NSF CSSI PI Meeting, Seattle, WA, Feb. 13-14, 2020

Award #: **1835267**

CSSI Element A Quantum Electromagnetics Simulation Toolbox (QuEST) for Active Heterogeneous Media by Design

PI: Carlo Piermarocchi, Co-PI: Shanker Balasubramaniam
Students: Elliot Lu, Connor Glosser, Thomas Bertus

Institution: Michigan State University

GOALS:

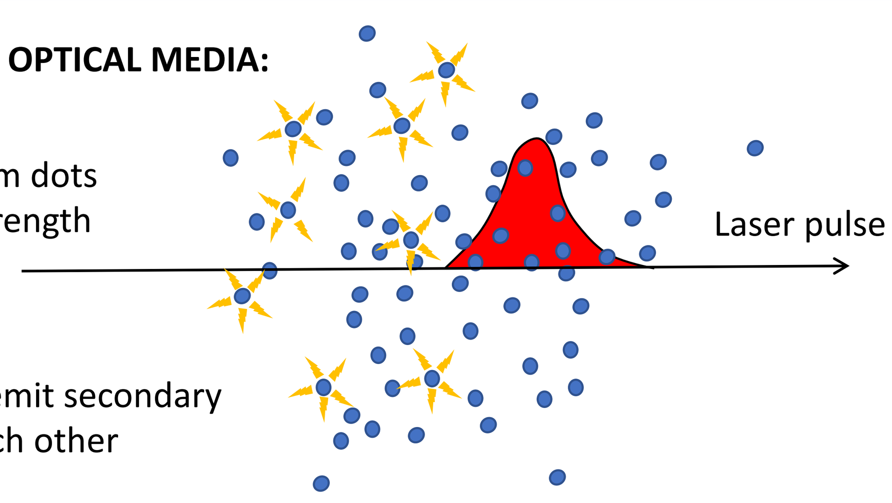
- Software elements for nano-photonics
- Simulating light propagation in complex non-linear media

INTELLECTUAL MERITS:

- Beyond homogeneous media: interacting quantum dots
- Time Domain Accelerated Algorithms: $O(N^2) \rightarrow O(N \ln N)$
- Localization/ Cooperative effects
- Material Optimization

MODEL SYSTEM FOR ACTIVE OPTICAL MEDIA:

Randomly distributed quantum dots with large optical oscillator strength



Laser-excited quantum dots emit secondary radiation and couple with each other

REQUIREMENTS:

Interaction: capture dot-dot electromagnetic coupling
Fast: Integral-based electromagnetics solvers
Self-consistent: calculation of the polarization dynamics
Scaling: describe 3D systems with a large number of dots
Microscopic: follow the evolution of each active center

APPROACH:

Semi-classical: A collection of two-level quantum systems described by density matrices interacting with a classical radiation field
Integral equation model: The radiation field is described in terms of a dyadic Green's function convolved with the polarization density acting as a source
Polarization: P(r) is calculated from optical the coherence in the density matrix

Liouville equation

$$\frac{\partial \hat{\rho}_\ell}{\partial t} = \left[\hat{\mathcal{H}}_\ell(\mathbf{E}(\mathbf{r}_\ell, t)), \hat{\rho}_\ell\right] - \hat{\mathcal{D}}[\hat{\rho}_\ell]$$

Integral propagator

$$\mathbf{E}(\mathbf{r}, t) = \frac{-\mu_0}{4\pi} \int \left(\bar{\mathbf{I}} - \hat{\mathbf{r}}\hat{\mathbf{r}}\right) \cdot \frac{\ddot{\mathbf{P}}(\rho)}{|\mathbf{r} - \mathbf{r}'|} + \left(\bar{\mathbf{I}} - 3\hat{\mathbf{r}}\hat{\mathbf{r}}\right) \cdot \left(\frac{c\dot{\mathbf{P}}(\rho)}{|\mathbf{r} - \mathbf{r}'|^2} + \frac{c^2\mathbf{P}(\rho)}{|\mathbf{r} - \mathbf{r}'|^3}\right) d^3\mathbf{r}'$$

