Machine Learning: A New Tool for the Physics Box?

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Machine learning: New tool in the box

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A recent burst of activity in applying machine learning to tackle fundamental questions in physics suggests that associated techniques may soon become as common in physics as numerical simulations or calculus.

Problem: energy transport in molecular networks

Model: HEOM

Supervised Learning application

Overview

- Research Goal: To understand energy transport in complex photosynthetic molecules and transfer the results to artificial systems

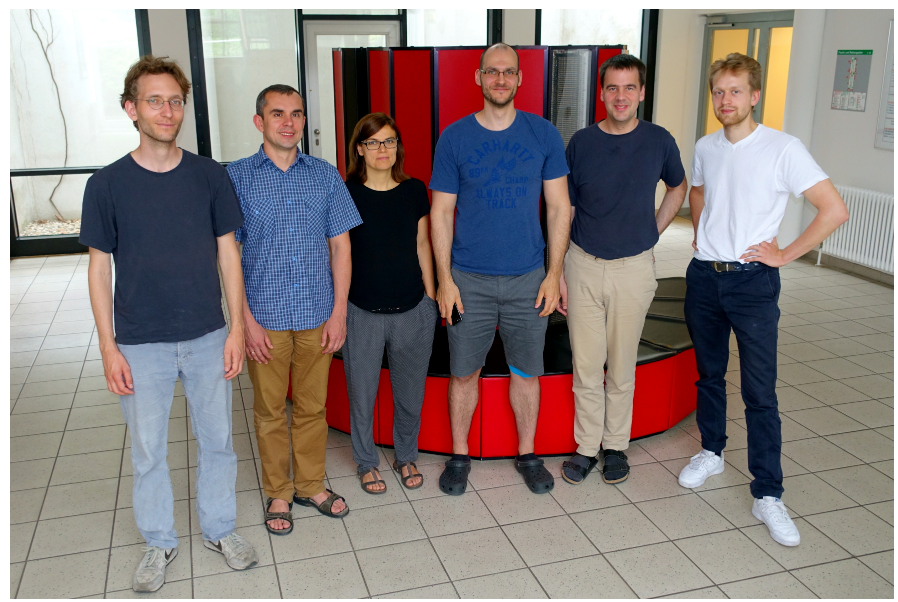
- Funding:

DFG-*Realistic Simulations of Photoactive Systems on HPC Clusters with Many-Core Processors* 2015-2017, Prof. A. Reinefeld, Dr. T. Kramer, Dr. Y. Zelinskyy, M. Noack

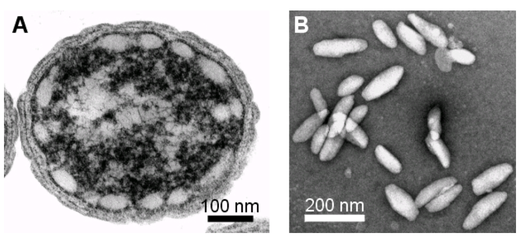
H2020-Marie Curie IF-*Control and optimization of energy flow in complex molecular networks*, April 2016-March 2018, Dr. M. Rodriguez

