WrightSim

Kyle Sunden

University of Wisconsin–Madison

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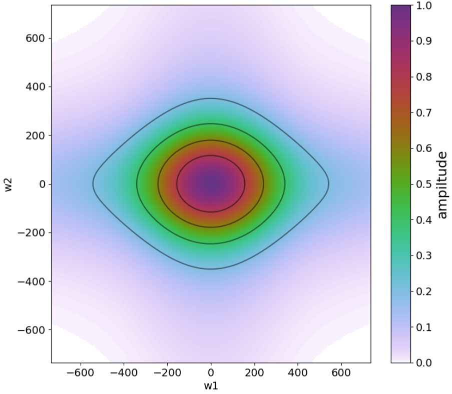
Goals

- Reproduce expermental spectra *in silico*.
- Designed with experimetalists in mind.
- Uses numerical integration for flexability, accuracy and interpretability.
- Focus on Frequency-domain spectroscopy, but techniques in principle extend to time-domain.
- Output retains frequency and phase information, can be combined with other simulations and measured similar to a monochromator.
- Selectivity in what portions of the overall signal are simulated, providing deeper understanding.

Sample Spectrum



Introduction

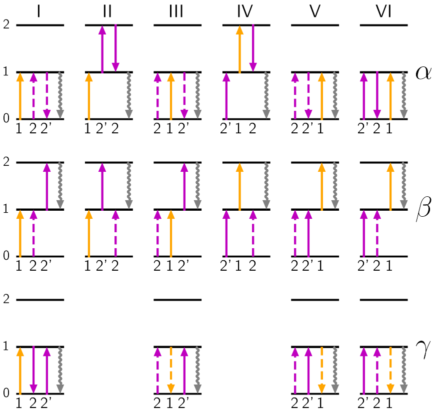
Presented here is a description of *what* is done to perform these simulations, to understand *why* it works, please refer to Kohler, Thompson, and Wright**Kohler_2017**.

The simulation uses a set number of electric fields (3, in the case of the simulation presented here).

These electric fields interact in combinitorically large different fashions.

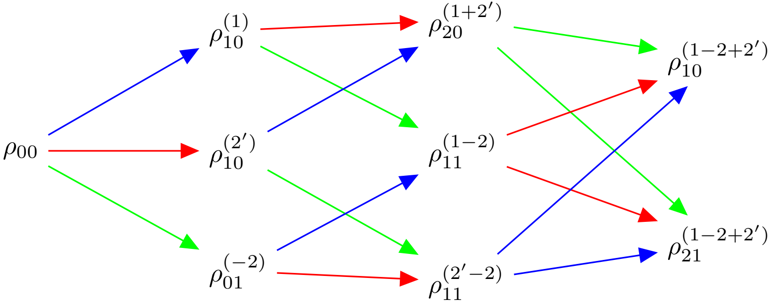
Interactions create superposition coherences and/or populations in material systems.

Pathways



There are six time orderings for interactions to occur (I-VI). There are 16 independant pathways possible for two positive (solid up/dashed down) and one negative (dashed up/solid down) interactions. Originally from **Kohler_2017**.

Finite state automaton



$$\overline{\rho} \equiv \begin{bmatrix} \tilde{\rho}_{00} \\ \tilde{\rho}_{01}^{-2} \\ \tilde{\rho}_{10}^{2'} \\ \tilde{\rho}_{10}^{1} \\ \tilde{\rho}_{20}^{1+2'} \\ \tilde{\rho}_{11}^{1-2} \\ \tilde{\rho}_{11}^{2'-2} \\ \tilde{\rho}_{10}^{1-2+2'} \\ \tilde{\rho}_{21}^{1-2+2'} \end{bmatrix}$$

Density elements, encoded with quantum state (subscript) and the electric fields which have ingeracted (superscript). Colored arrows represent the different electric fields. All possible states which have the desired conditions for the process simulated are included. These form the state vector (right).**Kohler_2017**

Hamiltonian Matrix

$$\overline{\overline{Q}} \equiv \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -A_2 & -\Gamma_{10} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ A_{2'} & 0 & -\Gamma_{10} & 0 & 0 & 0 & 0 & 0 & 0 \\ A_1 & 0 & 0 & -\Gamma_{10} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & B_1 & B_{2'} & -\Gamma_{20} & 0 & 0 & 0 & 0 \\ 0 & A_1 & 0 & -A_2 & 0 & -\Gamma_{11} & 0 & 0 & 0 \\ 0 & A_{2'} & -A_2 & 0 & 0 & 0 & -\Gamma_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & B_2 & -2A_{2'} & -2A_1 & -\Gamma_{10} & 0 \\ 0 & 0 & 0 & 0 & -A_2 & B_{2'} & B_1 & 0 & -\Gamma_{21} \end{bmatrix}$$

Defines the transition between states, dependant on the electric field. Γ represents the dephasing/population decay. A and B variables incorporate the dipole moment and electric field terms.**Kohler_2017**

The dot product of this matrix and the density vector, $\overline{\rho}$, gives the change in in the density vector. This is repeated over many small time periods to achieve the recorded results.

