Time-dependent method in laser material interactions
-- a hybrid method of using openmp + MPI + cuda C in Fortran

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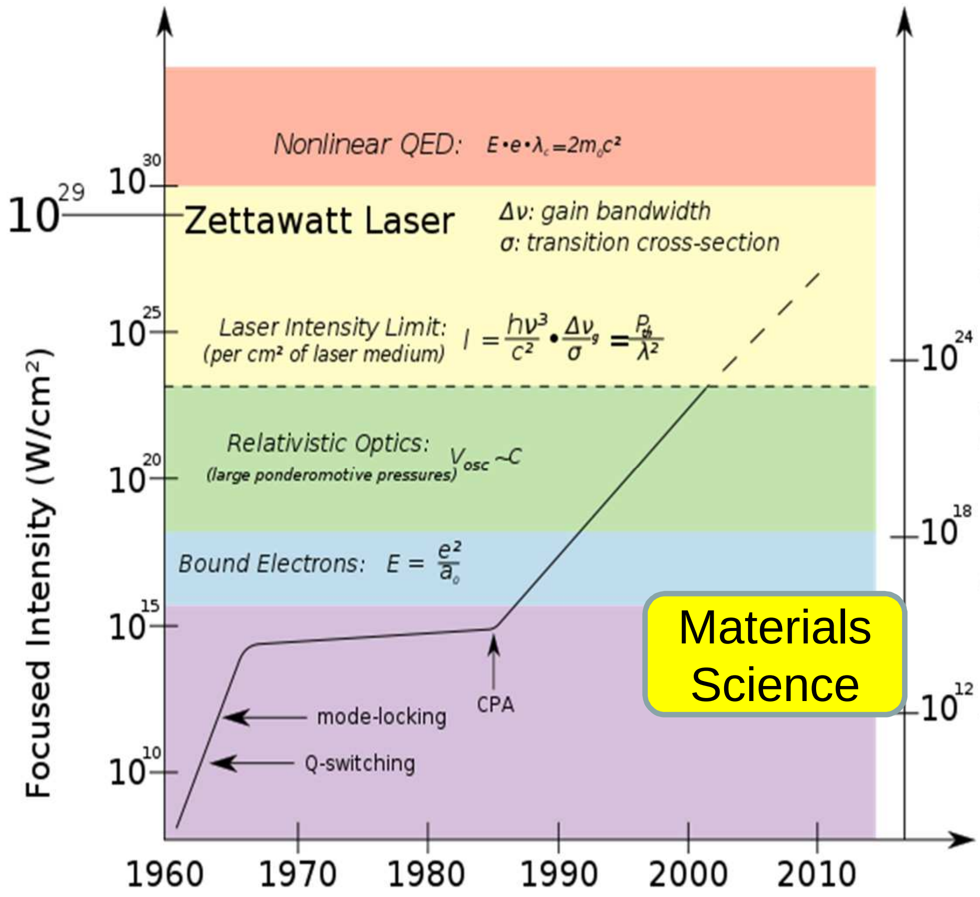
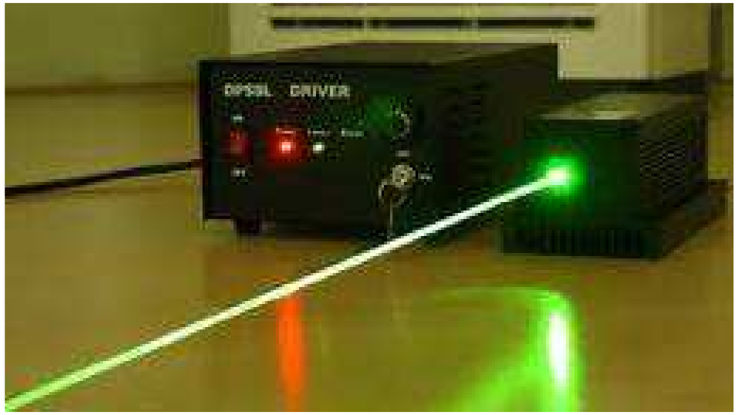
Outline

- What we are working on
  - **Understand** the mechanism of laser-material interactions
  - **Control** material properties in an ultrashort time scale
- Computational Methods
  - Working Equation: Time-dependent Schrodinger equation (PDE)
  - Space: dynamic important region (Inner, numerical simulation), asymptotical region (outer region, analytic treatment)
  - Many-electron effect: Model potential, Density-functional theory
  - **Code structure for HA-PACS (GPU cluster)**
- Results
  - Above threshold ionization in intense mid-IR field (80GB, 50x6 PFlops)
  - Control the transparency in attosecond time-scale

