Relativistic coupled cluster for a new generation of supercomputers

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I will present a new implementation of relativistic coupled cluster algorithms[1,2,3] that is based on the efficient GPU-adapted and parallel ExaTensor library of Lyakh[4,5]. I will discuss our design choices, required starting data, present capabilities and performance of the code. I will also give an outlook of our possible further developments. The code will be provided as open-source with the December 2019 release of DIRAC[6].

References
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