Compressed sensing in atomic simulations

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Introduction

- Real-time methods for atomic simulations:
  - Molecular dynamics
  - Electron dynamics (real-time TDDFT)
- Linear and non-linear response
- Good scaling and parallelizability
- Long propagation times
- Signal analysis techniques to reduce propagation time
Optimal sampling

- Often information is stored in compressed form
- Basis expansion where most coefficients are zero (or almost zero)
- Data acquisition is usually done in uncompressed form
- Measure more data than required
Compressed sensing

- Measure only the number of samples required
- Proportional to the number of coefficients in a compressed representation
- Concept of sparsity
- Un-coherent sampling
- General and flexible method
- Many applications in science and technology
Compressed sensing for Fourier coefficients

Consider the discrete Fourier transform

\[ g_k = \sum_{j=1}^{N_t} \Delta t \sin(\omega_k t_j) h_j. \]

This is a linear transform that can be considered a matrix inversion problem

\[ F g = h \]

Where \( F \) is the \( N_\omega \times N_t \) Fourier matrix with entries

\[ F_{jk} = \frac{2}{\pi} \Delta \omega \sin(\omega_j t_k) \]
We are interested in the case $N_\omega > N_t$

Undetermined problem: many solutions

Sparsity: select the solution with the largest number of zeros
The minimization of the number of zeros (0-norm) is numerically hard.

Use the 1-norm $|g|_1 = \sum_k |g_k|$ instead.

This is the Basis Pursuit problem:

$$\min_g |g|_1 \quad \text{subject to} \quad Fg = h$$
In practice a signal might have noise

\[ \min_{\mathbf{g}} |\mathbf{g}|_1 \quad \text{subject to} \quad |F\mathbf{g} - \mathbf{h}|_2 < \eta \]

Exact reconstruction
A simple case: vibration of N₂
Vibration of \( \text{N}_2 \): peak position
Vibrational spectrum of benzene from MD

- Fourier transform 5000 fs
- Compressed sensing 1000 fs
Absorption spectrum of benzene from RT-TDDFT

Absorption cross-section [arbitrary units]

Energy [eV]

1 fs
2.5 fs
5 fs
10 fs
25 fs

Exp.
Circular dichroism spectrum of (R)-methyloxirane
Compressed sensing for 2D spectroscopy

- Experimental data for different $t$ and $\tau$
- Fixed value of $T$
- Fourier transform in $t$ and $\tau$

2D spectra of an Rb atom
2D spectra peak-width

- Linewidth (rad/fs)
- Number of sampled points

- 2D discrete FT
- 2D CS with uniform grid sampling
- 2D CS with random grid sampling
Conclusions

- Compressed sensing for numerical applications: reduced computing time
- Improved Fourier transform: many applications
- Problems: peak shapes and widths, computational cost
- Other methods: maximum entropy, filter diagonalization
- Applications beyond Fourier
- Random sampling