Status of intense laser



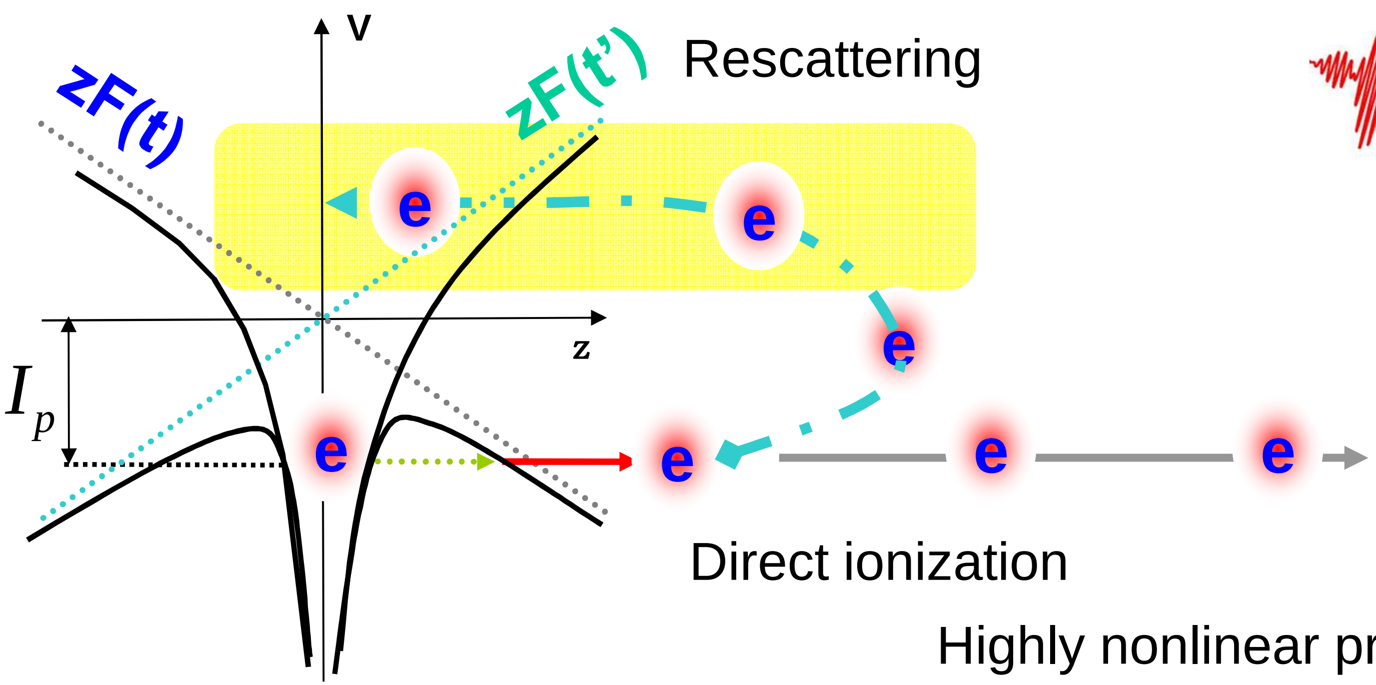


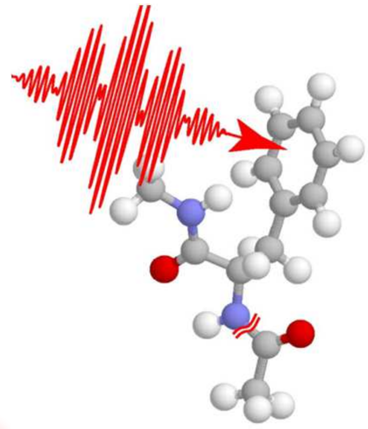
Laser intensity: $10^{12} \sim 10^{16}$ W/cm^2

Pulse duration: 4 fs (10^{-15} s) ~

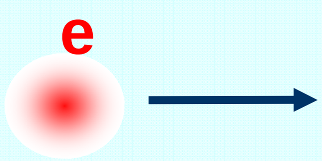
Wavelength: 200 nm ~ 4000 nm

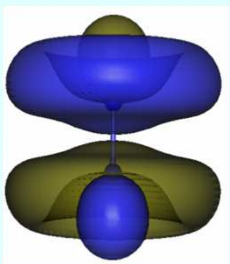
Main mechanism and its application: Rescattering





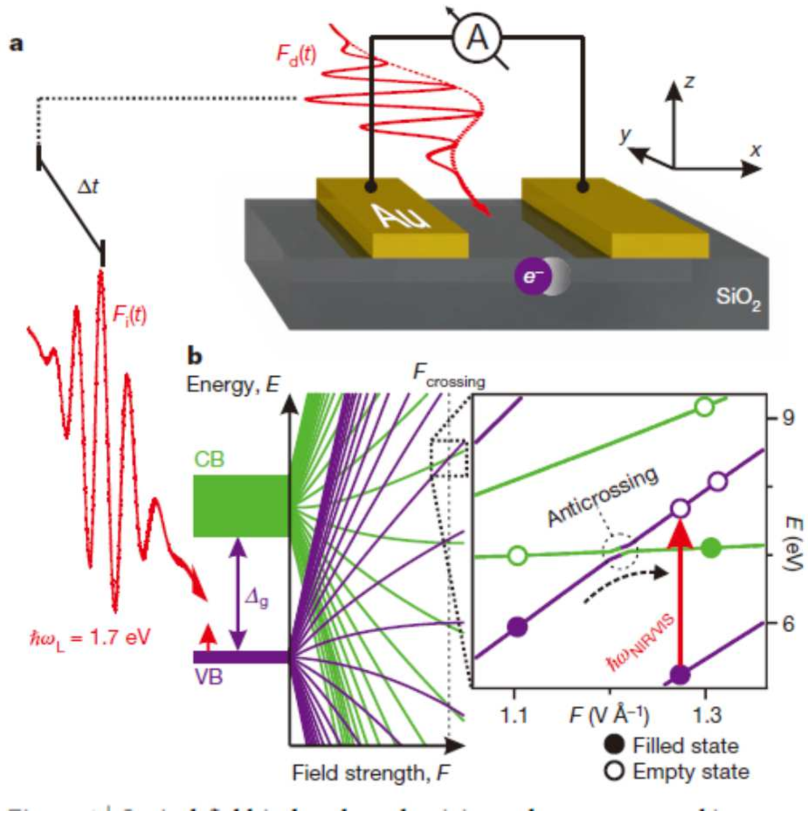
Highly nonlinear process



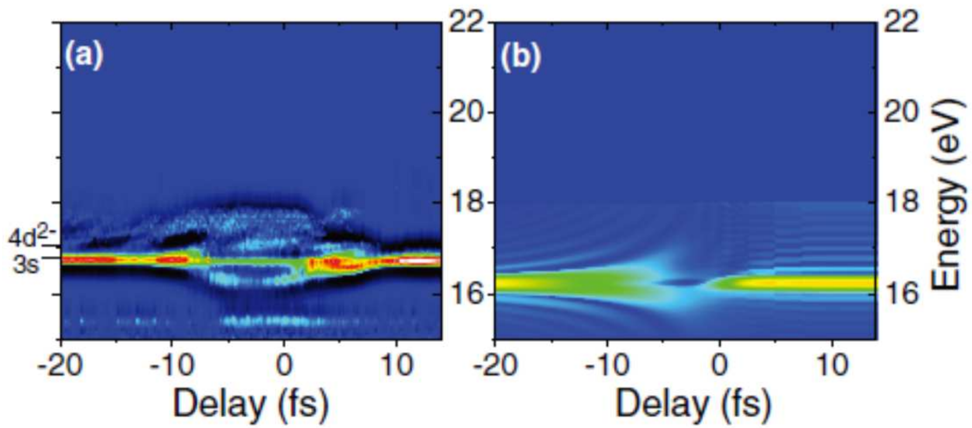


(a) High harmonic generation
(b) Ionization or dissociation
(c) Image the structure (holography)