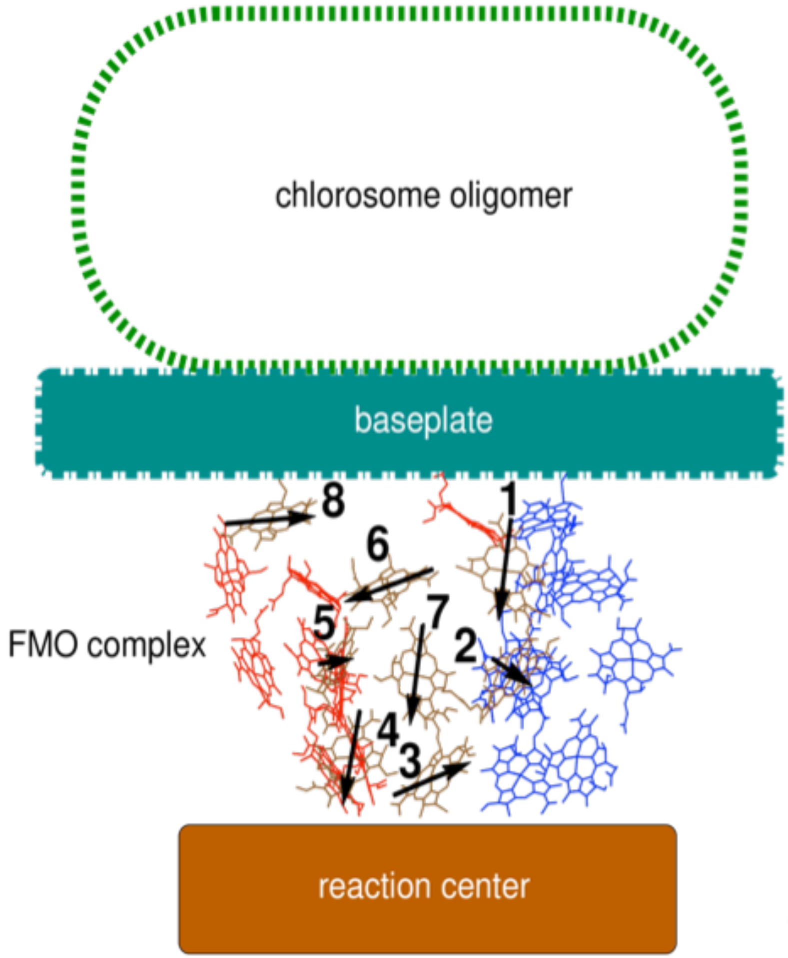
HORIZON 2020

DFG Deutsche Forschungsgemeinschaft



Photosynthesis in Green Sulfur Bacteria





Antenna

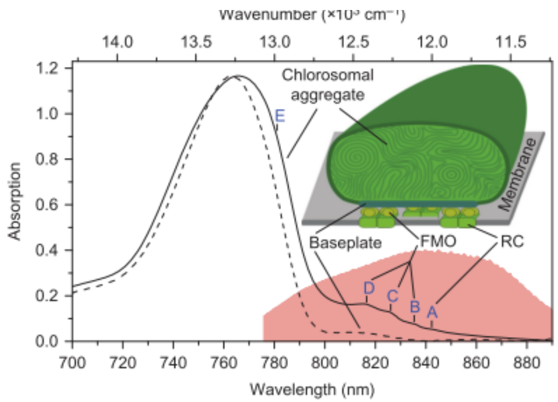
few photons per day

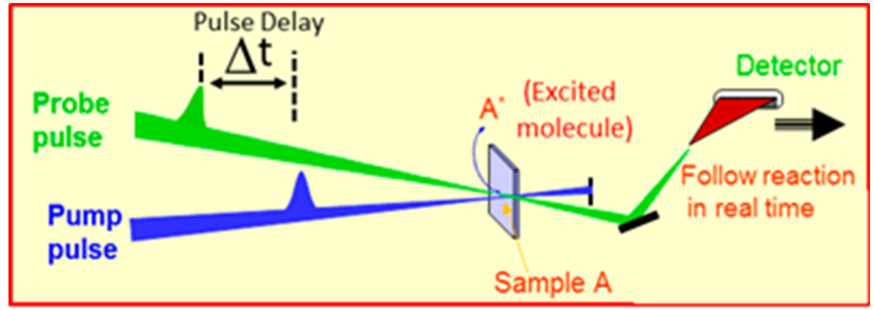
