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

(a) High harmonic generation
(b) Ionization or dissociation
(c) Image the structure (holography)
Control material properties in attosecond time scale


Insulator $\rightarrow$ conductor (1 fs)

Wang, et al., PRA (2013)

Simulation on HA-PACS

Photoabsorption or no (1 fs)
Working Equations (time-dependent Schrodinger equation)

Initial: \[ \Phi_0 \]

Differential: \[ i \frac{\partial}{\partial t} \Psi(t) = H(t) \Psi(t) \quad \Psi(t) = U(t, -\infty) \Phi_0 \]

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 \[ V^{ext}(t) = r \cdot E(t) \quad A(t) = \int_{t'}^{\infty} E(t') dt' \]

Velocity gauge \[ V^{ext}(t) = p \cdot A(t) \]
Key step: time-propagator (Split-Operator Method)

Time-propagation:

\[ \Psi(t + \Delta t) = e^{-iH(t)\Delta t} = U(t + \Delta t, t)\Psi(t) \]
\[ \approx e^{-iH_0\Delta t} e^{-iV(t)\Delta t} e^{-iH_0\Delta t}\Psi(t) + O(\Delta t^3) \]

Discretize space in pseudo-spectra grid:

\[ H_0 = H_{r_i,r_j}^0(\ell), \quad \Psi(r_i, \theta) = \sum_{\ell} R_{\ell}(r_i) Y_{\ell,m}(\hat{r}), \quad \Psi(r_i, \ell) = R_{\ell}(r_i) \]

Time-propagation → vector, matrix operations → blas

One time step: 2 zgemv (zgemm): \( NR^2 \times NL \times (Np) \) cublas_
2 zgemm : \( NR \times NL^2 \times (Np) \) cublas_
1 exponential : \( NR \times NL \times (Np) \) Cuda C
Total ops. Z \( 4 \times NR \times NL \times (NR+NL+1) \times (Np) \times NT \times K \) (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 \times \text{LperThread} \times 16
(4000^2 \times 16 \times 15 = 3.8 \text{ GB})

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

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

\Psi^a(r, \ell) = S_{r\rightarrow r'}(\ell)\Psi(r', \ell) \quad \text{zgemv(m)}

\Psi^b(r, \theta) = T_{\ell\rightarrow \theta}\Psi^a(r, \ell) \quad \text{zgemm}

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

\Psi^d(r, \ell) = T_{\theta\rightarrow \ell}\Psi^c(r, \theta) \quad \text{zgemm}

\Psi^a(r, \ell) = S_{r\rightarrow r'}(\ell)\Psi(r', \ell) \quad \text{zgemv(m)}
Structure of code (machine)

One MPI thread

OpenMP+ mkl

Cublas + CUDA C

HA-PACS

Device = mod(myid,4)

MPI
(node 0)
Thread 0
(Device 0)
Thread 1
(Device 1)
Thread 2
(Device 2)
Thread 3
(Device 3)

MPI
(node 1)
Thread 4
(Device 0)
Thread 5
(Device 1)
Thread 6
(Device 2)
Thread 7
(Device 3)

MPI
(node n)
Thread a
(Device 0)
Thread b
(Device 1)
Thread c
(Device 2)
Thread d
(Device 3)
Numerical accuracy:

Single-electron model:

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

Time propagation: systematic error:

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**Graph 1: Time step vs. 1-Norm.**

- X-axis: Time step

**Graph 2: Ionization probability vs. IR Laser Intensity.**

- X-axis: IR Laser Intensity (W/cm$^2$)
- Y-axis: Ionization probability

Legend:
- Integral
- Differential
- V-D
Memory and Work load

2D + Time propagation in spherical coordinates:

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

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


HA-PACS: 5 nodes, 20 hrs
Attosecond Streaking

Without IR field

With IR field
Control transparency in attosecond time scale

**A**

**XUV/IR Interferometer**

**B**

Reaction Microscope

EUV pulse 43 eV, ~5fs

IR pulse 1.5 ev, 30fs

ALuminum Foil

Beam Chopper

**APT + IR**

**COLTRIMS**
IR assistant Photoabsorption cross sections
Control transparency

Applications:

Generate a super-fast optical switch

in femto or atto second time domain

ON

OFF
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?