DARESBURY LABORATORY

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INFORMATION QUARTERLY for COMPUTER SIMULATION OF CONDENSED PHASES

An informal Newsletter associated with Collaborative Computational Project No. 5 on Molecular Dynamics, Monte Carlo and Lattice Simulations of Condensed Phases.

Number 33 January 1991

Contents

- General News 2
- BEYOND THE PAIR POTENTIAL REGISTRATION FORM 3
- Situations vacant 5
- THE CCP5 PROGRAM LIBRARY. E-mail Service 6
- TEQUILA molecular distance plot program A. Wilton F Müller-Plathe. 13
- Computer Simulation of Liquid Crystals Workshop report M. P. Allen 18
- Molecular dynamics on parallel computers K. M. Crennell 23
- C-language Program for the Irregular Close Packing of Hard Spheres M. Bargiel, J. Mościński 27
- C-language Molecular Dynamics Program for the Simulation of Lennard-Jones Particles M. Bargiel, W. Dzwinel, J. Kitowski, J. Mościński 42
- Microscale Hydrodynamics on Microcomputers J. Tarbaj, M. Zimnoch, J. Mościński, J. Kitowski, M. Bubak 62
- CCP5 Literature Survey 1989 71

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General News

RENEWAL PROPOSAL CCP5 has been renewed for a further three years. Funds have been allocated for holding meetings and workshops, for overseas visitors and for collaborations within the UK. If UK CCP5 members would like to set up a small **collaboration** funds are available for this purpose. Please send a brief account of the current or proposed research to the CCP5 secretary. Also it is possible to obtain funds for **overseas visitors** to the UK. If anyone in the UK has a visitor in mind, or if anyone would like to visit the UK from abroad please send details to the CCP5 secretary.

FUTURE MEETINGS AND WORKSHOPS CCP5 is planning two workshops and one meeting in the near future. A workshop is being held at the University of Keele on the topic "**Beyond the Pair Potential**". This will be held on 15th-16th April 1991. A registration form is included in this issue of the newsletter. A workshop on the "**Simulation of the Structure and Transport of Molecules in pores.**" will be held at the University of Southampton on Friday April 26th 1991. Anyone interested in attending should contact Professor D Tildesley, Department of Chemistry, University of Southampton, Southampton SO9 3PH. A meeting on "**Molecular Modelling of Solids and Surfaces**" will be held on 9th-11th July 1991. This will be held at the University of Glasgow. The contact for further details is Dr. N. Allan, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS.

CCP5 PROGRAM LIBRARY Details are contained in this issue of accessing the CCP5 program library through E-mail automatically. Also two new programs have been added to the library and have been documented in this issue.

National Centre News The major development during the past year has been the switch by RAL and ULCC to UNICOS on the CRAY computers. There has also been some discussion about the future of ULCC. It has now been recommended that a CRAY service should continue at ULCC.

CRAY TIME CCP5 participants are reminded that CCP5 has an annual allocation of Cray time at Rutherford (Cray XMP-48), which is available for the development of simulation programs which are of general use to the CCP5 community. Readers who wish to use some of this allocation should write to the CCP5 Secretary, Dr. M. Leslie, TCS Division, SERC Daresbury Laboratory, Daresbury, Warrington WA4 4AD.

SERC CCP5 Workshop

"BEYOND THE PAIR POTENTIAL"

PHYSICS DEPARTMENT
UNIVERSITY OF KEELE
15-16 APRIL 1991

This CCP5 workshop aims to bring to the attention of the simulation community new methods for modelling the energetics of condensed matter. Particular emphasis will be on the Car-Parrinello technique and other methods of ab initio simulation, including the Hartree-Fock approach, as well as semi-empirical methods such as tight-binding theory. The organisers seek contributed talks, and plan to hold a poster session given enough contributions. Please overwhelm us!