Control material properties in attosecond time scale



Simulation on HA-PACS



Photoabsorption or no (1 fs)

Insulator ➔ conductor (1 fs)

Wang, *et. al.,* PRA (2013)

A. Schiffrin, *et. al.,* Nature, (2012)

Working Equations (time-dependent Schrodinger equation)

Initial: Φ_0

Differential:
$$i\frac{\partial}{\partial t}\Psi(t) = H(t)\Psi(t) \qquad \Psi(t) = U(t,-\infty)\Phi_0$$

Integral:
$$\Psi(t) = -i\int_{-\infty}^{t} U(t,\tau)V_{in}(\tau)U_0(\tau,-\infty)\Phi_0 d\tau + U_0(t,-\infty)\Phi_0$$

Laser material interactions

Length gauge $V^{ext}(t) = \mathbf{r}\cdot\mathbf{E}(t)$

$$\boldsymbol{A}(t) = \int_{t'}^{\infty} \boldsymbol{E}(t')dt'.$$

Velocity gauge $V^{ext}(t) = \mathbf{p}\cdot\mathbf{A}(t)$

Key step: time-propagator (Split-Operator Method)

Time-propagation:

$$\begin{aligned}\Psi(t+\Delta t) &= e^{-iH(t)\Delta t} = U(t+\Delta t, t)\Psi(t) \\ &\approx e^{-iH_0\Delta t} e^{-iV(t)\Delta t} e^{-iH_0\Delta t}\Psi(t) + O(\Delta t^3)\end{aligned}$$

Discretize space in pseudo-spectra grid:

$$H_0 = H^0_{r_i,r_j}(\ell), \quad \Psi(r_i,\theta) = \sum_\ell R_\ell(r_i) Y_{\ell,m}(\hat{r}), \quad \Psi(r_i,\ell) = R_\ell(r_i)$$

Time-propagation → vector, matrix operations → blas

One time step:	2 zgemv (zgemm):	NR^2 x NL x (Np)	cublas_
	2 zgemm :	NR x NL^2 x (Np)	cublas_
	1 exponential :	NR*NL*(Np)	Cuda C
Total ops. Z		4*NR*NL*(NR+NL+1)*(Np) *NT***K** **(K=1,3)**	

Outline of the simulation code

MPI_init / GPU_device

Prepare pre-time-pro.

Copy data to GPU

Time -propagation

Output

Eigen value problem (MKL)
S: NR^2 * LperThread*16
(4000^2 x 16 x 15 = 3.8 GB)

$$\Psi_0, \quad S(\ell) = e^{-iH_0(\ell)\Delta t/2}$$

$$\Psi(t+\Delta t) \quad = \quad e^{-iH_0\Delta t} e^{-iV(t)\Delta t} e^{-iH_0\Delta t} \Psi(t)$$

$$\Psi^a(r,\ell) = S_{r\to r'}(\ell)\Psi(r',\ell) \quad \mathrm{zgemv(m)}$$

$$\Psi^b(r,\theta) = T_{\ell\to\theta}\Psi^a(r,\ell) \quad \mathrm{zgemm}$$

$$\Psi^c(r,\theta) = e^{-iV(r,\theta,t)\Delta t}\Psi^b(r,\theta) \quad \mathrm{Cuda\ C}$$

MPI_ALLREDUCE

$$\Psi^d(r,\ell) = T_{\theta\to\ell}\Psi^c(r,\theta) \quad \mathrm{zgemm}$$

$$\Psi^a(r,\ell) = S_{r\to r'}(\ell)\Psi(r',\ell) \quad \mathrm{zgemv(m)}$$

Structure of code (machine)

One MPI thread

OpenMP+ mkl

Cublas + CUDA C

HA-PACS

Device = mod(myid,4)

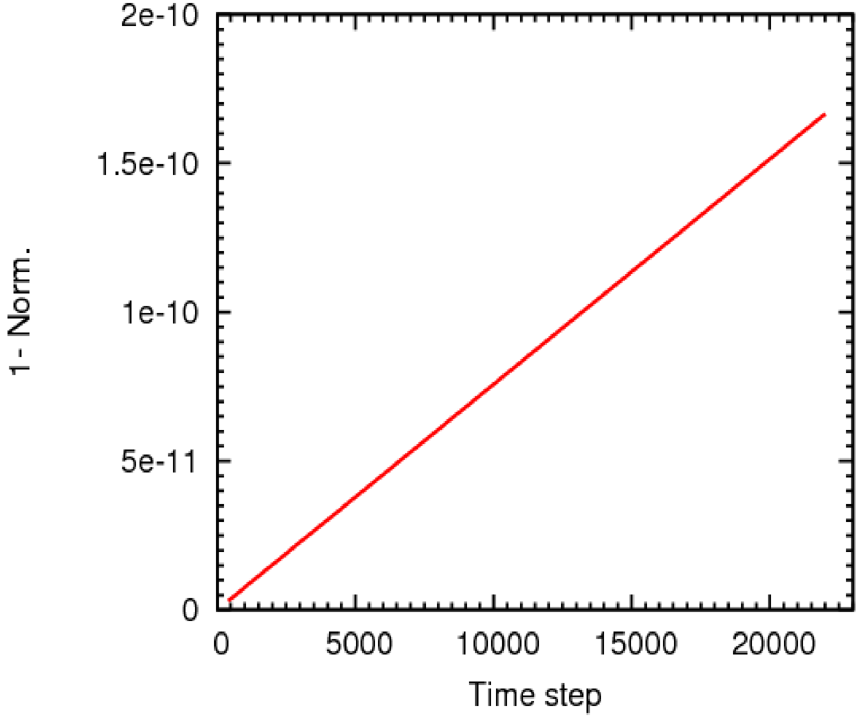
MPI (node 0)	MPI (node 1)	......	MPI (node n)
Thread 0 (Device 0)	**Thread 4** (Device 0)		**Thread a** (Device 0)
Thread 1 (Device 1)	**Thread 5** (Device 1)		**Thread b** (Device 1)
Thread 2 (Device 2)	**Thread 6** (Device 2)		**Thread c** (Device 2)
Thread 3 (Device 3)	**Thread 7** (Device 3)		**Thread d** (Device 3)

