Compressed sensing in atomic simulations

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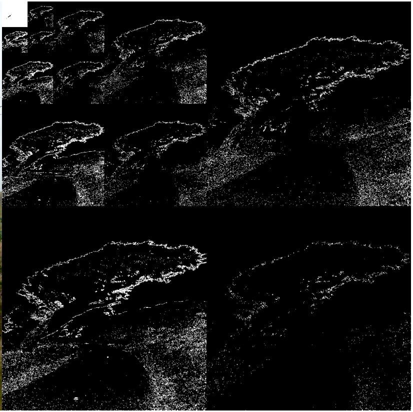
Introduction

- 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

$$F\boldsymbol{g} = \boldsymbol{h}$$

- Where F is the $N_\omega \times N_t$ Fourier matrix with entries

$$F_{jk} = \frac{2}{\pi} \Delta\omega \sin(\omega_j t_k)$$

Undetermined problem

- We are interested in the case $N_\omega > N_t$
- Undetermined problem: many solutions
- Sparsity: select the solution with the largest number of zeros

Basis pursuit problem

- 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

$$\min_{\boldsymbol{g}} |\boldsymbol{g}|_1 \quad \text{subject to} \quad F\boldsymbol{g} = \boldsymbol{h}$$

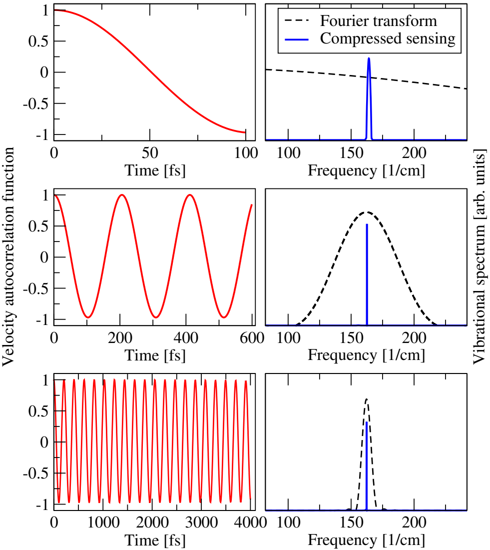
Basis pursuit de-noising (BPDN)

- In practice a signal might have noise

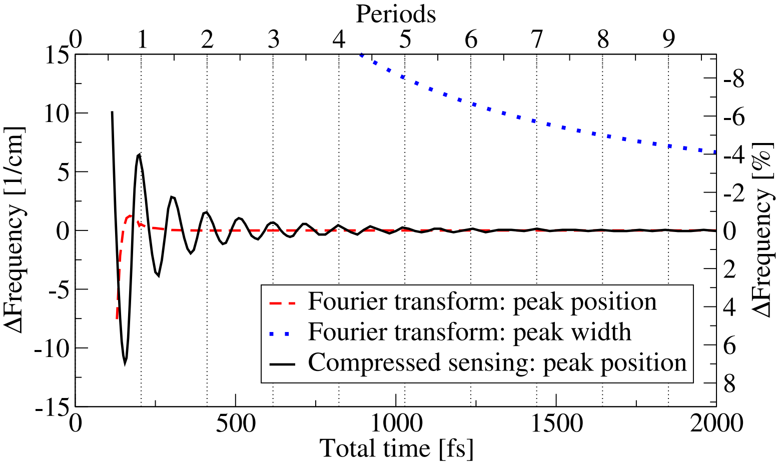
$$\min_{\boldsymbol{g}} |\boldsymbol{g}|_1 \quad \text{subject to} \quad |F\boldsymbol{g} - \boldsymbol{h}|_2 < \eta$$

