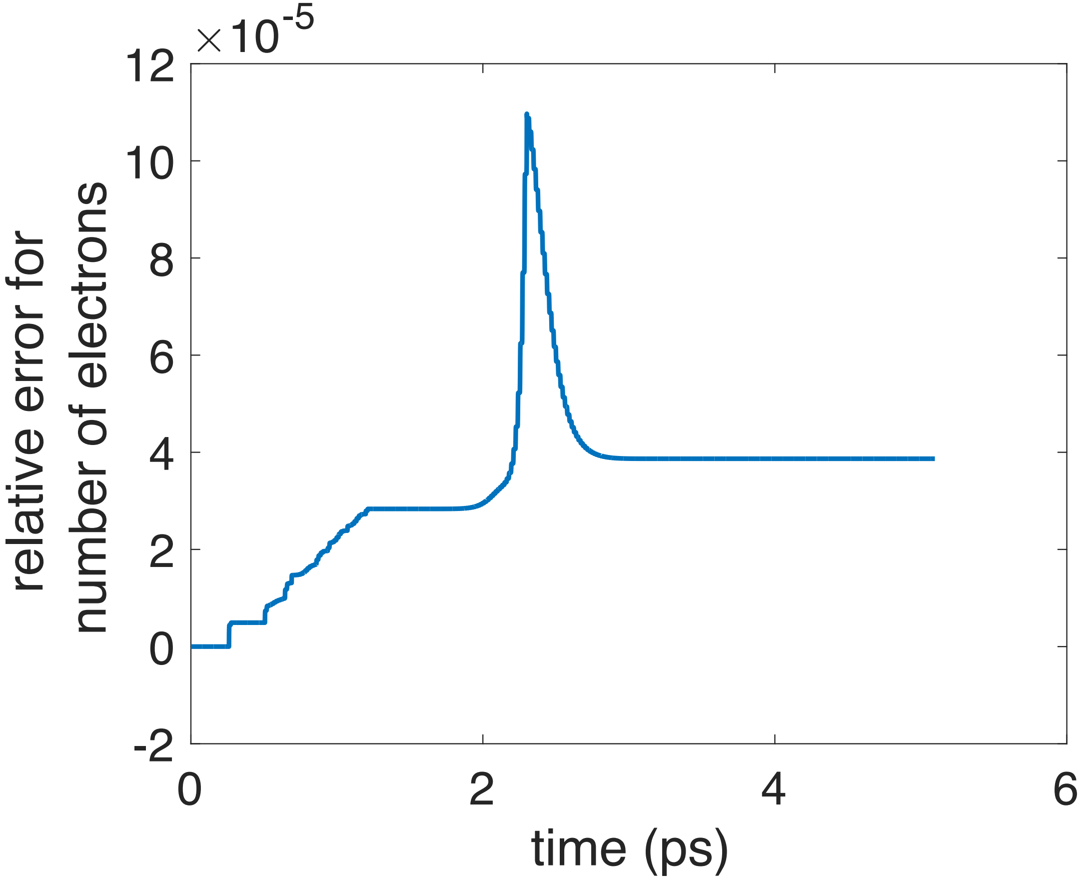
Algorithm: Reduced ODE system

procedure SOLVE NUMBER DENSITY
- $\mathbf{n} \leftarrow$ 4 level of *number density*
- $p \leftarrow$ *lowest ionization level*
- $\mathbf{W} \leftarrow$ ionization probability
- *loop*: solve 4-level ODE update $\mathbf{n}$
- add electron from new number density
- **if** $n[1] \approx 0$ **then**
  - $n[1,2,3] = n[2,3,4]$.
  - $n[4] = 0$.
  - $p = p + 1$.

Verification of reduced-4 level

- From example using Kr and CO2 laser
- Largest error happens around peak of laser, but overall < 0.01%





Implementation in the 3D, relativistic, parallel code SPACE

- EM-PIC module
  - physics models describing atomic processes and transformations
  - tracking particles of numerous species
  - parallel solver optimization for field solver and particle mover
- ES module - Adaptive Particle-in-Cloud method (AP-Cloud)
  - highly adaptive, fully particle replacement of PIC, for arbitrary geometry domains
  - adaptive computational nodes or particles with an octree data structure
  - particle quantity assigned to computational nodes by weighted least square approximation
  - PDE discretized using generalized finite difference method and solved with fast linear solvers