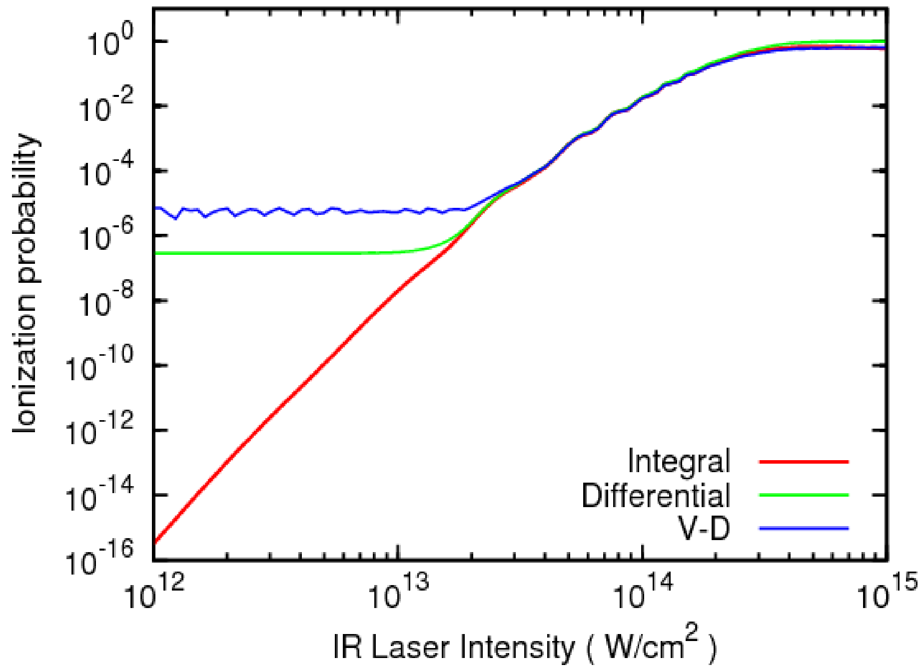
Numerical accuracy:

Single-electron model:

One time-step: random, round-off, double-complex, 10^{-14} (norm)

Time propagation: systematic error:





Memory and Work load

2D + Time propagation in spherical coordinates:

Memory: $k*16*N_r^2 * N_L$ (0.5 GB ~ 100.0 GB)
(800, 50 ~ 4000, 300)

Flops: $k*N_r^2 * N_L * N_t$ (0.5N_p PFlops, ~ 100N_p PFlops)

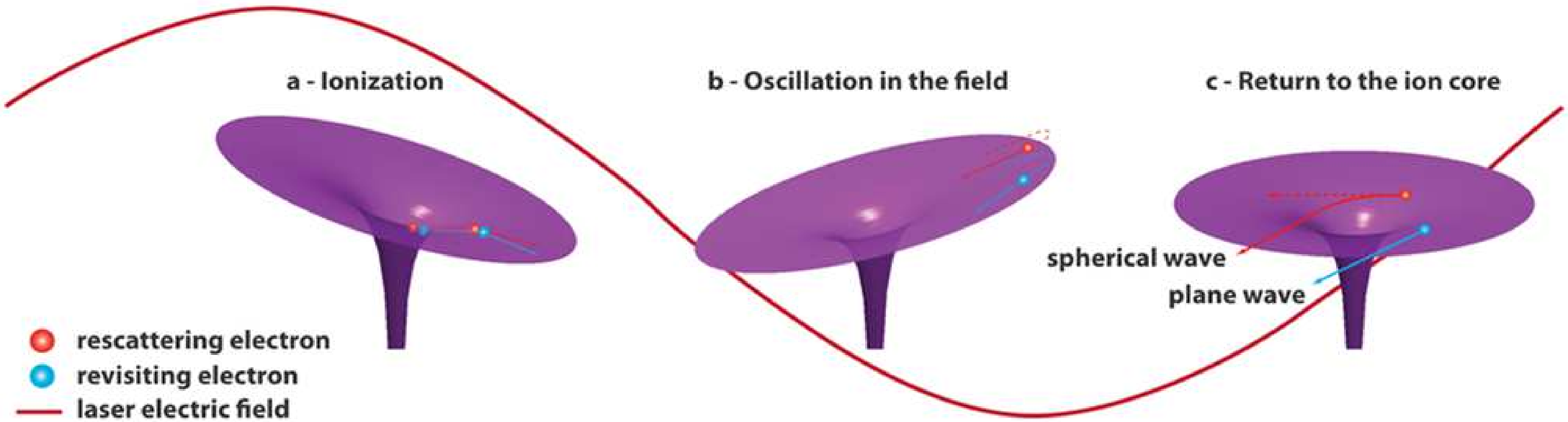
Speed: Double complex:

- Small Job (5 nodes, NO GPU comm) : 68% , 1.7x6 TFlops
- Large Job: (20 nodes, With GPU comm): 10% , 1.0x6 TFlops

