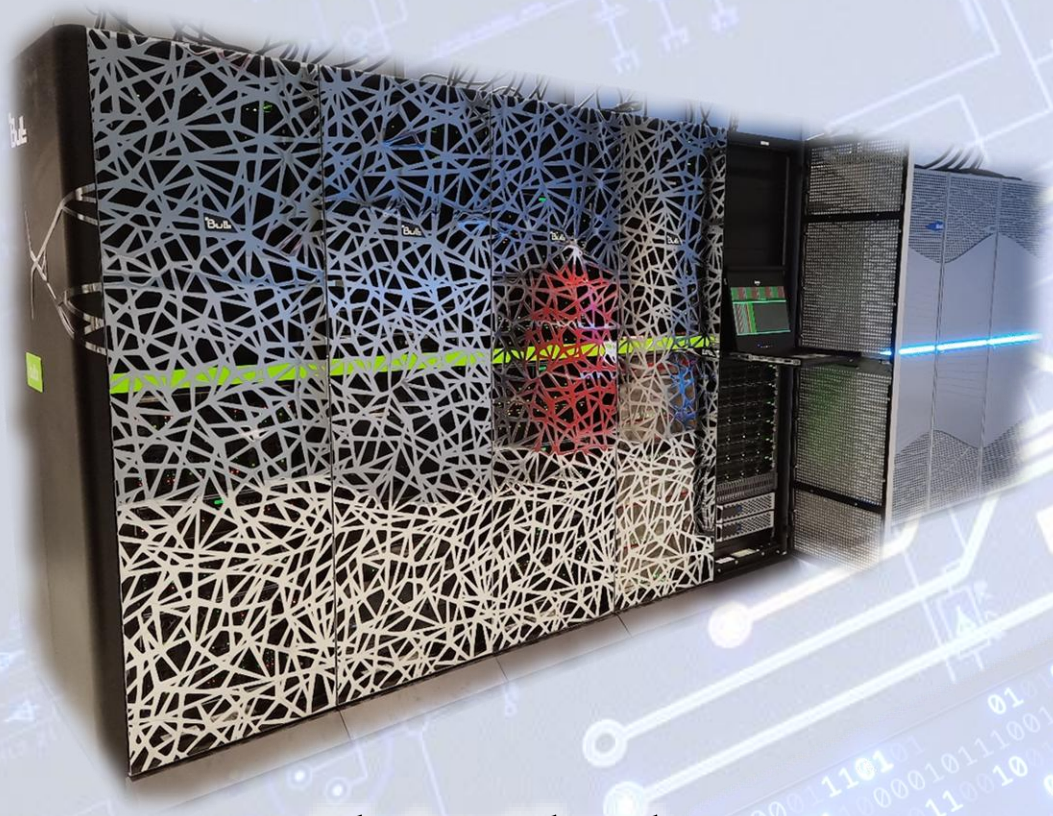
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Molecular aggregates at various intensities of optical fields: from absorption to six-wave mixing 2DES

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Perturbative expansion in powers to the excitation field is a powerful tool for non-linear spectra analysis. While such an approach allows to calculate induced polarization at an arbitrary order. It fails to account for nonlinear processes that react to change in optical field intensity such as exciton – exciton annihilation (EEA).

EEA is an excitation density dependent process as it involves 2 separate excitations interacting and forming a short lived doubly excited state. This state quickly decays and only a single excitation remains. The effect is a nonlinear decay in excitation density.

One way to treat this problem is by using nonlinear exciton equations (NEE) which allows to generate hierarchy of equations. The hierarchy is endless and needs to be cut at some point either by dropping terms (with reasoning that EEA limits the number of excitations in the system) or factorizing them in lower order terms while preserving the dependence on optical field intensity.

We have expanded the NEE equation with EEA terms[1]. We compared a few factorizations that should simplify calculations, but it was only for a molecular dimer. Since then we have made several developments. The equations were expanded to generalized(from paulion to boson) particles[2]. NEE were applied to study EEA signatures in 2D electron spectra calculations with up to six-wave mixing [3]. We made studies of the effects of various factorizations schemes on larger aggregates with varying excitation intensity [4] and additional possible simplifications to the NEE [2].

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