NISE

NISE (Numerical Integration of the Schrödinger Equation) is an existing open-source implementation of the simulation for these kinds of spectra.**nise**

It was written by Kohler and Thompson while preparing their manuscript.**Kohler_2017**

NISE uses a slight variation on the algorithm presented, which allows for a 7-element state vector, but requires two simulations.

The end result is the same.

NISE is included as a reference for prior implementations.

Algorithmic Improvements

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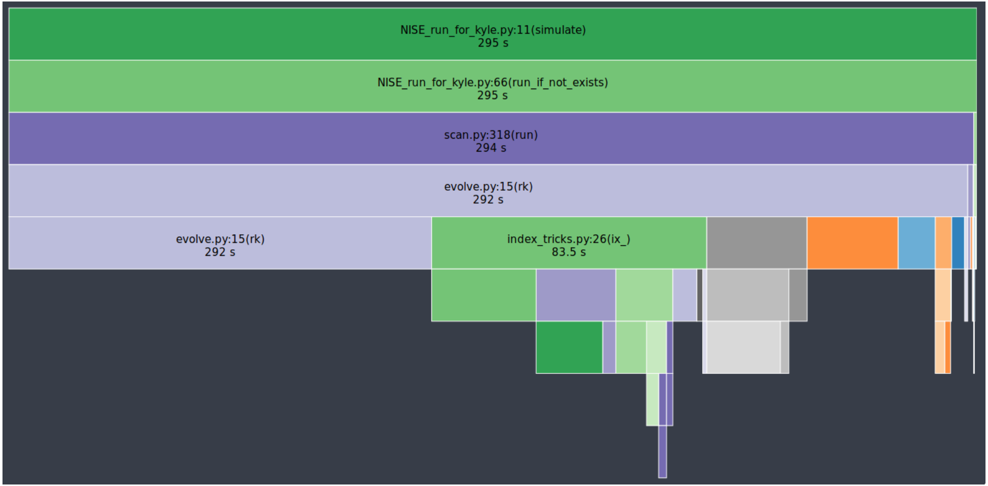
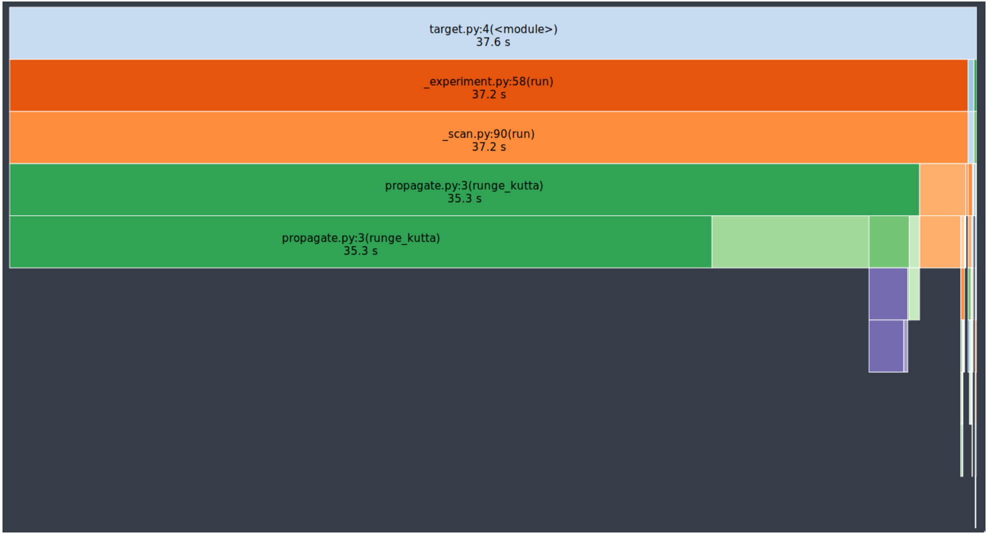
Profile trace of NISE



Profile trace of `WrightSim`



Parallel Implementations

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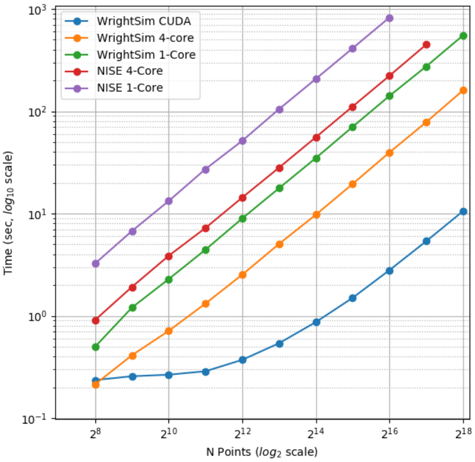
Scaling Analysis



Limitations

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