ATI in intense mid-IR field

ATI: above-threshold ionization

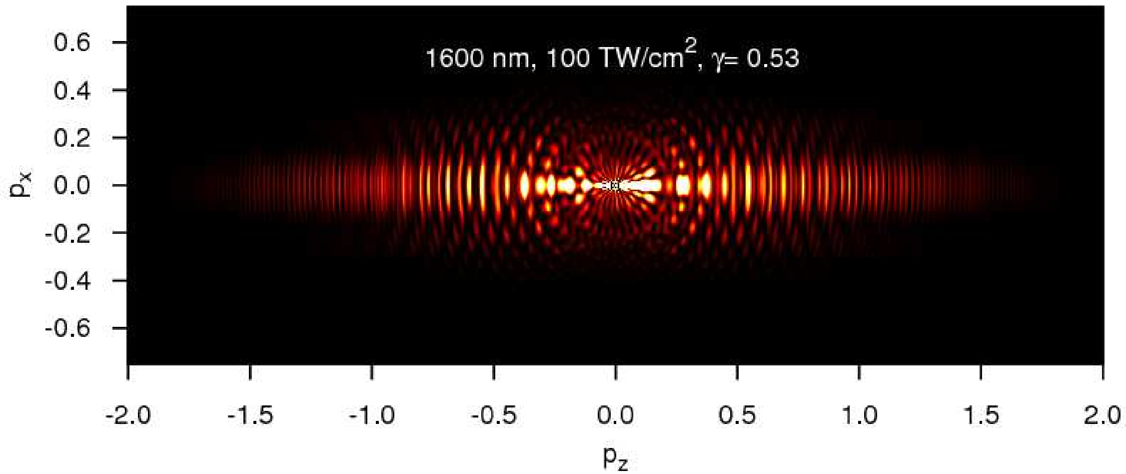
Physical Process: $A \; + n \; h\nu \; \rightarrow \; A^{+} + e$



ATI in intense mid-IR field

Memory: $\propto \lambda^3$

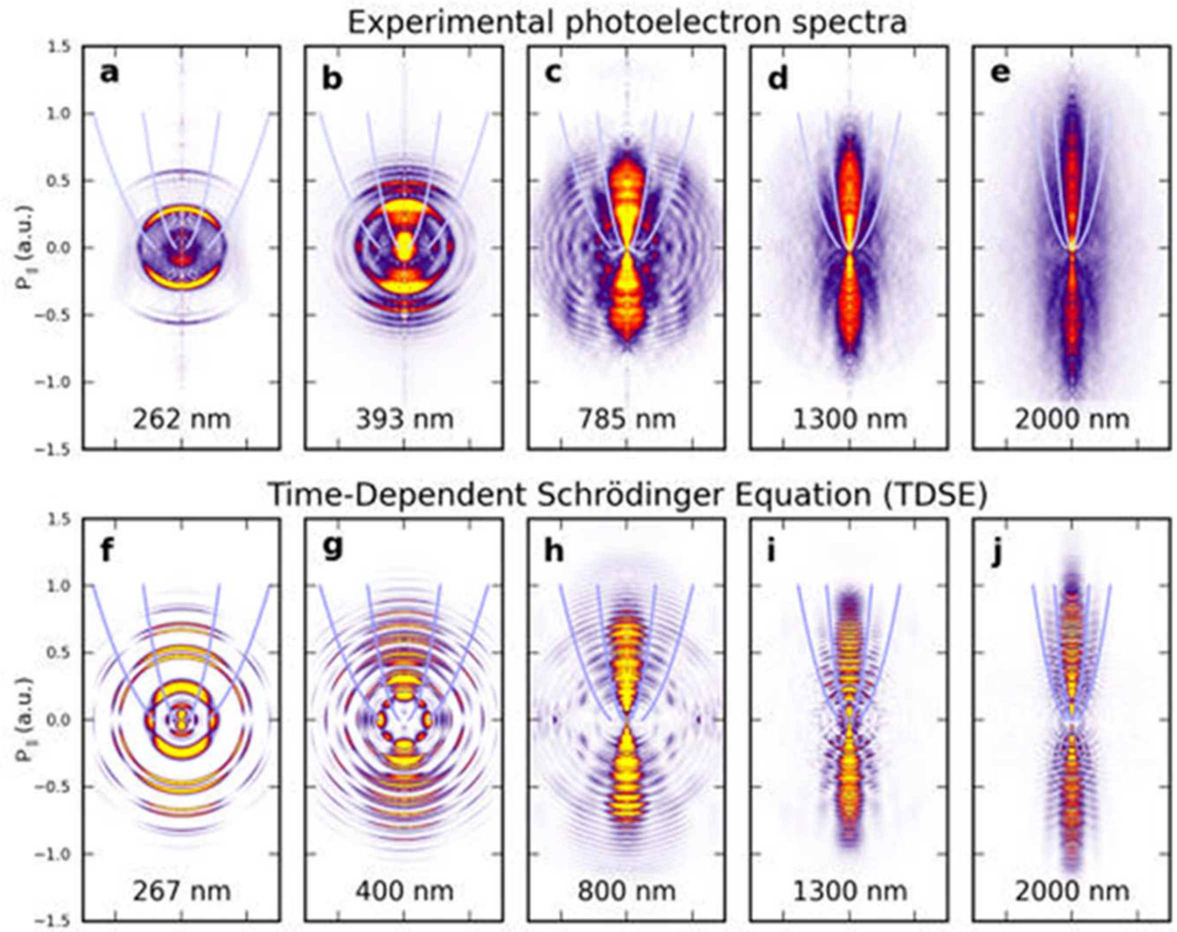
A typical ATI spectra:

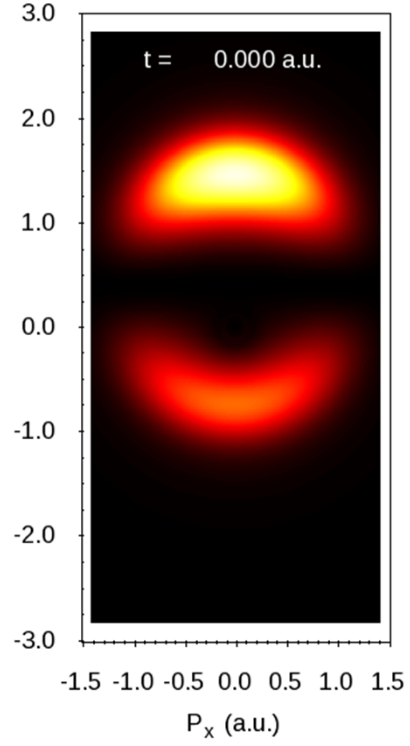


Goal:

- understand the structure:
  interference between the returning and rescattering electrons
- Information encoded in the structure:
  inner-work: how the electron interacts with the parent core

