Generating coupled cluster code for modern distributed memory tensor software

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The goal of this project is to design a set of software tools for elegant development of relativistic coupled clusters methods.

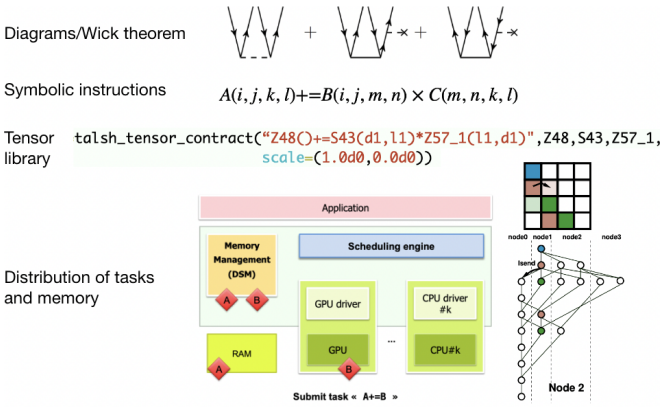

Figure 1: The workflow scheme of the **tenpi** toolchain includes a code generator, intermediate optimizer and a unified interface towards tensor libraries. Fig. from [1]

Modern computer architectures are composed of heterogeneous processing and memory hierarchies. Data movement cost often dominates the cost of computation and only a fraction of peak CPU/GPU power is used. Despite this, most software still uses programming systems lacking any reasoning about the placement and movement of data.

Unlike BLAS for matrix operations, there is no unified tensor interface/library used by the community. Available distributed memory libraries used for chemical applications are not adapted to heterogeneous architectures. The **tenpi** toolchain addresses this problem.

Motto: *"Separate science from the computational platform."*

The first application of the **tenpi** toolchain is on molecular properties as part of the HAMP-vQED project [2]. Studies so far indicate that QED-effects (electron self-energy and vacuum polarization) reduce relativistic effects by about 1%. However, such investigations have been limited to valence properties, since there are currently no reliable tools for general molecules to study the core region, where QED-effects are generated [3].

[1] https://starpu.gitlabpages.inria.fr, visited 2. 6. 2023.
[2] A. Sunaga, M. Salman, T. Saue, J. Chem. Phys., **157** (2022), 164101.
[3] P. Pyykkö, J. F. Stanton, Chem. Rev., **112** (2012), 1.