

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Efficient GPU calculation of 2D-echo spectra of excitonic energy-transfer in systems with large reorganization energy BIRGIT HEIN, CHRISTOPH KREISBECK, TOBIAS KRAMER, University of Regensburg, Germany, MIRTA RODRIGUEZ, IEM, CSIC, Madrid, Spain — Using the Fenna-Matthews-Olson light harvesting complex as example, we calculate the two dimensional echo spectra (2D echo) of a multi-site system coupled to phonon baths using the propagation scheme suggested by Ishizaki and Fleming in 2009 which works for large system-bath couplings. We study the anti-correlations in the shapes of the 2D spectrum peaks which are seen as evidence for exciton energy transfer. This computationally demanding calculation uses 2.6 h GPU (graphics processing unit) time compared to 2.8 weeks time on a high performance conventional CPU cluster. The efficient implementation of the exact hierarchical equations obliterates the need for approximative methods and facilitates the interpretation and comparison of theory and experiment for systems with large reorganization energies. References see www.quantumdynamics.de

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Date submitted: 24 Nov 2010

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