Light-harvesting complex

Reaction Center

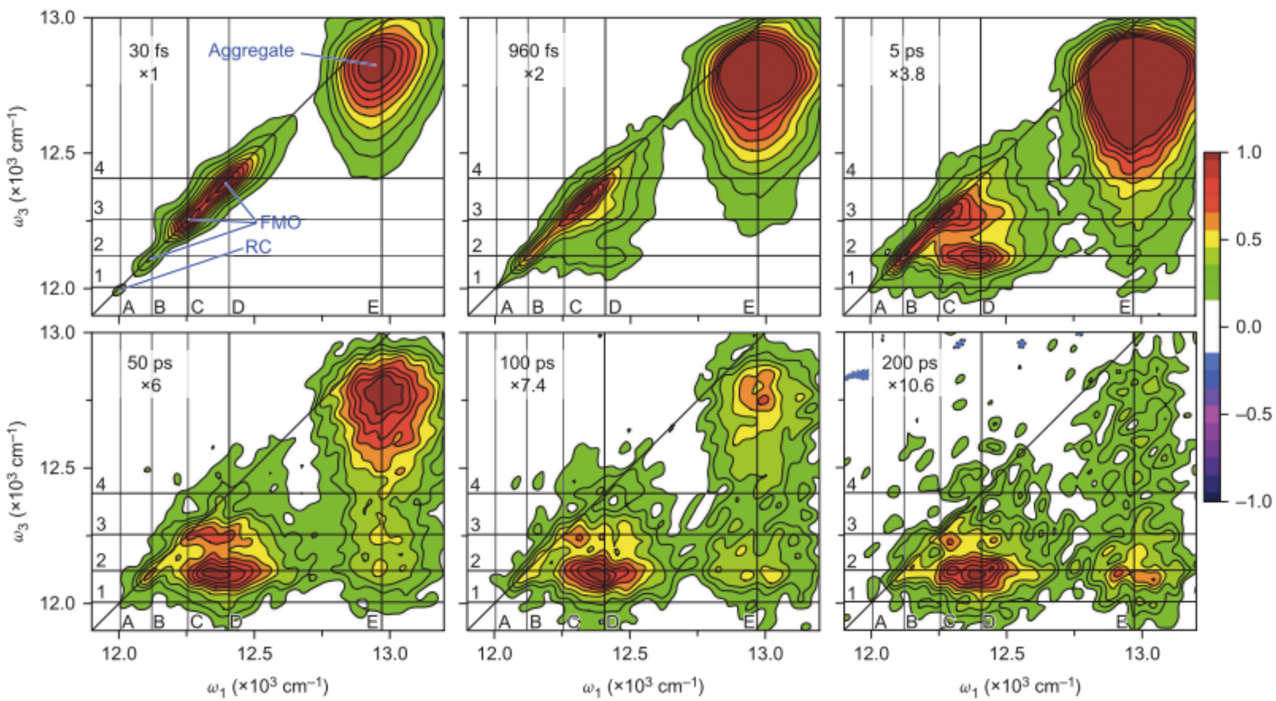
pico (10^{-12}) seconds time scale

Optical probes are used to map the flow through the molecular network

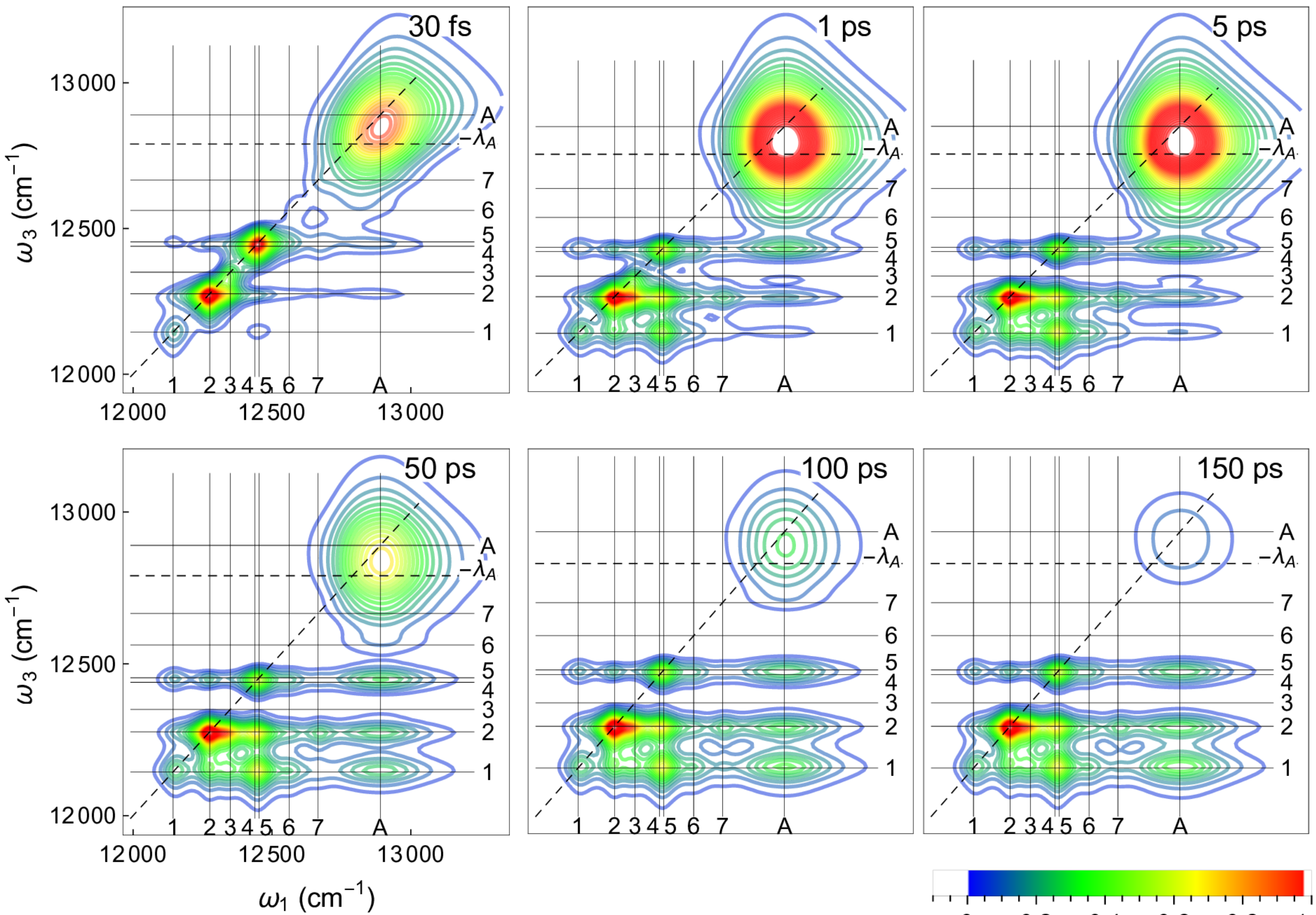




2D spectra map population in network