Two level system Hamiltonian

$$\hat{\mathcal{H}}(t) \equiv \begin{pmatrix} 0 & \mathbf{d} \cdot \mathbf{E}(t) \\ \mathbf{d}^* \cdot \mathbf{E}^*(t) & \hbar\omega_0 \end{pmatrix}$$

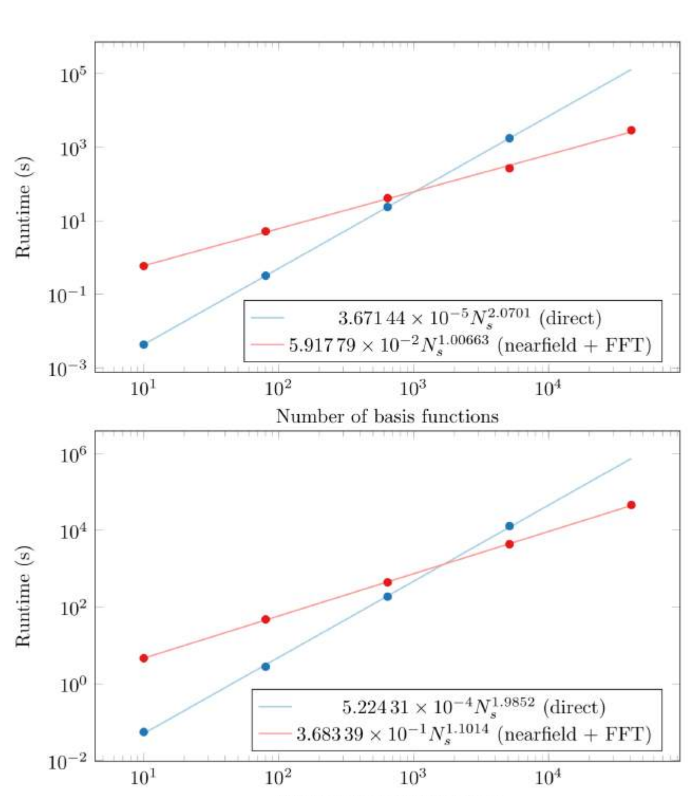
Dissipation and decoherence

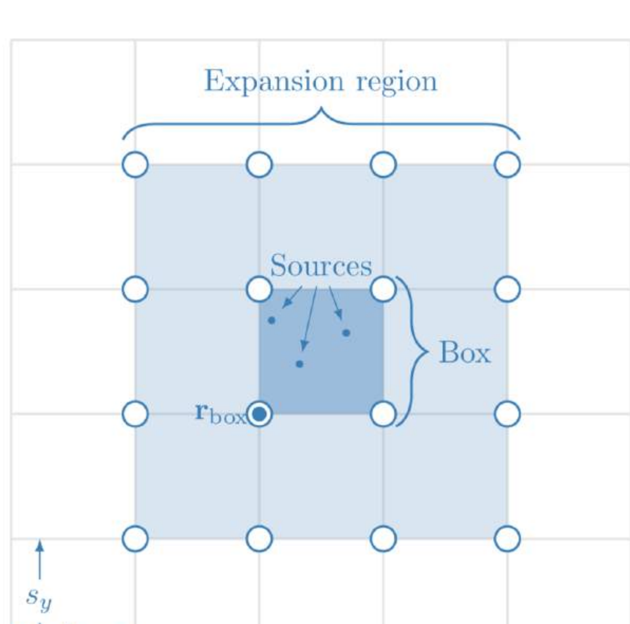
$$\hat{\mathcal{D}}[\hat{\rho}] \equiv \begin{pmatrix} (\rho_{00} - 1)/T_1 & \rho_{01}/T_2 \\ \rho_{10}/T_2 & \rho_{11}/T_1 \end{pmatrix}$$

