July 31, 2000

To whom it may concern,

I would like to ask for support in order to participate in the ACTS Toolkit Workshop, organized by NERSC at the Lawrence Berkeley National Laboratory, September 28-30, 2000.

Please find attached a breafly description of my work, list of publications and references.

Sincerely,

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Research Interest

During the past three years I have performed Postdoctoral research in several aspects of theoretical atomic physics, at the Atomic Physics group at Auburn University, USA, together with Profs. M.S. Pindzola and F. Robicheaux. As is shown in my publication list, I am currently carrying on investigations in electron-ion recombination processes and in atomic collision theory. In many of these investigations we wish to apply advanced computational methods and parallel computing to the study of atomic dynamics. Central to these efforts are studies in atomic collision physics in which further theoretical and computational developments and the effective use of the latest massively parallel computers could contribute significantly to the solution of long-standing problems in the field and embody the sate-of-the-art.

One of the most powerful theoretical approaches to the electron collisions problem is based on the R-matrix solution for an antisymmetrized product of an N–electron target wavefunction and a free-electron scattering wavefunction. For applications to electron-impact excitation and ionization of atoms and ions, we make use of five of the modules or stages in the Belfast RMATRX I package. Recently, I rewrote the most time-consuming stages from the RMATRX I packgage, adapting them for use on distributed-memory parallel computers. For STG3, the $(N+1)$-electron Hamiltonian matrix for each $LS\pi$ symmetry is directly partitioned over the many processors of a distributed-memory parallel computer. An advantage of partitioning the Hamiltonian matrix is that the memory requirements per processor are minimized. The global Hamiltonian matrix is never constructed; only a local portion resides on each processor. Second, the partitioned eigenvectors are used to calculate the R-matrix surface amplitudes in parallel. Thus global eigenvectors are never constructed. Finally, since the $LS\pi$ symmetries are completely independent, they may also be run in parallel for ultimate wall clock minimization. I also adapted the further stages of the R-matrix suite for use on massively parallel computers. The calculation of the K-matrices and cross-sections (in STGF and STGIC) is partitioned over the processors according to incident electron energy. The new parallel package has allowed us to study convergence of the R-matrix pseudo-state method as a function of the angular momentum of the pseudo states.

Concerning electron-ion recombination, I am participating in research on field enhanced dielectronic recombinations and on the effect of overlapping resonances. This research demands also diagonalization of very large complex matrices. The size of the matrices involved in these calculations, requires extremely time-consuming calculations, beyond the capabilities of regular computers.

I am also becoming familiar with the methods that solve the time–dependent Schrodinger equation on a partitioned lattice. This technique has been employed in the Auburn University atomic physics group for solving many different problems (*e.g.* electron impact ionization, photoionization, electron-impact double-ionization, and even to solve the Gross-Pitaevskii equation for the calculation of Bose-Einstein condensates).

For my actual and further work, my computation requirements include diagonalization of dense, banded and sparse matrices, equation solver of dense, banded and sparse matrices, differential equation solvers and Fast-Fourier transformers. I will also need different tools for visualization of the results.

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