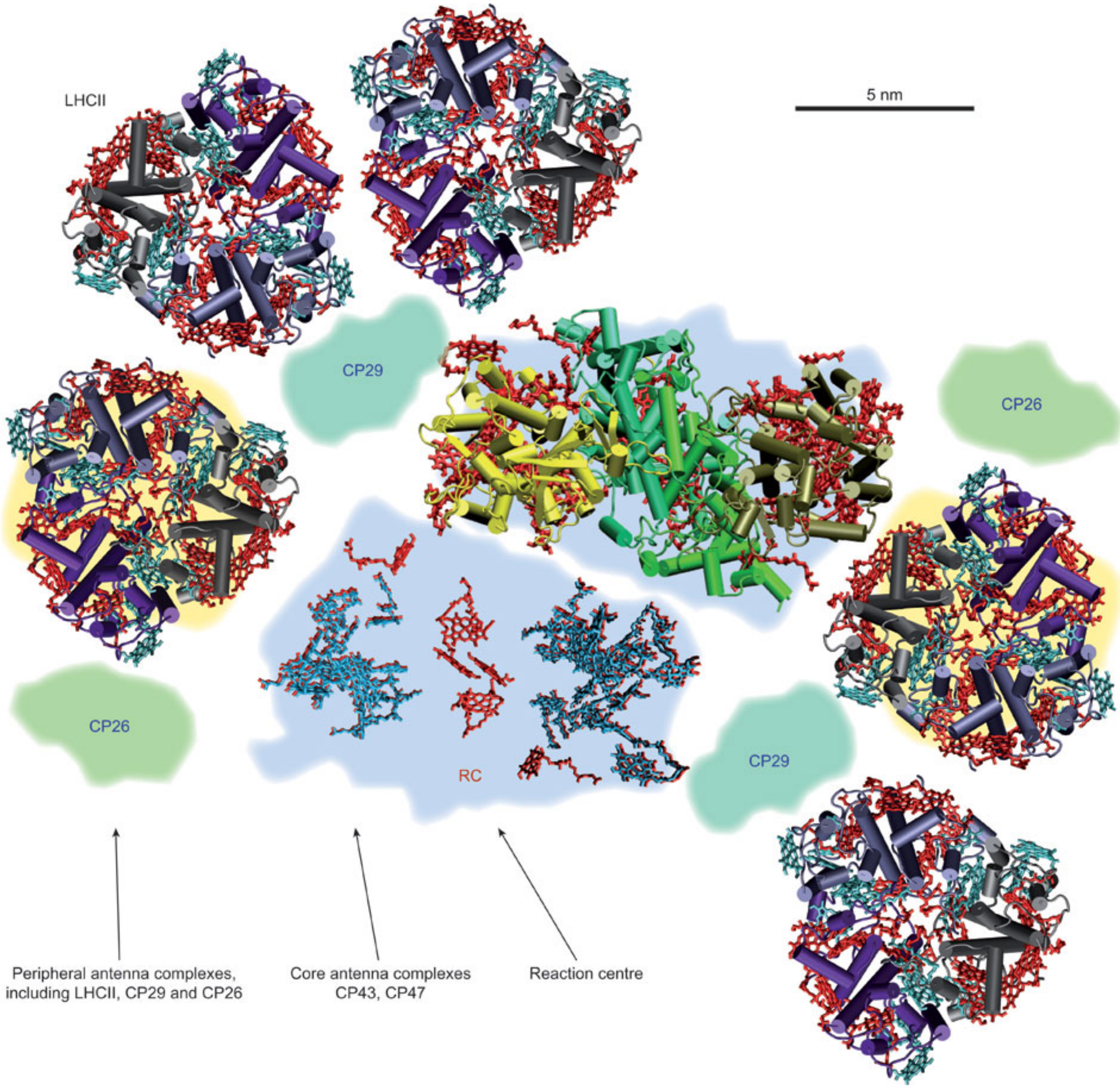


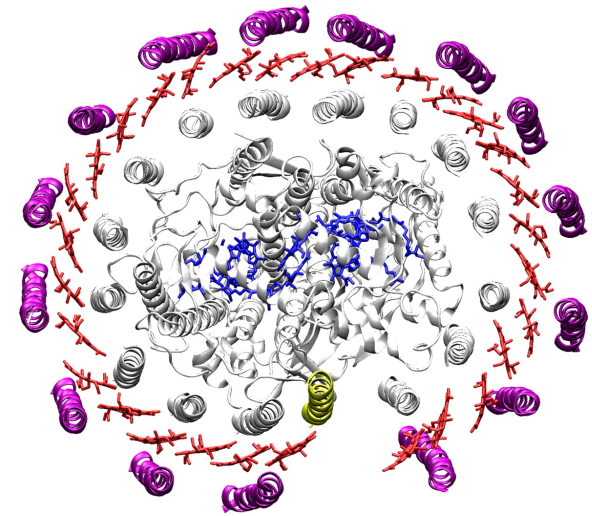
Theoretical results

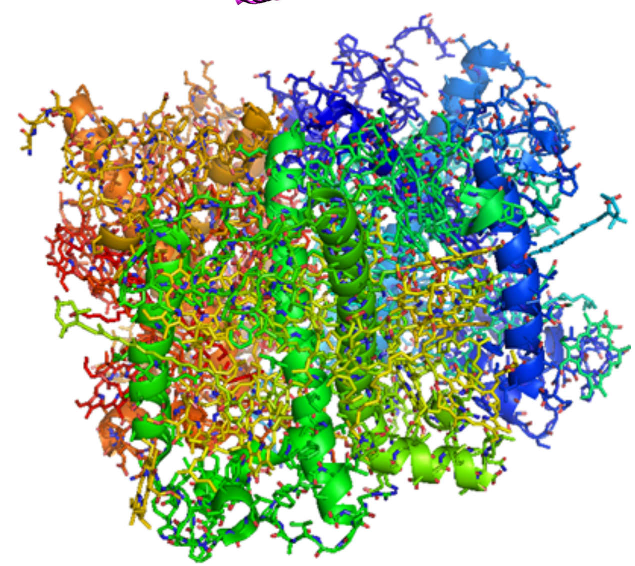


Tobias Kramer and **Mirta Rodriguez**, Scientific Reports Feb 2017 accepted
https://arxiv.org/abs/1702.06948