- Exact reconstruction

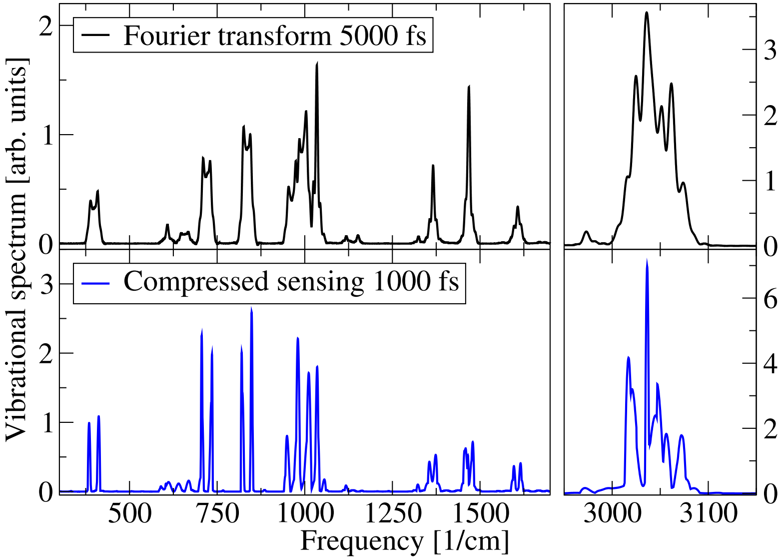
A simple case: vibration of N_2



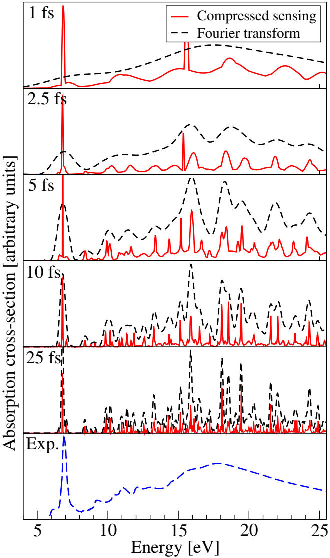
Vibration of N_2: peak position



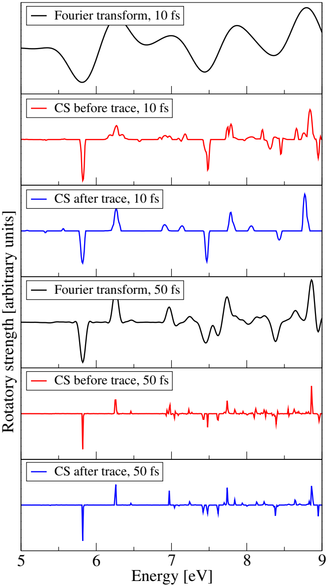
Vibrational spectrum of benzene from MD



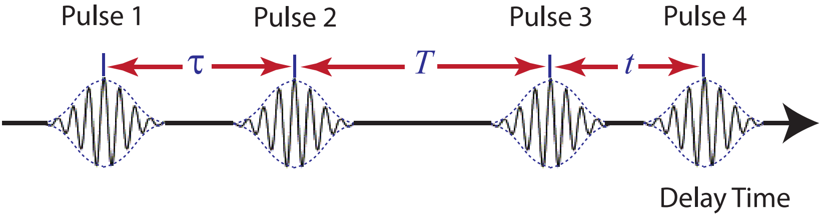
Absorption spectrum of benzene from RT-TDDFT



Circular dichroism spectrum of (*R*)-methyloxirane



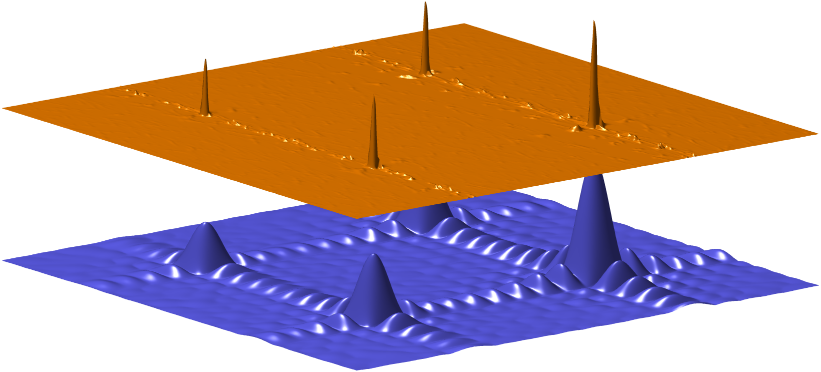
Compressed sensing for 2D spectroscopy[1]



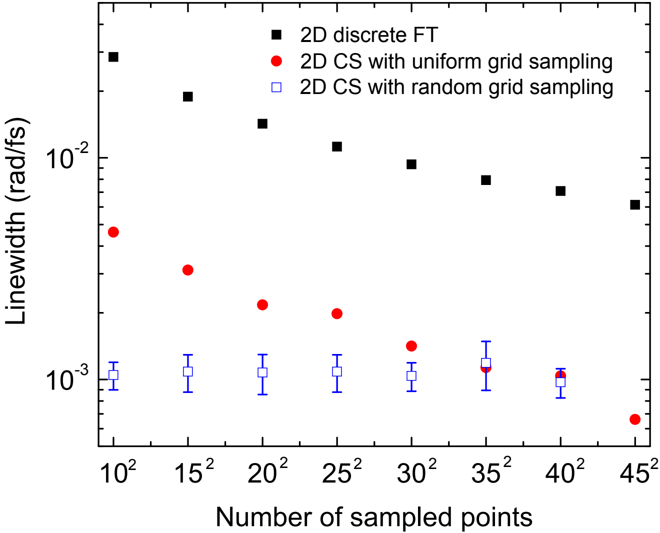
- Experimental data for different t and τ
- Fixed value of T
- Fourier transform in t and τ

[1] J. N. Sanders et al, J. Phys. Chem. Lett. **3**, 2697 – 2702 (2012)

2D spectra of an Rb atom



2D spectra peak-width



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

X. Andrade, J. N. Sanders and A. Aspuru-Guzik, Proc. Nat. Acad. Sci. **109**, 13928 – 13933 (2012).