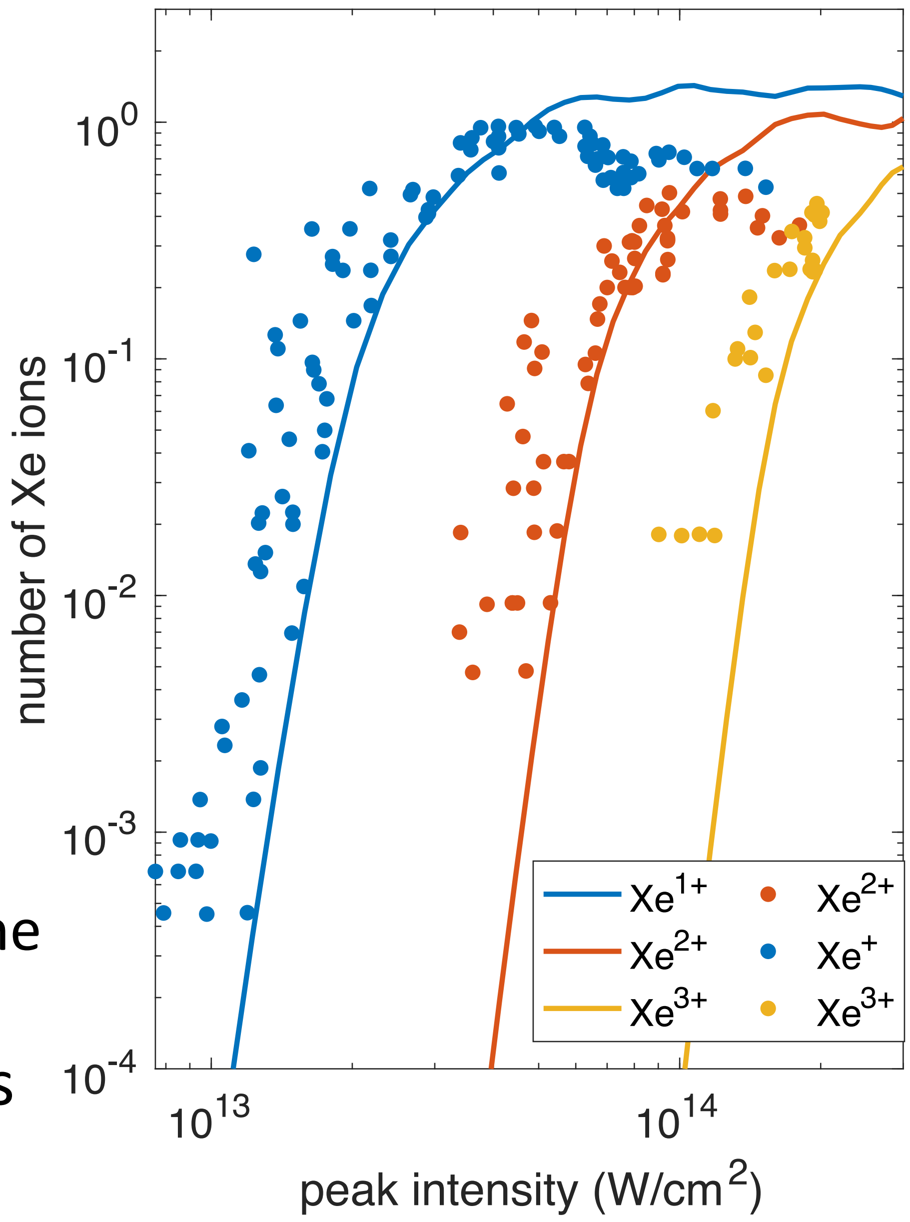
[4] K. Yu, P. Kumar, S. Yuan, A. Cheng, and R. Samulyak, SPACE: 3D parallel solvers for Vlasov-Maxwell and Vlasov-Poisson equations for Relativistic Plasmas with Atomic Transformations, Comp. Phy. Comm., Aug. 2022, doi: 10.1016/j.cpc.2022.108396.