Our goal: Any size light harvesting complexes







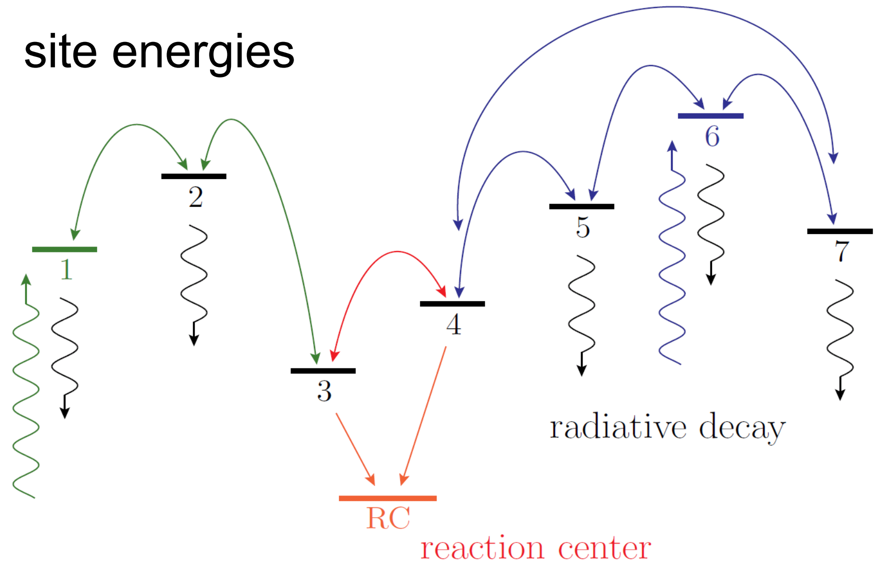
GD Scholes et al, Lessons from Nature about solar harvesting, Nature Chemistry 3, 763 (2011)

Model:

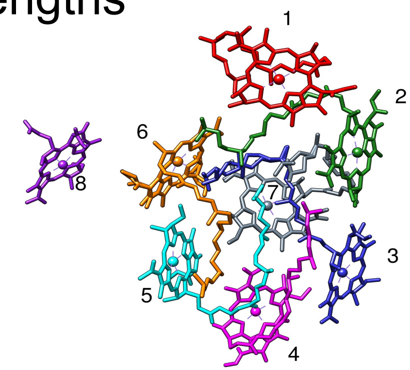
» Quantum transport across a network with strong environmental noise

Model for energy transfer

site energies



hopping strengths



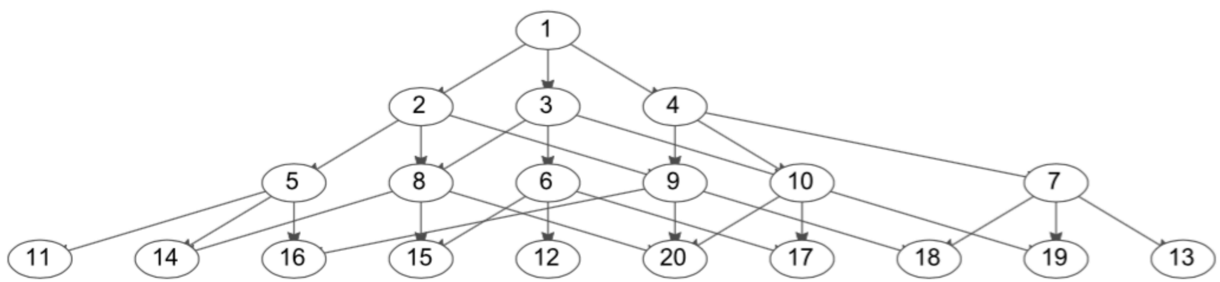
Network + Environmental Noise

$$\mathcal{H}=\underbrace{\sum_{m=1}^{d}\varepsilon_m|m\rangle\langle m|+\sum_{m>n}J_{mn}(|m\rangle\langle n|+|n\rangle\langle m|)}_{\text{exciton dynamics }(7\times 7\text{ matrix})}+\underbrace{\sum_{m,i}|m\rangle\langle m|\lambda_i\,(b^{\dagger}_{i,m}+b_{i,m})+\sum_{m,i}\hbar\omega_i b^{\dagger}_i b_i}_{\text{vibrational coupling}}$$

Hierarchical Equations of Motion (HEOM)

Quantum dynamics described in terms of a hierarchy of time-dependent differential equations labeled with d-tuples $\vec{n} = (n_1, \ldots, n_{\text{baths}}),\ n_i \in N^0$

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma^{\vec{n}}(t) = -\frac{\mathrm{i}}{\hbar}\left[\mathcal{H}, \sigma^{\vec{n}}(t)\right] + \sum_i^{n_{\text{baths}}} \mathcal{A}_i \sigma^{\vec{n}^-}(t) + \sum_i^{n_{\text{baths}}} \mathcal{B}_i \sigma^{\vec{n}^+}(t)$$