Comparison with experiment



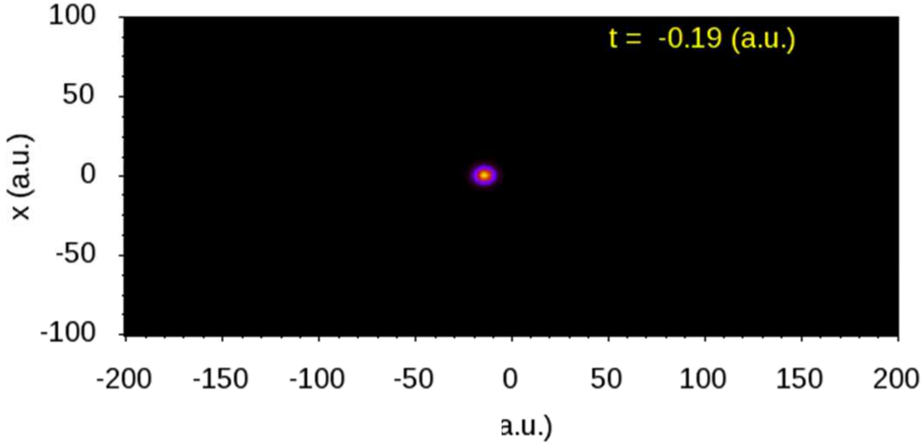


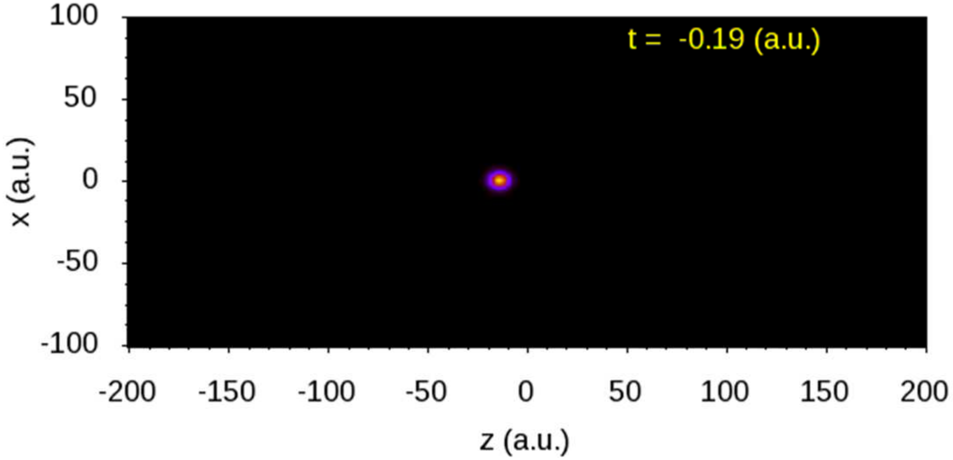
D. D. Hichstein, *et. al.*, PRL (2012).