Validation of solution

- Yergeau experiment (1987)
  - CO2 laser, pulse duration 1.1ns, beam waist 65um
  - Xe ion (dots)
- Estimated gaussian-Lorentz laser profile

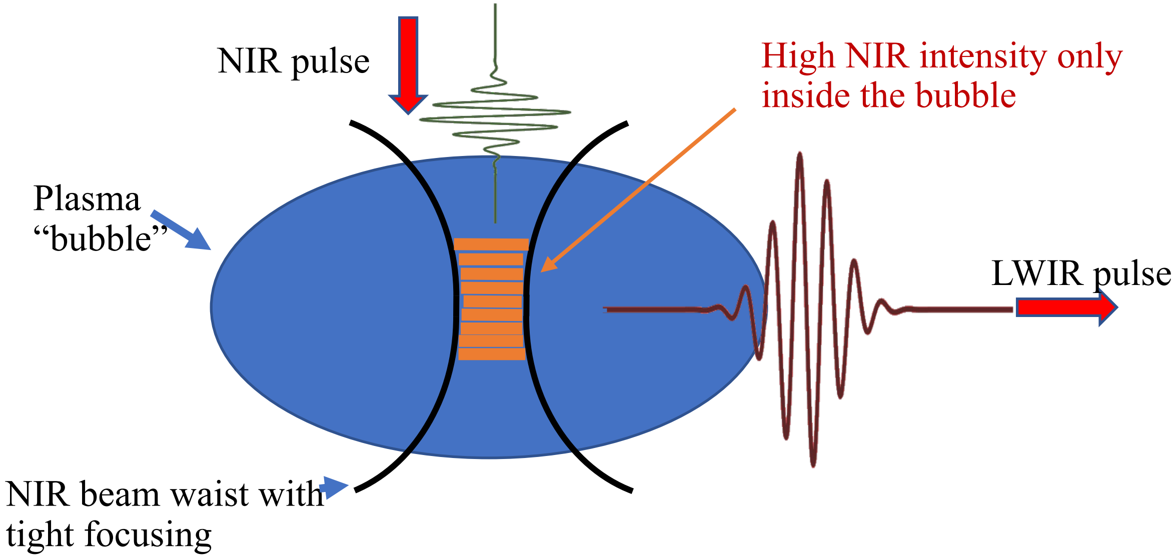
$$I(r,z,t) = I_0\, F(r,z)T(t)$$

- Integrate number of ions over a finite 3D volume around the laser focus location (lines)
- Good qualitative agreement
  - saturation features of each ion level
  - same slope of #ion vs. peak intensity comparing to the experimental data
- Slight shift to the right due to accumulation of errors



[3] F. Yergeau, S. L. Chin, and P. Lavigne, "Multiple ionisation of rare-gas atoms by an intense CO_2 laser (10^14W/cm^2)," *J. Phys. B: Atom. Mol. Phys.*, vol. 20, no. 4, pp. 723–739, Feb. 1987, doi: 10.1088/0022-3700/20/4/013.