SPEAKERS WILL INCLUDE:

R. Car	IRRMA, Lausanne
R. Catlow	Royal Institution, London
R. Jones	University of Exeter
M. Payne	Cavendish Laboratory, Cambridge
D. Pettifor	Imperial College, London
A. M. Stoneham	AEA Technology, Harwell

Further information from:

Mike Gillan,
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Keele, Staffordshire, ST5 5BG

Phone: 0782 621111 ext. 3911

E-mail: pha71@keele.seql

UNIVERSITY OF KEELE

'BEYOND THE PAIR POTENTIAL'

UNIVERSITY OF KEELE, 15 - 16 APRIL 1991

REGISTRATION FORM

NAME: .....

ADDRESS: .....

.....

.....

TELEPHONE: .....

ELECTRONIC MAIL: .....

****

CONFERENCE CHARGES:

REGISTRATION FEE (25 pounds) .....pounds
(Includes 2 lunches and
light refreshments. Students: see below.)

ACCOMMODATION (18 pounds per night) .....pounds

DINNER ON 15. APRIL (9 pounds) .....pounds

TOTAL .....pounds
(Cheques payable to 'CCP5 Keele Workshop')

The registration fee will be waived for students (i.e. students do not pay for lunches); supervisor's letter is required.

The accommodation charge includes breakfast. Please indicate here which nights you require accomodation: .....

Special dietary requirements? Make a note here: .....

****

CONTRIBUTED PAPERS:

I do / do not wish to contribute a presentation entitled:

.....

Please enclose an abstract with this form.

****

Please send this form, together with a cheque for the appropriate amount, payable to 'CCP5 Keele Workshop', together with your abstract, if any, to arrive no later than 15. March 1991, to:

Professor M. J. Gillan
Department of Physics, University of Keele
Keele, Staffordshire ST5 5BG

UNIVERSITY OF DUBLIN

TELEPHONE No. 772941
EXTENSION 1726

Professor of Physical Chemistry
and Head of Department:
JOHN CORISH

DEPARTMENT OF CHEMISTRY
TRINITY COLLEGE
DUBLIN 2
IRELAND

Short term Postdoctoral position available until 30 September 1991. The work is in the general area of the simulation of polymeric material containing dopant ions and could involve either static lattice methods or quantum mechanical calculations.

Apply to:

Professor J. Corish,
Department of Chemistry,
Trinity College,
Dublin 2.

Telephone Dublin 772941, Ext 1726

FAX Dublin 712826.

23.11.90

The CCP5 Program Library

W. Smith

December 10, 1990

News.

We are pleased to announce the following additions to the Program Library:
From Prof. Jacek Mościński's group at the Institute of Computer Science, Cracow, we have received two C-language programs:

- MD3DLJ - by M. Bargiel, W. Dzwinel, J. Kitowski and J. Mościński. A molecular dynamics program for Lennard-Jones atoms using the link-cell method with other refinements to enhance performance.
- NSCP3D - by M. Bargiel and J. Mościński. A program for irregular close packing of hard spheres.

Both programs are suitable for IBM PCs and are fully documented. The programs are descibed in detail in this issue of the newsletter.
We have also received a simple graphics program: TEQUILA - a molecular distance plot program, by A. Wilton and F. Müller-Plathe. It is suitable for unix graphics workstations and is also described in this issue of the newsletter.

Our thanks go to the above mentioned for their support.

CCP5 Program Library E-Mail Service

From January 1 1991 it will be possible for CCP5 members to get copies of CCP5 programs through E-mail *automatically*. To do so they should send an E-mail message to **info-server@uk.ac.daresbury**. The contents of the e-mail message should be as follows (Note: the use of upper and lower case is significant - this is a unix system!):

request sources
topic index CCP/ccp5
topic CCP/ccp5/program-name

Where program-name is the name of the desired source code. A mail server will automatically process this message and return a copy of the source code to your e-mail address. Please note the following however:

The program source will be returned to you in **uue** format, which is a form of encoding most suitable for mail messages. It can easily be decoded on any unix system using the uudecode command. (Check your local unix *man* file for details). Also, to speed the transfer, the source will be split into files of 1200 records each, so expect two or three such files for the average CCP5 program. Once again, uudecode will help you to sort things out.