ACCELERATION WITH THE ADAPTIVE INTEGRAL METHOD (AIM)

To ensure scalability to large numbers of dots, we reduce the $O(N^2)$ complexity of the discrete convolution step to O(N logN). The AIM algorithm achieves this by:

- Projecting the spatial basis functions onto auxiliary basis functions on points of a grid
- Evaluating the discrete convolution between grid points using a FFT

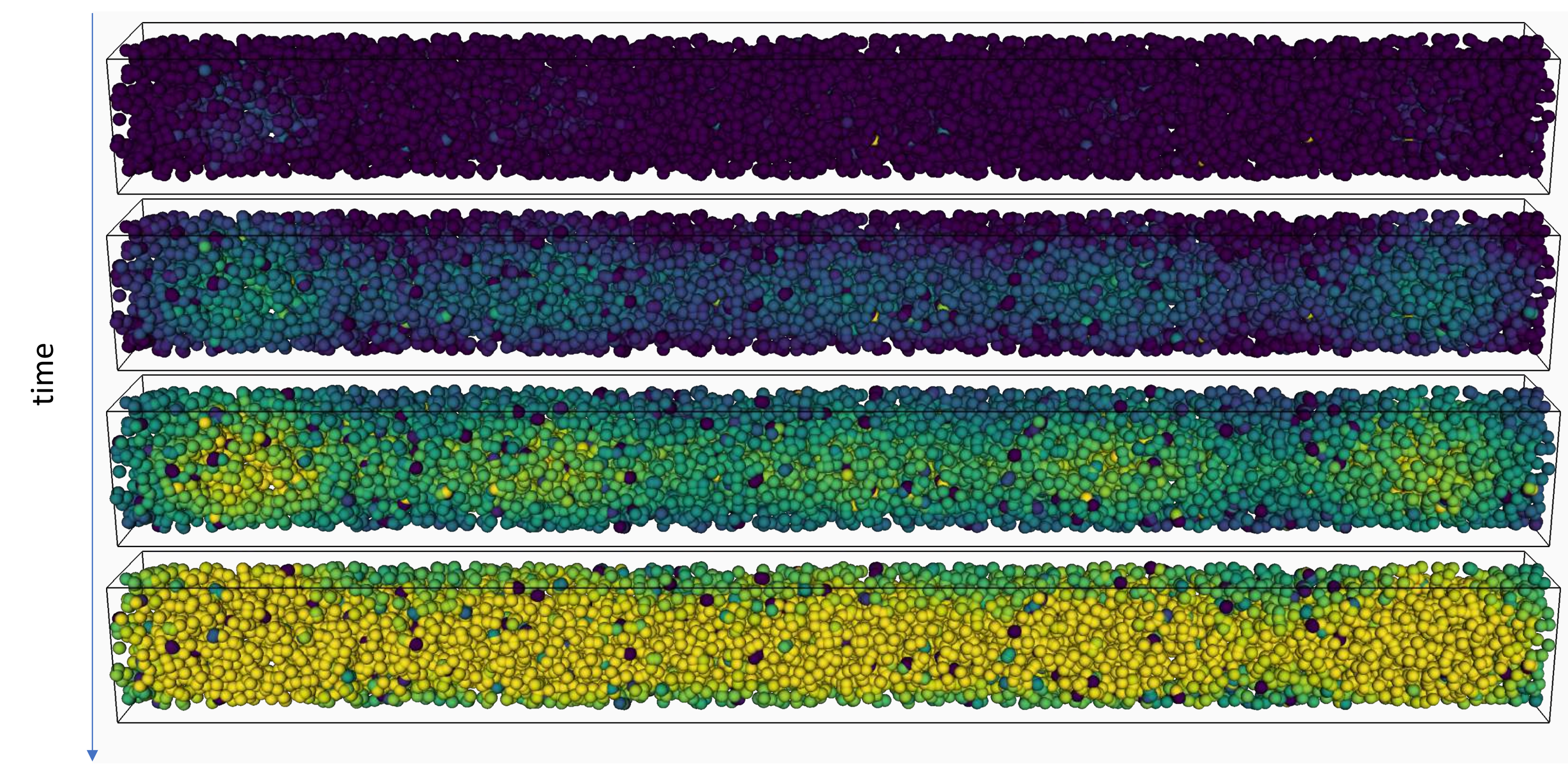




FFT runtime (excluding setup time) using a third-order expansion. (Top left) 1024 time steps with grid mesh of Δs = λ/400 and prescribed polarizations in the fixed frame. (Bottom left) 1000 time steps with Δs = λ/10 and Liouville-dynamics polarization in the rotating