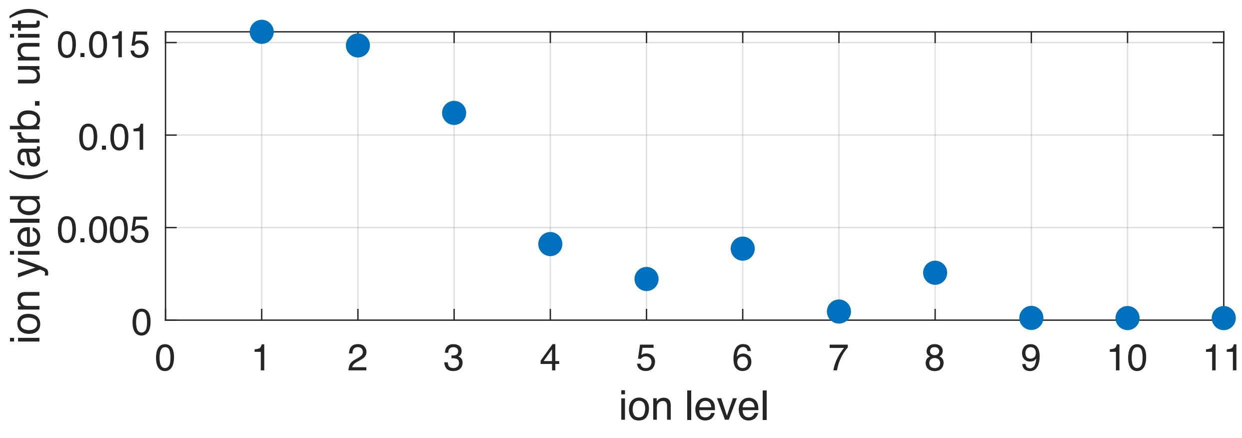
Ionization injection experiment setup



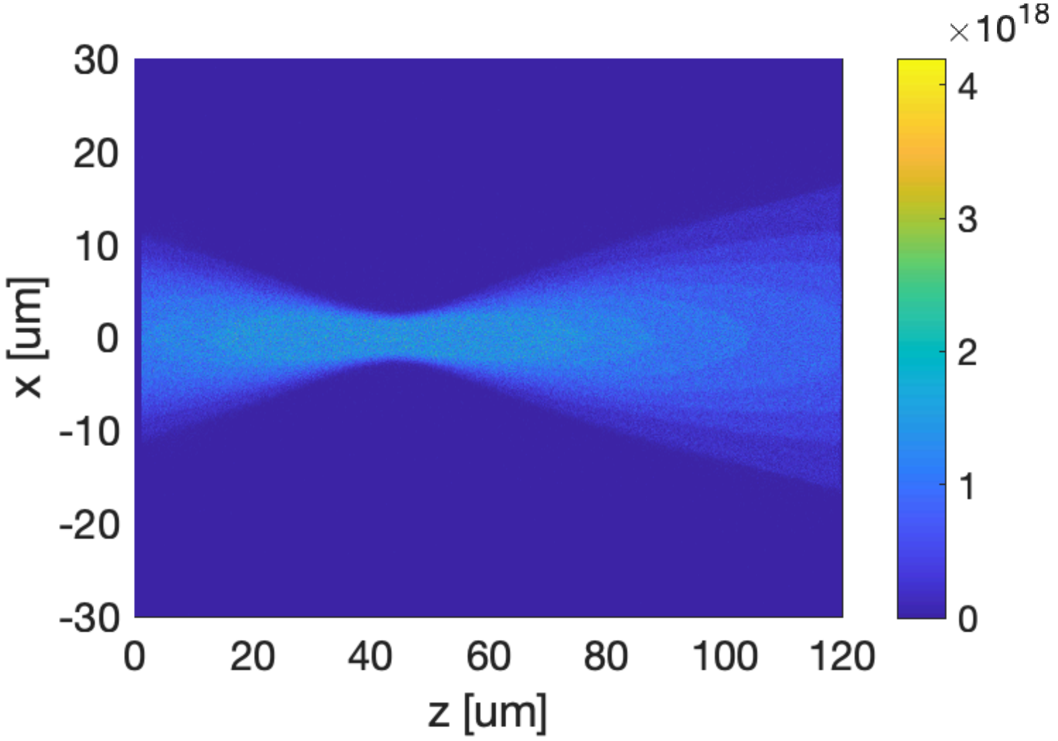
- High-Z gas target (Kr): high amplitude wakes, high acceleration and low emittance
- NIR: low a_0 with high intensity to ionize the plasma at a trapping wake phase.
- LWIR: high a_0 with low intensity long wavelength to drive the wake in self-modulated rigime, without fully ionize the gas

Study of ionization injection (3D implementation)