Readers who do not have unix facilities should include the following lines at the start of the above message:

line-limit: nnnnn
coding: off

Where nnnnn is the number of records in the source (in most cases 6000 should be enough). The program will be sent in plain FORTRAN as a single file. It may take a while to arrive, but be patient! Also beware in case your system mailer cannot handle messages of this size.

Readers must realise that the terms of use and distrubution of the CCP5 programs that have applied hitherto will be maintained. Users should not redistribute or sell the programs, nor is any liability accepted for their use, either by SERC or the program authors. It is a requirement on the user that the programs be fully tested for their intended purpose. Any bugs found should be reported to the librarian, for the benefit of other users.

Lastly readers should realise that this means of transfer does not include any program documentation. So if you are unable to make sense of the programs, write for the documentation!

We are grateful to Mr. P. Griffiths of Daresbury's ITS Division for implementing this facility.

CCP5 Program Library Contents

The CCP5 Program Library provides programs and documentation free of charge to academic centres upon application to Dr. W. Smith, TCS Division, S.E.R.C. Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K.. Listings of programs are available if required but it is recommended that magnetic tapes (supplied by the applicant) be used. It may also be possible to transfer a small number of programs over the JANET network to other computer centres in the U.K.. Please note that use of inappropriate packing for magnetic tapes (e.g. padded bags) may result in them being considered unusable by Daresbury Computing Division and returned without the required software. Please ensure that these forms of packaging are not used. A list of programs available is presented in the following pages.

Readers should also note that we are authorised to supply the example programs originally published in the book "Computer Simulation of Liquids", by M.P. Allen and D.J. Tildesley (Clarendon Press, Oxford 1987). These are supplied in the same manner as the resident CCP5 programs. We are grateful to Mike Allen and Dominic Tildesley for their permission.

We should also like to remind our readers that we would welcome further contributions to the Program Library. The Library exists to provide support for the research efforts of everyone active in computer simulation and to this end we are always pleased to extend the range of software available. If any of our readers have any programs they would like to make available, please would they contact Dr. Smith.

Please Note: For copyright reasons we are not able to supply the programs CASCADE, SYMLAT, THBFIT,THBPHON and THBREL free of charge to Universities outside the United Kingdom.

Program from the Book: "Computer Simulation of Liquids" by M.P. Allen and D. Tildesley, Clarendon Press, Oxford 1987.

These programs originally appeared on microfiche in the book "Computer Simulation of Liquids" by M. P. Allen and D. J. Tildesley, published by Oxford University Press, 1987. They are made freely available to members of CCP5, in the hope that they will be useful. The intention is to clarify points made in the text, rather than to provide a piece of code suitable for direct use in a research application. We ascribe no commercial value to the programs themselves. Although a few complete programs are provided, our aim has been to offer building blocks rather than black boxes. As far as we are aware, the programs work correctly, but we can accept no responsibility for the consequences of any errors, and would be grateful to hear from you if you find any. You should always check out a routine for your particular application. The programs contain some explanatory comments, and are written, in the main, in FORTRAN-77. One or two routines are written in BASIC, for use on microcomputers. In the absence of any universally agreed standard for BASIC, we have chosen a very rudimentary dialect. These programs have been run on an Acorn model B computer. Hopefully the translation of these programs into more sophisticated languages such as PASCAL or C should not be difficult.