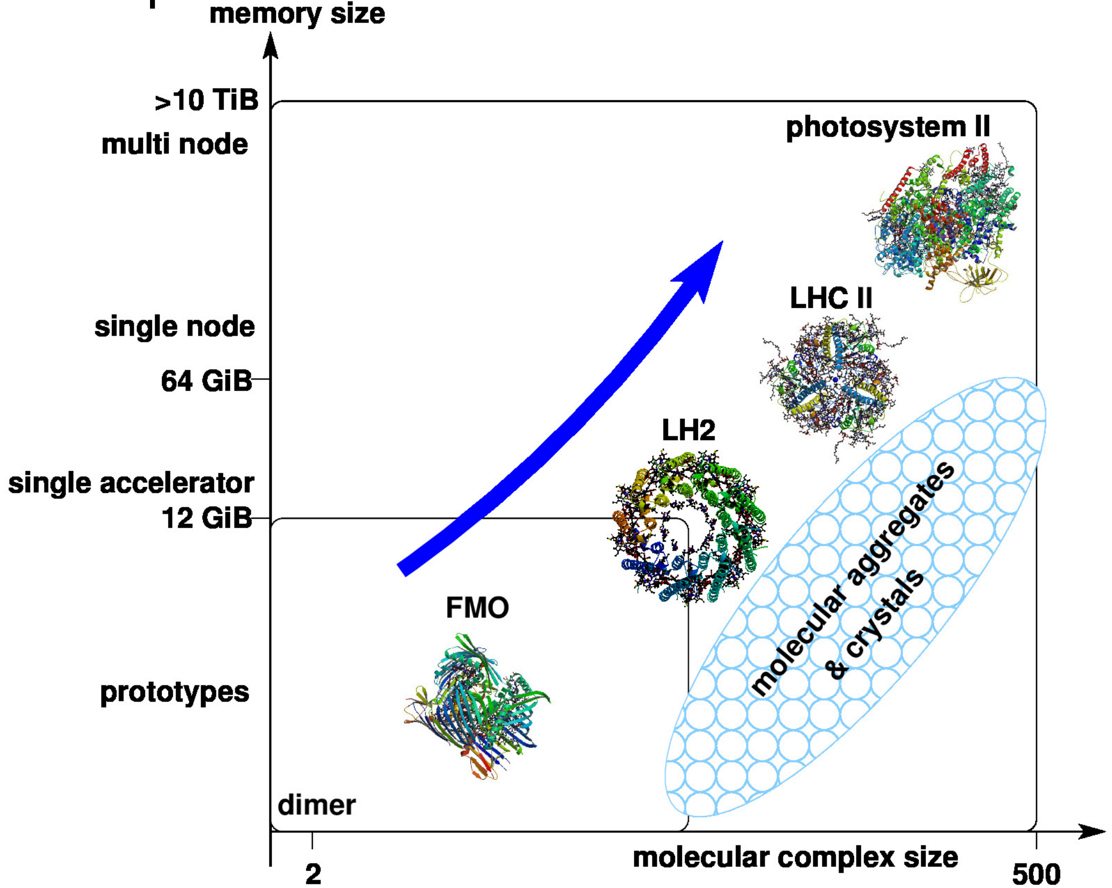


each box represents a $d \times d$ complex-valued matrix for a different excitation level

1	0	0	0	5	2	0	0	9	1	0	1	13	0	0	3	17	1	0	2
2	1	0	0	6	0	2	0	10	0	1	1	14	2	1	0	18	0	2	1
3	0	1	0	7	0	0	2	11	3	0	0	15	1	2	0	19	0	1	2
4	0	0	1	8	1	1	0	12	0	3	0	16	2	0	1	20	1	1	1

Progress towards large system sizes

- HEOM performance model: FLOP ~16 d^3 d^k Memory use ~ 2x2x8 d^k d^2
  Computational intensity =d/2 FLOP/byte
  d: system dimension k: coupling to environment
- Scalable implementation of the HEOM