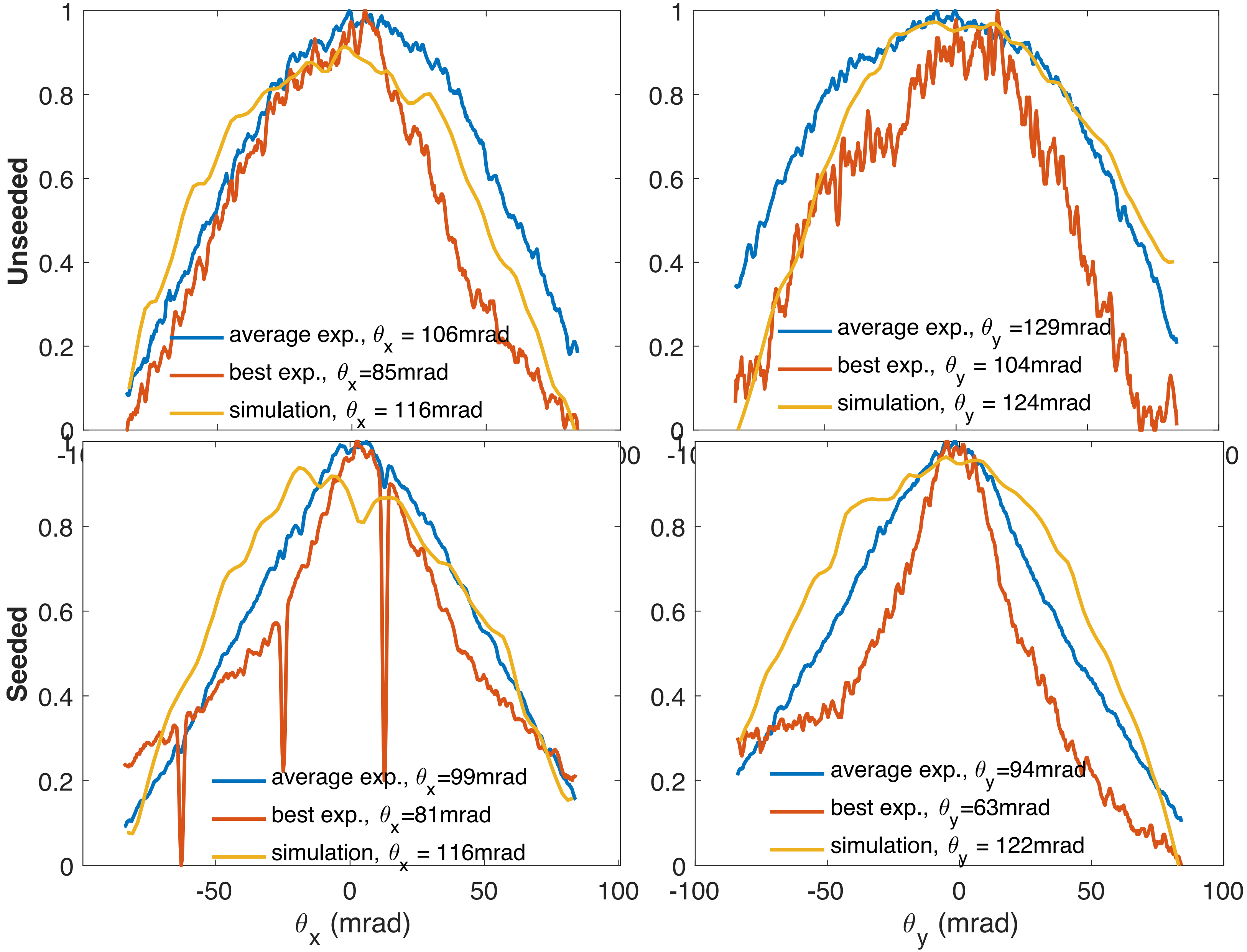
Ion yield by Ti:Sapph laser with 3mJ, 70fs



Charge distribution by Ti:Sapph laser (2ps after laser pass focus location)