M.P.Allen

THE CCP5 PROGRAM LIBRARY.

```
ADMIXT     [MD,LJA/MIX,LF,TH+MSD+RDF]          W. Smith
CARLOS     [MC,VS+Aquo,TH]    B. Jonsson & S. Romano
CARLAN     [DA,CARLOS structure analysis]  B. Jonsson
                                          & S. Romano
CASCADE    [LS,DIL,EM,TH+STR]    M. Leslie & W. Smith
CURDEN     [DA,Current Density Correlations] W. Smith
DENCOR     [DA,Density Correlations]    W. Smith
HLJ1       [MD,LJA,LF,TH+MSD+RDF]    D.M. Heyes
HLJ2       [MD,LJA,LF,TH+MSD+RDF+VACF]    D.M. Heyes
HLJ3       [MD,LJA,LF/LC,TH+MSD+RDF]    D.M. Heyes
HLJ4       [MD,LJA,LF/CP+CT,TH+MSD+RDF]    D.M. Heyes
HLJ5       [MD,LJA/SF,LF,TH+MSD+RDF]    D.M. Heyes
HLJ6       [MD,LJA,TA,TH+MSD+RDF]    D.M. Heyes
HMDIAT     [MD,LJD,G5+Q4,TH+MSD+QC]    S.M. Thompson
HSTOCH     [MD/SD,VS+BA,LF+CA,TH]    W.F. van Gunsteren
                                   & D.M. Heyes
MCN        [MC,LJA,TH]    N. Corbin
MCLSU      [MC,LJA,TH]    C.P. Williams & S. Gupta
MCMOLDYN   [MD/MC,LJS+FC+AQ,LF+QF/G5+QS,TH+RDF] A. Laaksonen
MCRPM      [MC,RPE,TH+RDF]    D.M. Heyes
MDATOM     [MD,LJA,G5,TH+RDF+MSD+QC]    S.M. Thompson
MDATOM     [MD,LJA,LF,TH+MSD+RDF]    D. Fincham
MDCSPC4B     [PRMD,BHM+FC,G5+G4,TH+STF+RDF]    W. Smith
MDDIAT     [MD,LJD,LF+CA,TH+MSD]    D. Fincham
MDDIATQ    [MD,LJD+PQ,LF+CA,TH+MSD]    D. Fincham
MDIONS     [MD,BHM,LF,TH+MSD+RDF+STF] D. Fincham
                                    & N. Anastasiou
MDLIN      [MD,LJL,G5+Q4,TH+MSD+QC]    S.M. Thompson.
MDLINQ     [MD,LJL+PQ,G5+Q4,TH+MSD+QC]    S.M. Thompson
MD3DLJ_C   [MD,LJA/MIX,LF/LC,TH+MSD+RDF]  M. Bargiel,
           W. Dzwinel, J. Kitowski and J. Moscinski
MDMANY     [MD,LJS+FC,LF+QF,TH] D. Fincham & W. Smith
MDMIXT     [MD,LJS/MIX,LF+QF,TH]    W. Smith
MDMPOL     [MD,LJS+FC/MIX,LF+QF,TH]    W. Smith & D. Fincham
MDNACL     [MD,BHM,LF,TH+MSD+RDF]    W. Smith
MDPOLY     [MD,LJS,G5+Q4,TH+MSD+QC]    S.M. Thompson
MDMULP     [MD,LJS+PD+PQ/MIX,LF+QF,TH]    W. Smith
MDSGWP     [MD,LJA/SGWP,LF,TH+VACF+RDF+QC]    W. Smith
                                          & K. Singer
MDTETRA    [MD,LJT,G5+Q4,TH+MSD+QC]    S.M. Thompson
MDZOID     [MD,GAU,LF+QF,TH+MSD+RDF+VACF]    W. Smith
NAMELIST   [UT, Namelist emulation]     K. Refson
NSCP3D     [UT, Hard sphere packing] M. Bargiel & J. Moscinski
PIMCLJ     [PIMC,LJA,MC,TH+RDF+QC] K. Singer & W. Smith
SCN        [MC,LJA,RFD,TH]    N. Corbin
SURF       [MD,BHM/TF/2D,LF,TH+RDF]    D.M. Heyes
```