frame. Both cases have a quasi-quadratic scaling in the direct calculation, whereas the FFT-accelerated calculation performs slightly worse than linear. (Right) Schematics of expansion grid.

RESULTS: Local and wavelength-scale features

- 10k dots; 0.2 μm x 4 μm cylinder oriented along the laser pulse propagation k vector
- Snapshots at -50 fs, 0 fs, 50 fs and 100 fs relative to pulse peak
- Hotspots separated by λ appear

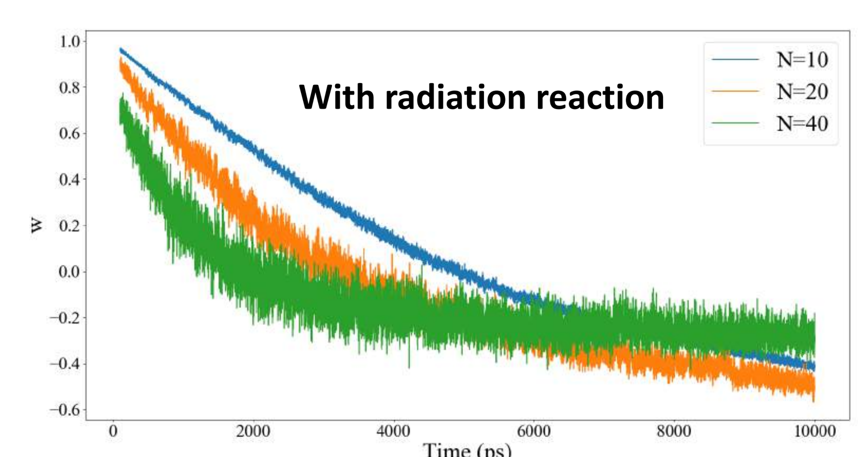


RESULTS: Super-radiant behavior in the time domain

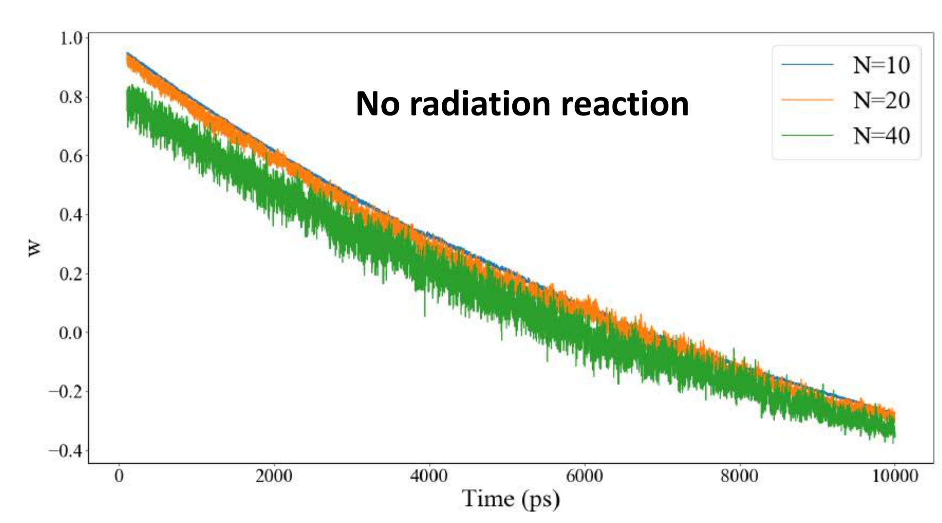
Radiation reaction field: Derived from expansion of Helmholtz dyadic Green's function for dots well within λ (including a self term).