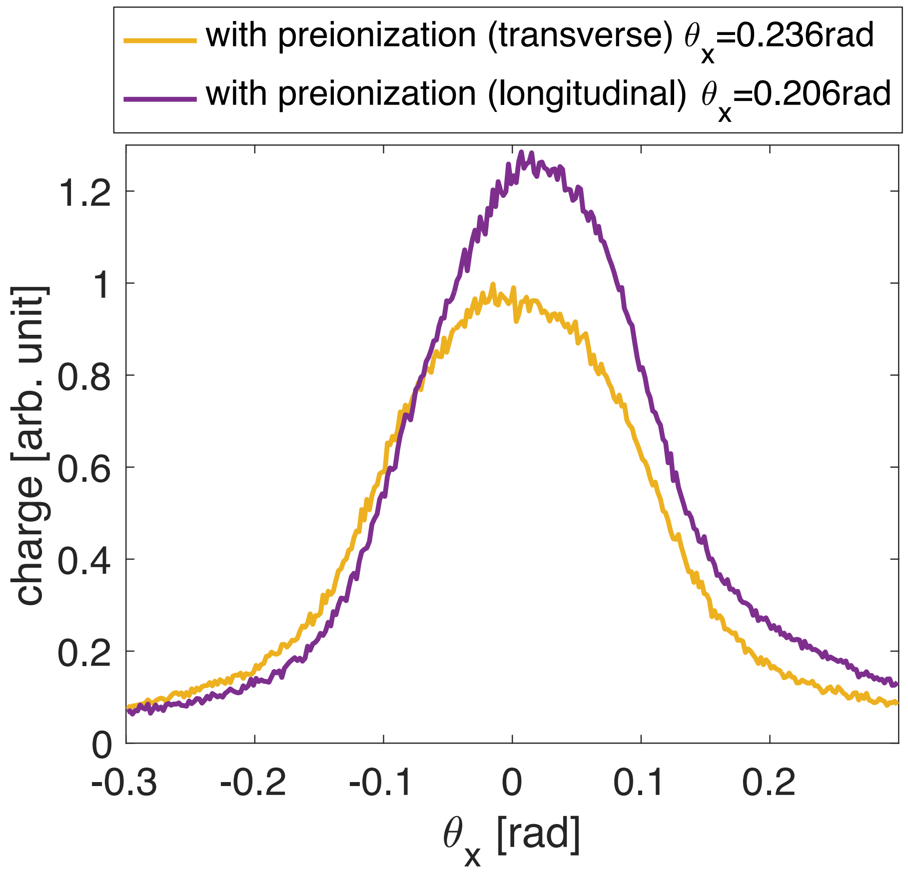


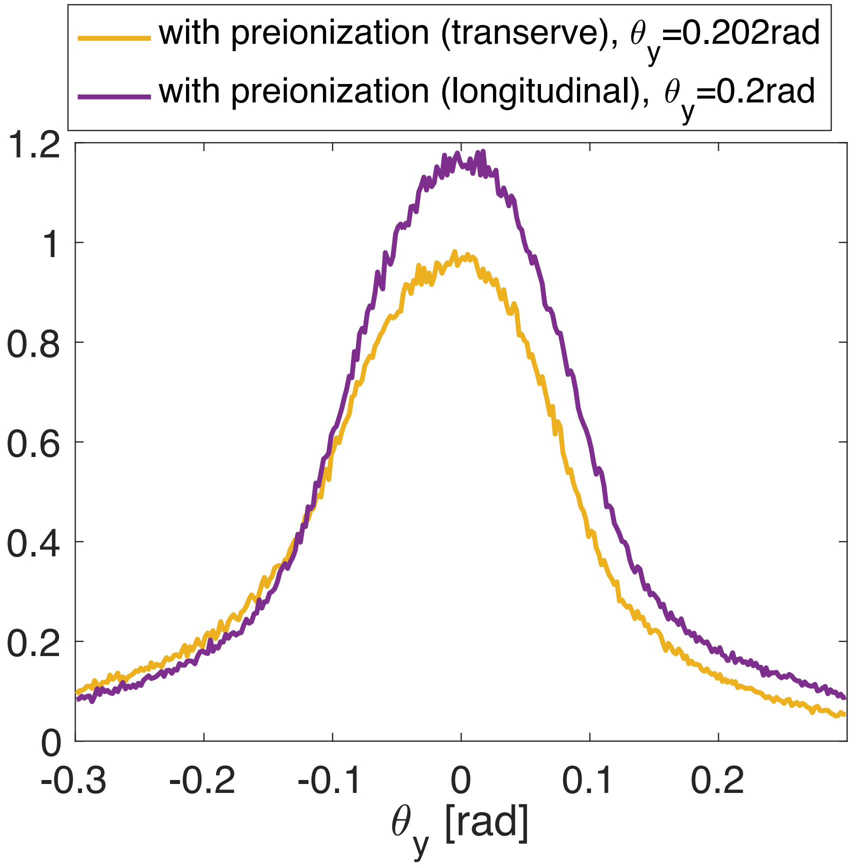
Divergence comparison with experiment



From plasma wakes driven by the CO2 laser in **self-modulated regime**

Simulation of ionization injection





Two laser	**perpendicular**	**Co-propagate**
charge/ charge without ionization laser	1.00	1.18
θ/θ_0 without ionization laser	x:0.98, y:1.02	x:0.85, y:1.01

Conclusion

- Developed efficient multi-level ionization algorithm with low error
- Validated model by comparing to experimental results
- Preliminary results for the study of ionization injection

Future Work

- Sensitively test on ion generations with various parameters
- Improve resolution and memory allocation efficiency in the 3D code
- Support ionization injection experiments in various settings

References

- M.V. Ammosov, N.B. Delone, V.P. Krainov, Sov. Phys. JETP 64 (1986) 1191.
- M.Chen, Numerical modeling of laser tunneling ionization in explicit particle-in-cell codes Journal of Computational Physics, 2013.
- F. Yergeau, S. L. Chin, and P. Lavigne, “Multiple ionisation of rare-gas atoms by an intense CO_2 laser (10^14W/cm^2),” *J. Phys. B: Atom. Mol. Phys.*, vol. 20, no. 4, pp. 723–739, Feb. 1987, doi: 10.1088/0022-3700/20/4/013.
- K. Yu, P. Kumar, S. Yuan, A. Cheng, and R. Samulyak, SPACE: 3D parallel solvers for Vlasov-Maxwell and Vlasov-Poisson equations for Relativistic Plasmas with Atomic Transformations, Comp. Phy. Comm., Aug. 2022, doi: 10.1016/j.cpc.2022.108396.

Acknowledgment

This work is supported by U.S. Department of Energy, Office of Science under Award No. DE-SC-0014043.