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SYMLAT    [LS,PIL,EM+SYM,TH+STR]   Harwell
THBFIT    [LS,PIL,EM,Potential fitting]   Harwell
THBPHON   [LS,PIL/3B,EM,Phonon dispersion]   Harwell
THBREL    [LS,PIL,EM,TH+STR]   Harwell
```

Key:

Program types:	MD	Molecular dynamics
	MC	Monte Carlo
	PRMD	Parrinello-Rahman MD
	LS	Lattice simulations
	SD	Stochastic dynamics
	DA	Data analysis
	UT	Utility package
	PIMC	Path Integral Monte Carlo
System models:	LJA	Lennard-Jones atoms
	LJD	Lennard-Jones diatomic molecules
	LJL	Lennard-Jones linear molecules
	LJT	Lennard-Jones tetrahedral molecules
	LJS	Lennard-Jones site molecules
	RPE	Restricted primitive electrolyte
	BHM	Born-Huggins-Meyer ionics
	SGWP	Spherical gaussian wavepackets
	TF	Tosi-Fumi ionics
	VS	Variable site-site model
	BA	Bond angle model
	PD	Point dipole model
	PQ	Point quadrupole model
	MIX	Mixtures of molecules
	GAU	Gaussian molecule model
	FC	Fractional charge model
	PIL	Perfect ionic lattice model
	DIL	Defective ionic lattice model
	3B	3-body force model
	2D	Two dimensional simulation
	SF	Shifted force potential
	FC	Fractional charge model
	AQ	Aqueous solutions
Algorithm:	G5	Gear 5th order predictor-corrector
	Q4	Quaternion plus 4th. order Gear P-C.
	LF	Leapfrog (Verlet)
	QF	Fincham Quaternion algorithm
	QS	Sonnenschein Quaternion algorithm
	LC	Link-cells MD algorithm
	CP	Constant pressure

	CT	Constant temperature
	TA	Toxvaerd MD algorithm
	CA	Constraint algorithm
	EM	Energy minimisation
	SYM	Symmetry adapted algorithm
	RFD	Rossky-Friedman-Doll algorithm
Properties:	TH	Thermodynamic properties.
	MSD	Mean-square-displacement
	RDF	Radial distribution function
	STF	Structure factor
	VACF	Velocity autocorrelation function
	QC	Quantum corrections
	STR	Lattice stresses

Programs from the Book "Computer Simulation of Liquids"

F.1 Periodic boundary conditions in various geometries
F.2 5-value Gear predictor-corrector algorithm
F.3 Low-storage MD programs using leapfrog Verlet algorithm
F.4 Velocity version of Verlet algorithm
F.5 Quaternion parameter predictor-corrector algorithm
F.6 Leapfrog algorithms for rotational motion
F.7 Constraint dynamics for a nonlinear triatomic molecule
F.8 Shake algorithm for constraint dynamics of a chain molecule
F.9 Rattle algorithm for constraint dynamics of a chain molecule
F.10 Hard sphere molecular dynamics program
F.11 Constant-NVT Monte Carlo for Lennard-Jones atoms
F.12 Constant-NPT Monte Carlo algorithm
F.13 The heart of a constant μVT Monte Carlo program
F.14 Algorithm to handle indices in constant μVT Monte Carlo
F.15 Routines to randomly rotate molecules
F.16 Hard dumb-bell Monte Carlo program
F.17 A simple Lennard-Jones force routine
F.18 Algorithm for avoiding the square root operation
F.19 The Verlet neighbour list
F.20 Routines to construct and use cell linked-list method
F.21 Multiple timestep molecular dynamics
F.22 Routines to perform the Ewald sum
F.23 Routine to set up alpha fcc lattice of linear molecules
F.24 Initial velocity distribution
F.25 Routine to calculate translational order parameter
F.26 Routines to fold/unfold trajectories in periodic boundaries
F.27 Program to compute time correlation functions
F.28 Constant-NVT molecular dynamics - extended system method
F.29 Constant-NVT molecular dynamics - constraint method
F.30 Constant-NPH molecular dynamics - extended system method
F.31 Constant-NPT molecular dynamics - constraint method
F.32 Cell linked-lists in sheared boundaries
F.33 Brownian dynamics for a Lennard-Jones fluid
F.34 An efficient clustering routine
F.35 The Voronoi construction in 2d and 3d
F.36 Monte Carlo simulation of hard lines in 2d
F.37 Routines to calculate Fourier transforms

TEQUILA molecular distance plot program

This program can be obtained from the CCP5 program library at the above address. It uses the VOGLE public-domain graphics library by Eric H. Echidna, which at the time this note is written can be obtained from: The Software Support Programmer, Dept. of Engineering Computer Resources, Faculty of Engineering, University of Melbourne Vic 3052, Australia, email: echidna@munnari.OZ.AU.

REFERENCE MANUAL FOR TEQUILA.F

INTRODUCTION.

