FFT-based methods for Time-Dependent Density Functional Theory (TDDFT)

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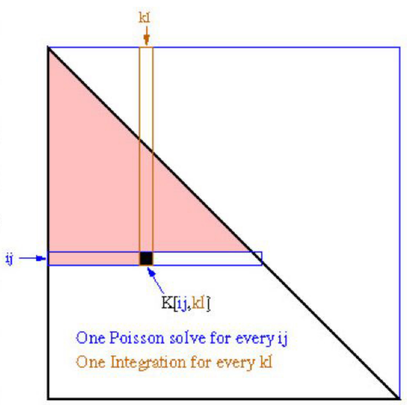
Background. Time-Dependent Density Functional Theory methods are used for studying excited state properties which cannot be obtained by standard DFT. We employ a method based on a frequency space representation. In this technique a large coupling matrix K is to be computed, and this constitutes a major computation when the number of atoms increases. Starting in 1999, our group implemented an initial parallel code which enabled the largest TDDFT computation at that time.

New Approach. Later the same code was optimized with the help of the Computer Science team achieving a factor of about 5 gain in execution time as well as substantial gains in memory usage. Recently, we moved to a new method which exploits FFT to solve the linear systems arising in the construction of K. The initial computational time went from a few days, to 15 hours, to 1.5 hours (most recent result).

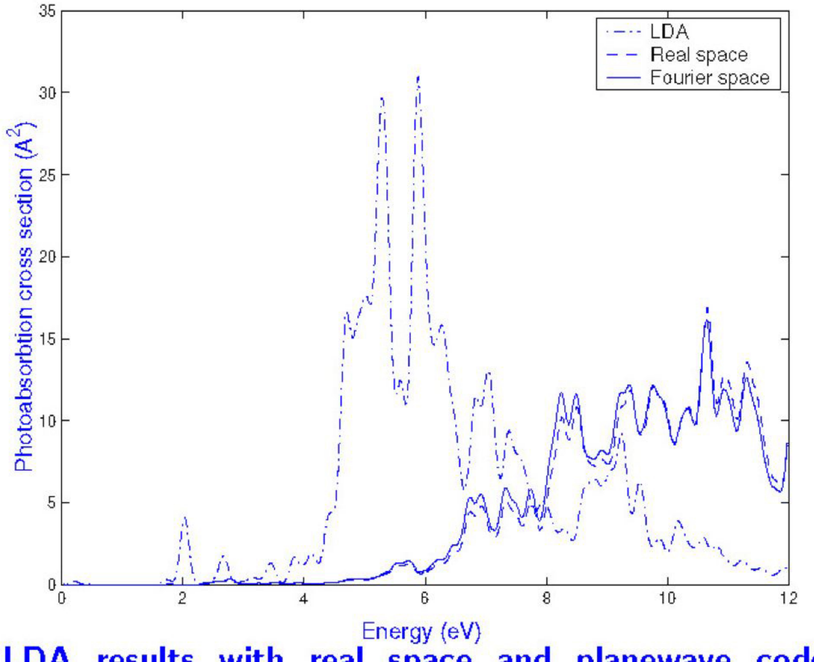
Results. The table shows wall-clock time of the parallel TDLDA code using Fourier space and Real Space for the Si34H36 test case running on 8 processors

Method	Wall-Clock Time (hours)
Real Space Code	15:30
PW: Initial Implementation	3:30
PW: Optimized load balancing	1:30



Coupling Matrix K

Each row of the coupling matrix requires solving a Poisson Equation which translate into a (sparse) linear system on the whole domain. Our initial approach used Conjugate Gradient. The new approach exploits the FFT and knowldge about the decay of the wavefunctions to solve these systems efficiently.



TDLDA results with real space and planewave codes ($Si34H36$). Also shown are results obtained with LDA.