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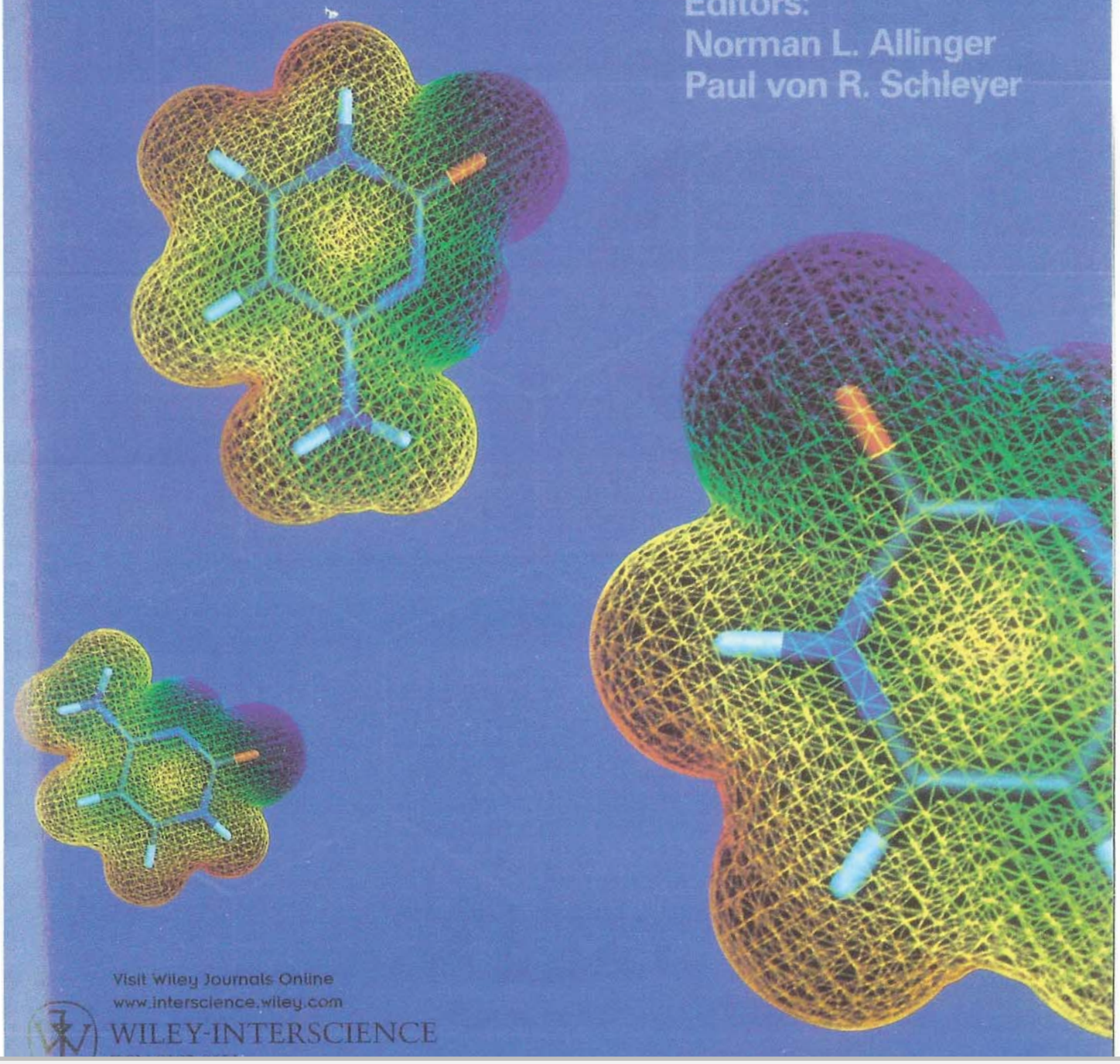

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(*Continued*)

Development of a Parallel Molecular Dynamics Code on SIMD Computers: Algorithm for Use of Pair List Criterion

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ABSTRACT: In recent years several implementations of molecular dynamics (MD) codes have been reported on multiple instruction multiple data (MIMD) machines. However, very few implementations of MD codes on single instruction multiple data (SIMD) machines have been reported. The difficulty in using pair lists of nonbonded interactions is the major problem with MD codes for SIMD machines, such that, generally, the full connectivity computation has been used. We present an algorithm, the global cut-off algorithm (GCA), which permits the use of pair lists on SIMD machines. GCA is based on a probabilistic approach and requires the cut-off condition to be simultaneously verified on all nodes of the machine. The MD code used was taken from the GROMOS package; only the routines involved in the pair lists and in the computation of nonbonded interactions were rewritten for a parallel architecture. The remaining calculations were performed on the host computer. The algorithm has been tested on Quadrics computers for configurations of 32, 128, and 512 processors and for systems of 4000, 8000, 15,000, and 30,000 particles. Quadrics was developed by Istituto Nazionale di Fisica Nucleare (INFN) and marketed by Alenia Spazio.
 J Comput Chem 19: 685–694, 1998

Keywords: molecular dynamics; domain decomposition algorithm; parallel computers; pair list for molecular dynamics code on SIMD machines; array processor elaborator (APE)

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