Brookhaven files contain information concerning protein structure. The file lists each atom in the molecule, starting from one end and progressing towards the other, atom by atom. The atom number, atom name, residue name, residue number and the x,y and z co-ordinates are all quoted for each. The files therefore contain detailed information on protein structure.

The information for these files is gathered in a number of ways. X-ray diffraction is widely used, with the sample in a crystalline form. The X-rays scatter off electrons, giving the best readings where there are abundant electrons (heavy metals give excellent results). Since there is a high electron density around the nucleus of an atom, it is possible to see where the atoms are located in a molecule by this method. Different atoms will give different diffraction patterns, depending on the arrangement of their electron shields.Hydrogen atoms however are practically invisible to this diffraction method, since they have a single electron. Neutrons, having electro-chemical neutrality, are able to pass unaffected through electron clouds. They scatter at the nucleus of the atoms, and interact best with atoms of a similar mass to themselves. Therefore hydrogen atoms are easily detected by this method, being the smallest of the atoms.

Reading the file,however, does not give much ofa clue as to what the protein actually looks like. It would be useful,then, to be able to use the proteindata to produce some form of visualisation of the protein molecule.

It is possible to 'draw' a 3-D representation of the molecule, using graphics packages such as Biograf. This gives an image that can be rotated , so that the protein's structure can be viewed from all angles. However, it is difficult to distinguish between two somewhat similar proteins by this method, since both may show identical

structural characteristics. The 3-D representation does not give any indication as which residues are present, which is most likely where any differences lie.

This program gives a more diagrammatic representation of a protein molecule, and whilst the 3-D structural characteristics are lost, they are still apparent in the diagram. Using the colour key, it is possible to see areas in which the atoms are closer than expected. A thick band of close atoms, generally along the diagonal of the plot, indicates a helix. Other features, such as beta pleats and hair-pin loops can also be identified. It is also possible to access the name of the residue that the atom is in. This makes it possible to see the visible differences between two proteins and whether there is any residue differences.

MAIN PROGRAM.

The program contained in the file tequila.f has been designed to read Brookhaven files. It does this line by line, disregarding any lines that do not begin with the keywords ATOM or HETATM. Each line consists of a string of data which gives information on each of the constituent atoms. This information is broken down into:-

ATOM NUMBER
ATOM LABEL
RESIDUE NAME
RESIDUE NUMBER
X \
Y - CO-ORDINATES
Z /

These portions of the line are returned to the main program in the file. Each portion is an array of dimension <natom>. <natom> is the number of lines within the Brookhaven file that begin with ATOM or HETATM. This means that part of the file has effectively been disposed of, and only the lines of interest are left.

The Brookhaven file is sorted further, with only the information regarding alpha carbons being acted upon. The x,y and z co-ordinates of these alpha carbons are renamed as xa,ya and za and are passed down into subroutine vector. Here the co-ordinates are used to calculate the distances between the alpha carbons.

These distances are passed back up to the main program contained in the two dimensional array <r>. <r> now contains an array of information which can now be transfered to subroutine triangle. Within this subroutine the contents of <r> are translated into colours, and these are displayed on the screen.

Subroutine triangle, as its name suggests, displays the array as a triangle. The triangle consists of small squares. The value of each of the array elements of <r> is effectively stored within these squares. The triangle is constructed from a square situated in the bottom left-hand corner of the graphics screen. This square is then repeated via a nested do-loop, which increases the value of the y co-ordinates, and then increases the value of the x co-ordinates. Since the array is duplicated i.e r(4,5) is the same as r(5,4) etc., then the resulting output need only be a triangle and not a large square, which would fill the entire screen.