HA-PACS: 5 nodes, 20 hrs

Attosecond Streaking

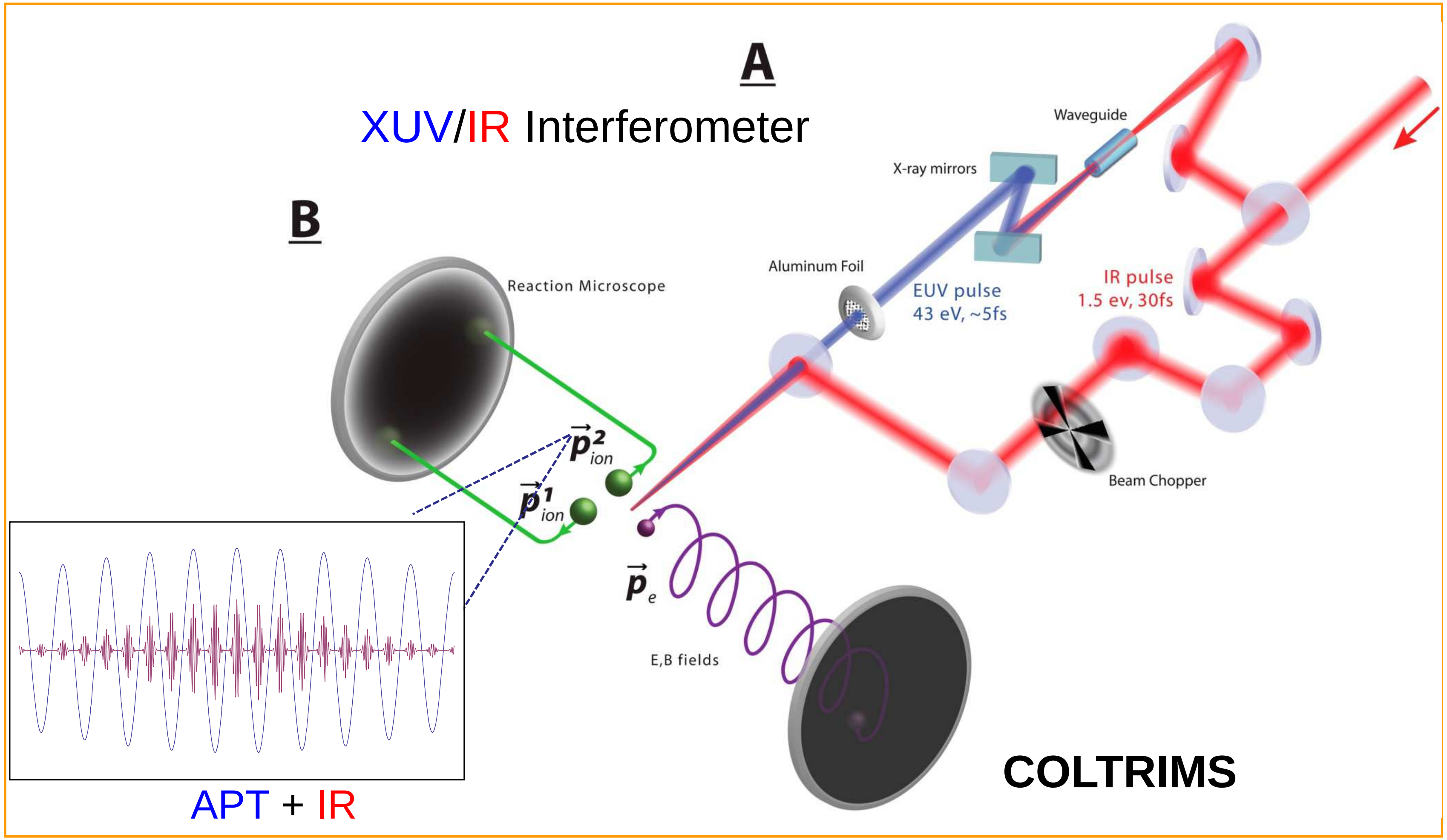
Without IR field



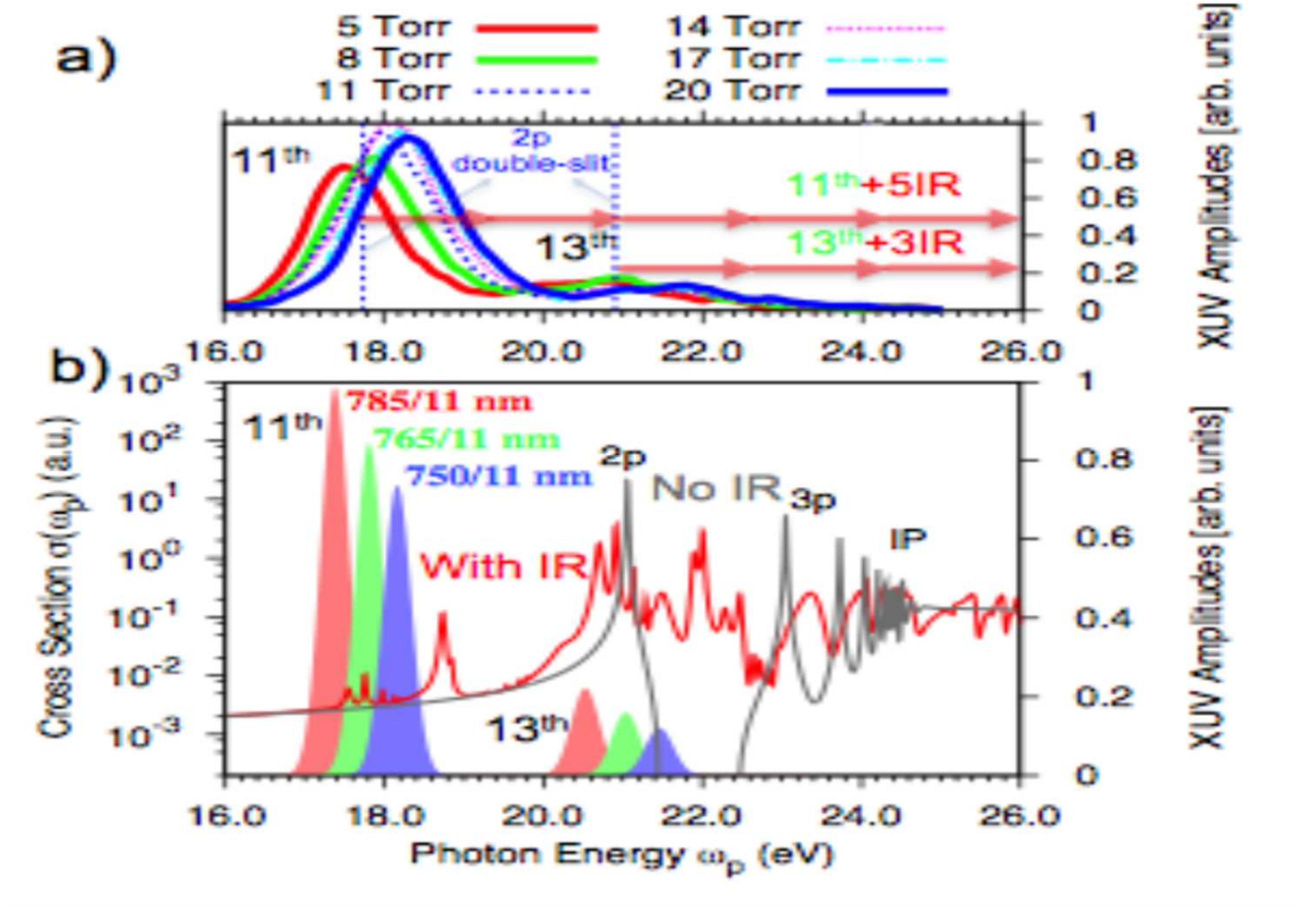


With IR field

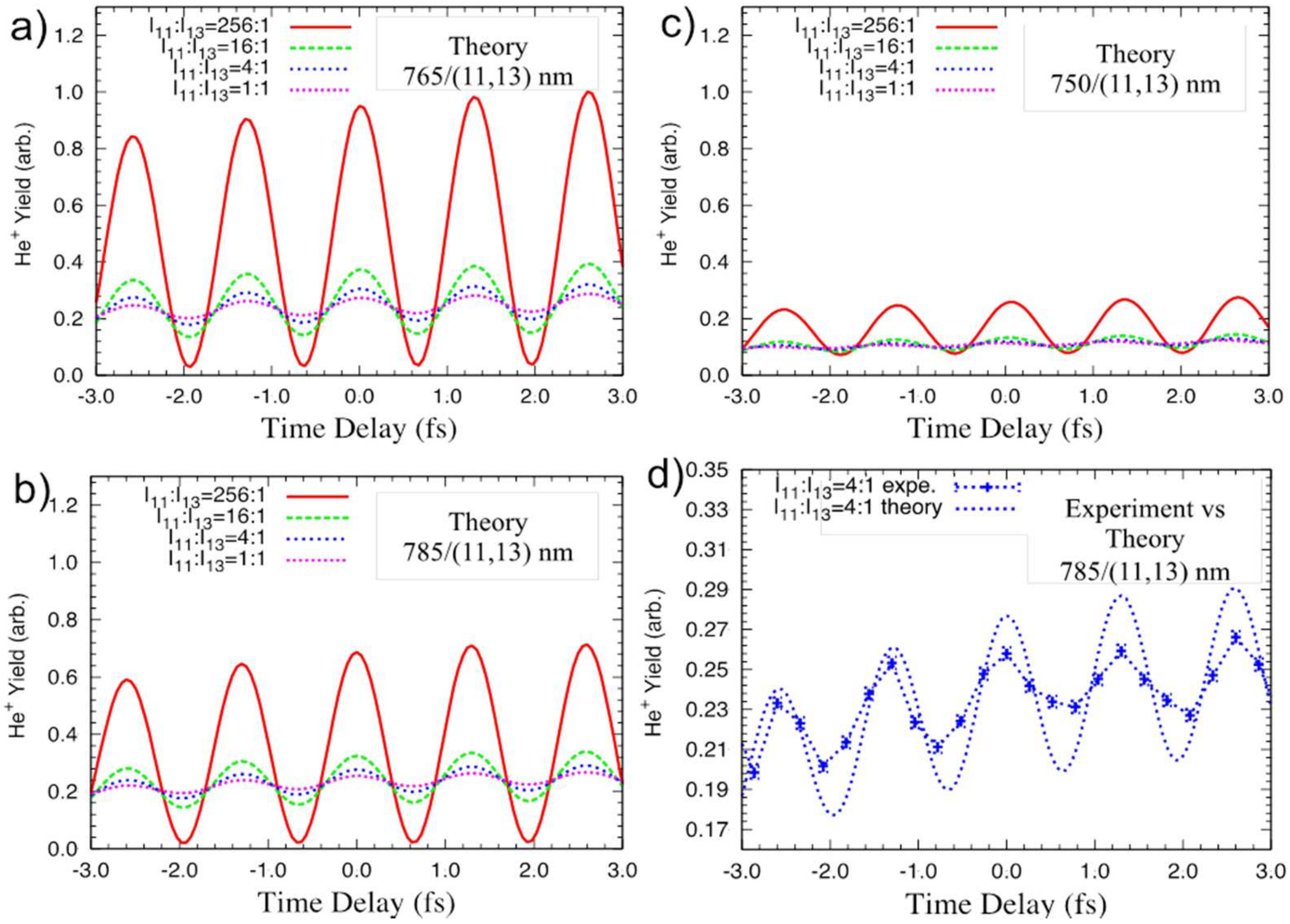
Control transparency in attosecond time scale



IR assistant Photoabsorption cross sections



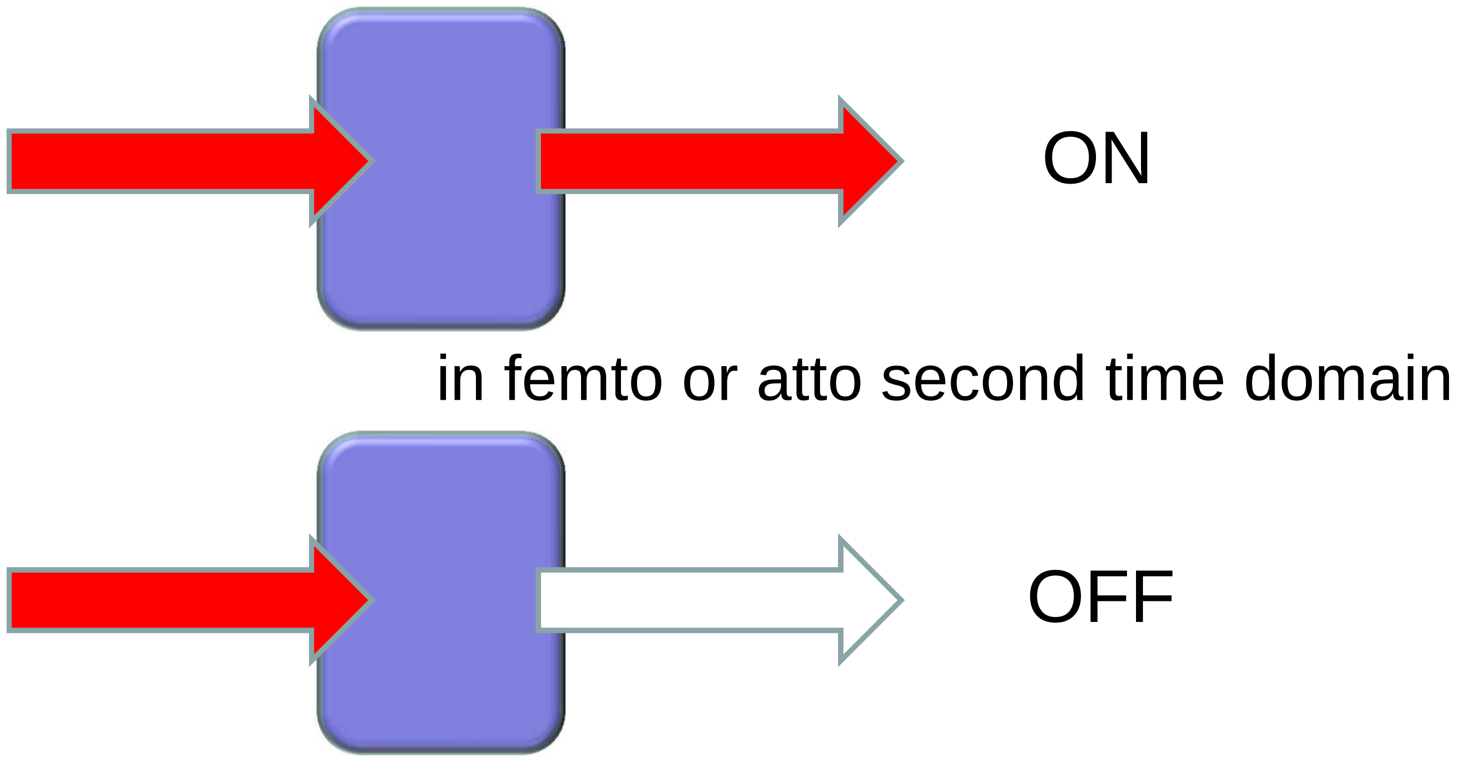
Control transparency



P. Ranitovic, et. al., PRL (2011).

Applications:

Generate a super-fast optical switch



Future works

- Code work: move to K20, 2.5~3 times faster than Fermi20
- Extend the present method to TDDFT-SIC
- Search the best way to generate HHG
- Search a way to control molecular dynamics from as to ps
- …
- how to minimize the communication time

  MPI on the GPU level ?