Collective effects: The radiation reaction leads to a nonlinear damping effect.

Super-radiance: Population of excited dots decays with time scaling as 1/N.



Magnitude of population inversion $w = 1 - 2\rho_{00}$ averaged over all dots, for N = 10/20/40.

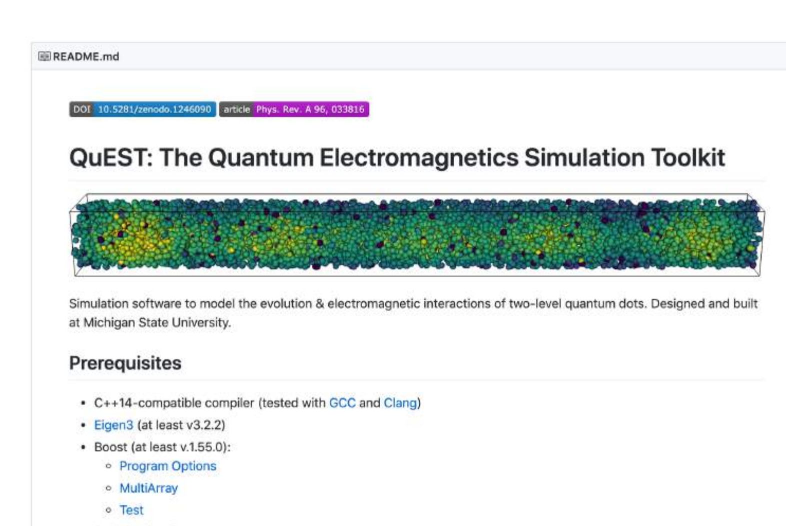


Note that without radiation reaction there is no apparent shortening of the decay with increasing N.

CONCLUSIONS

So far we have:

- Developed software elements to discover novel photonic materials
- Implemented and tested accelerated methods that led us to simulate systems with 100,000+ centers
- Included radiation reaction effects
- Observed coherent collective effects both in the space and time domain



AIM code available on:
https://github.com/cglosser/QuEST QuEST: v0.2.1. (2018). doi:10.5281/zenodo.1246090

REFERENCES AND CONTACT

Carlo Piermarocchi: piermaro@msu.edu
Shanker Balasubramaniam: bshanker@msu.edu

Lu, E., Piermarocchi, C., & Shanker, B. (2020). Modeling Radiation Reaction Induced Superradiance in Quantum Dot Systems (submitted).

Glosser, C., Lu, E., Bertus, T. J., Piermarocchi, C., & Shanker, B. (2019). Acceleration techniques for semiclassical Maxwell-Bloch systems: An application to discrete quantum dot ensembles. *arXiv preprint arXiv:1910.08594*.

Glosser, Connor, Carlo Piermarocchi, and B. Shanker. "Acceleration techniques for semiclassical Maxwell-Bloch systems." In *2018 IEEE MTT-S International Conference on Numerical Electromagnetic and Multiphysics Modeling and Optimization (NEMO)*, pp. 1-3. IEEE, 2018.

Glosser, Connor, B. Shanker, and Carlo Piermarocchi. "Collective Rabi dynamics of electromagnetically coupled quantum-dot ensembles." *Physical Review A* 96, no. 3 (2017): 033816.