

PACKAGE ID - 000826NCUBE00 PARBOND

KWIC TITLE - Parallel Molecular Dynamics Program for
Molecules

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LIMITATION CODE -COPY **AUDIENCE CODE** - LIM

COMPLETION DATE - 06/01/1993 **PUBLICATION DATE** - 03/13/1995

DESCRIPTION - ParBond is a parallel classical molecular dynamics code that models bonded molecular systems, typically of an organic nature. It uses classical force fields for both non-bonded Coulombic and Van der Waals interactions and for 2-, 3-, and 4-body bonded (bond, angle, dihedral, and improper) interactions. It integrates Newton's equation of motion for the molecular system and evaluates various thermodynamical properties of the system as it progresses.

PACKAGE CONTENTS - Media Directory; Software Abstract; Media Includes Source Code, User's Guide;

SOURCE CODE INCLUDED? - Yes

MEDIA QUANTITY - 1 3.5 Diskette

METHOD OF SOLUTION - The force fields used by ParBond are the standard harmonic equations commonly used by commercial and academic codes such as CHARMM, AMBER, and DISCOVER. The method of timestep integration is velocity Verlet. The parallelization method for the non-bonded and bonded interactions is force-decomposition or replicated-data.

COMPUTER - NCUBE 2

OPERATING SYSTEMS - ParBond is written in a high-level language and thus compiles on the nCUBE 2 under whatever current version of the OS is being used.

PROGRAMMING LANGUAGES - FORTRAN 77

SOFTWARE LIMITATIONS - ParBond is limited to running problems that can fit in available memory on a single processor of the nCUBE 2. Since all of the data structures (atom lists, neighbor lists) are distributed, this means very large problems (ten to hundreds of thousands of atoms) can be run on large number processors. Array bounds are fixed by parameter statements in the top of the include files used by the source code.

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SOURCE CODE AVAILABLE (Y/N) - Y

UNIQUE FEATURES - The use of the force-decomposition parallelization strategy is the only unique feature of ParBond. This enables large number of processors to be used more effectively for many problems.

RELATED SOFTWARE - There is a pre-processing program 'prep' which is not part of this ParBond distribution package, but which is useful for creating one of the input data files that ParBond uses. Users can contact the author directly for a copy of prep and its associated documentation.

OTHER PROG/OPER SYS INFO - Parabond is written in F77 with only a few simple extensions (longer-than-6-character variable names, uses of enddo) that are supported by virtually all F77 compilers.

HARDWARE REQS - This distribution of ParBond software runs on the nCUBE 2 parallel computer.

TIME REQUIREMENTS - The time for a particular run scales roughly linearly with the number of timesteps and number of atoms.

REFERENCES - Informal documentation

ABSTRACT STATUS - Submitted 3/13/95. Released screened 4/09/96.

SUBJECT CLASS CODE - W

KEYWORDS -

COMPUTER PROGRAM DOCUMENTATION
P CODES
EQUATIONS OF MOTION
DYNAMICS
MOLECULES
COLLISIONS

EDB SUBJECT CATEGORIES -
990200 664300

SPONSOR - DOE/ER

PACKAGE TYPE - SCREENED