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Electron-impact calculations of near-neutral atomic systems utilising Petascale computer architectures[1]

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Over the last couple of decades, a number of advanced non-perturbative approaches such as the R-matrix[1,2,3], TDCC[4] and CCC[5] methods have made great strides in terms of improved target representation and investigating fundamental 2-4 electron problems. However, for the electron-impact excitation of near-neutral species or complicated open-shell atomic systems we are forced to make certain compromises in terms of the atomic structure and/or the number of channels included in close-coupling expansion of the subsequent scattering calculation. The availability of modern supercomputing architectures with hundreds of thousands of cores, and the emergence new opportunities through GPU usauge offers one possibility to address some of these issues. To effectively harness this computational power will require significant revision of the existing code structures. I shall discuss some effective strategies within a non-relativistic and relativistic R-matrix framework using the examples detailed below. The goal is to extend existing R-matrix methods from 1-2 thousand close coupled channels to 10,000 channels. With the construction of the ITER[6] experiment in Cadarache, which will have Tungsten plasma-facing components, there is an urgent diagnostic need for the collisional rates for the near-neutral ion stages. In particular, spectroscopic diagnostics of impurity influx require accurate electron-impact excitation and ionisation as well as a good target representation. There have been only a few non-perturbative collisional calculations for this system, and the open-f shell ion stages provide a daunting challenge even for perturbative approaches [7]. I shall present non-perturbative results for for the excitation and ionisation of W^{3+} and illustrate how these fundamental calculations can be integrated into a meaningful diagnostic for the ITER device.

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