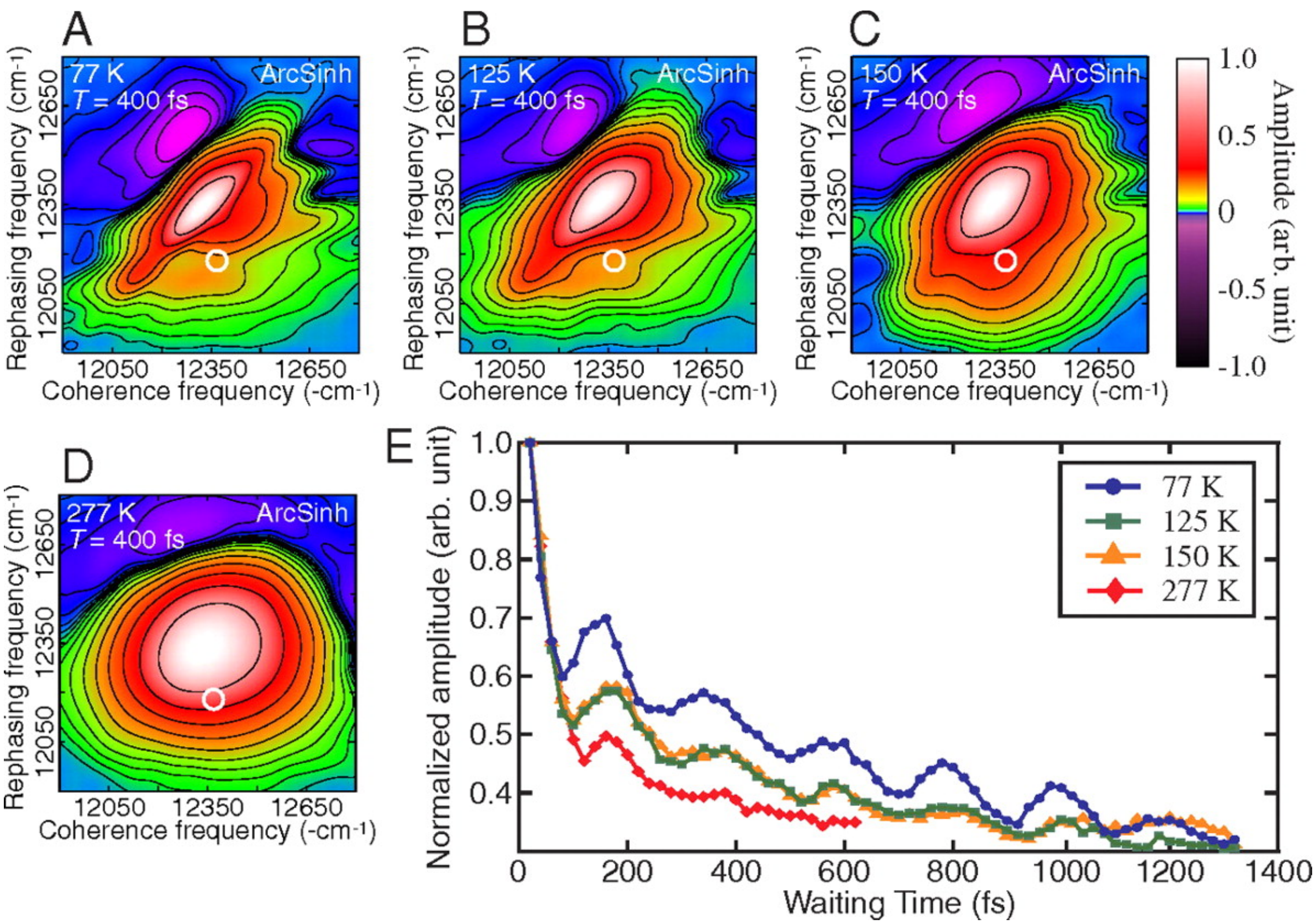
Machine Learning in Theoretical Physics

– We need to generate the training data
– We have very good theoretical models

+ Models are expensive ~ N^6 scaling
+ It may save computational time for disorder/noise averaging
+ Picks interesting patterns, missed by the models or parametrisation
+ Neural Networks accurately describe non-linear processes (key in most Physics problems)
+ It may provide size-independent solutions

» Can Machine Learning predict Quantum behaviour in light harvesting complexes?

Quantum behavior in photosynthesis



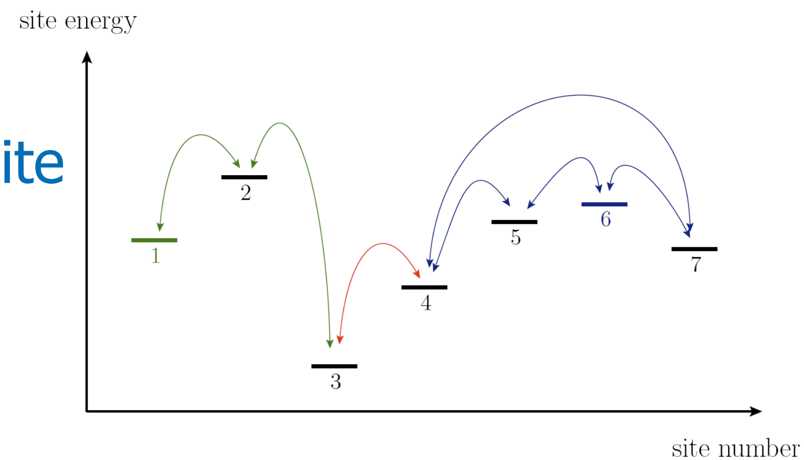
Gitt Panitchayangkoon et al. PNAS 2010;107:12766-12770

PNAS

Supervised learning of transfer probability within a molecular network

1) Initialize the network in site 1

3) Measure the probabilities at end-site



3) Training set:

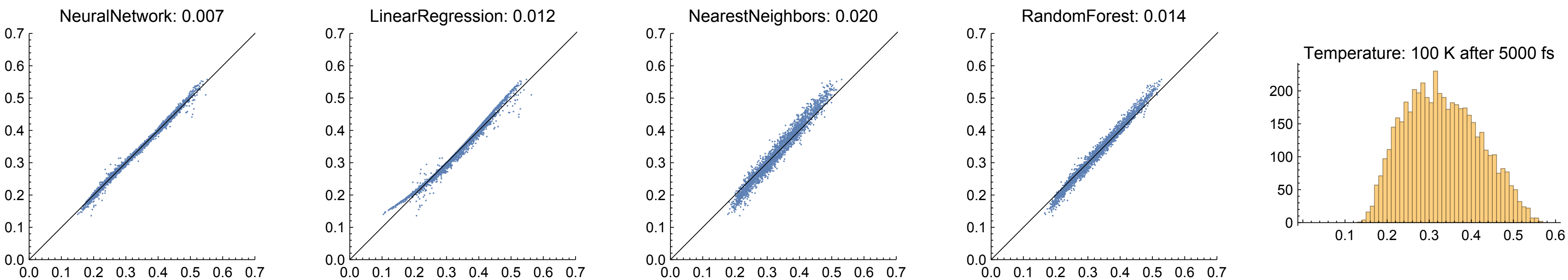
(site energies, hopping strengths)→ transfer probability

10^4 random realizations of hopping and site energies

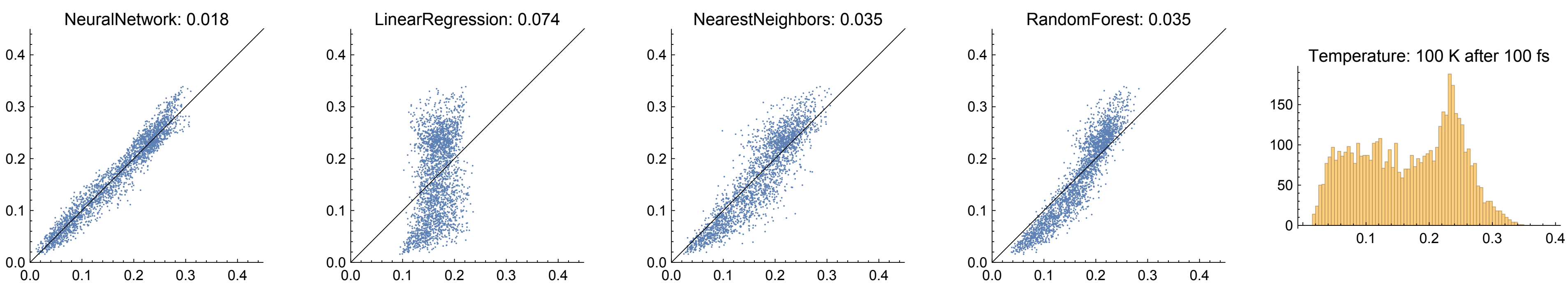
Fixed temperature (100K), fixed environmental coupling

Quantum vs. classical/thermal behaviour

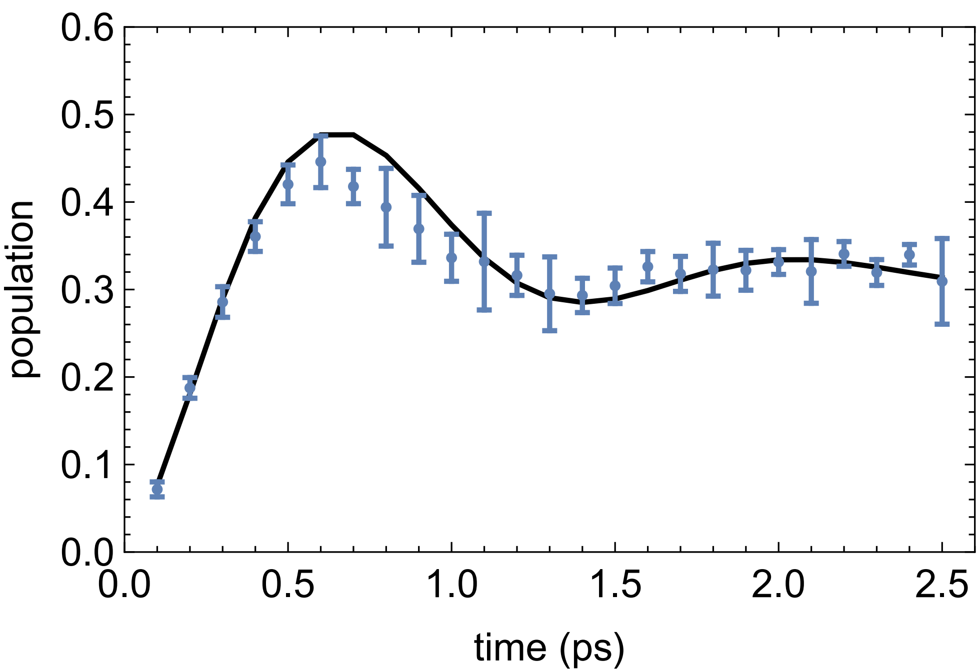
- classical thermalisation



- quantum



Supervised Learning is able to predict quantum behaviour in the network



Wolfram Mathematica 11

Amazon MXNet Learning Framework

- Physics model calculation

° SL preliminary results

» Thank you very much for your attention!