The size of the squares is determined by how many elements are held within the array <r>. The screen runs from position -0.9 to position 0.9 in screen co-ordinates. This distance (which is equivalent to 1.8) is divided by the number of alpha carbons (ntom). This value is used to increment the x and y co-ordinates, so that the resulting triangle will make the most effective use of the space available.

As the squares are drawn, they are filled with a colour. The colour chosen is relevant to the distance that is contained within the array element that the square represents. The colours are set in subroutine setmap, and are accessed via the function colmap. Function colmap contains a series of statements, which if fulfilled will return a value for the colour, to the triangle subroutine. The colours have been graded from red (for the closest atoms) through orange, yellow, green and blue to deep purple. White is used to colour any squares that contain a value that is less than the first set of boundaries. If the value exceeds the highest boundary, then the square is not coloured, but becomes the screen background colour (in this case, black).

A colour key is portrayed in the top right-hand segment of the screen, showing the limits of the boundaries (in Angstroms) and the associated colour. Thus the closest atoms can be identified at a glance, as can areas where the atoms are furher apart than expected.

THE OPTIONS.

The program allows for a series of optional jobs to be carried out.

The options are called upon using the keyboard characters. Key 'd' displays a screen which lists the various options within the program. The options are as follows:-

CHARACTER	FUNCTION
q	When this key is pressed, the graphics screen is exited, and control is passed back to the standard output.
s	This key enables the second screen to be accessed. This triangle consists of an array that contains information on the minimum distance between the residues.
a	This key returns the screen to the initial screen which denotes the distance between alpha carbons.
p	This writes the output to a postscript file.
h	This writes the output to a HP file.
c	This writes the output to a colour postscript file.
r	This enables a more detailed examination of the triangle. When 'r' is pressed, option control is passed to the mouse. If the left hand side or the central mouse buttons are clicked, then the residue names, numbers and the actual distance between the two atoms represented at that mouse position, will be returned to the standard output. The right hand

side mouse button will return control to the keyboard.

KEY 's'

The screen pattern is built up in the same way as before. This time however, the array <r> contains the shortest distance between the atoms in one residue and the atoms in the others. These distances are calculated in subroutine shortdist, in the same way as subroutine vector calculates its distances. Here, however, the distances between all of the atoms is calculated and the shortest ones are retained.

KEYS 'p','c' and 'h'

These allow the output screen to be written to a file. This means that it is possible to obtain a hard copy of the screen, which can be kept.Since each screen is unique to the file being read, and each output screen is lost once the program is exited, this is very useful.

KEY 'r'

The output screen provides a useful representation of a proteins structure. It also provides a quick comparison between two different proteins. The user may, however, want to beable to obtain more information than can be shown on the screen. Using the mouse, it is possible to move to the cursor to an area of interest, ans access further information. If the left hand side or the central mouse buttons are clicked, then the residue names and numbers of the atoms that are stored at that location will be printed into the standard output. The actual distance between the two atoms will also be printed. To exit from this facility, the right hand side mouse button must be pressed. This will return the control to the keyboard. This option can be used for both the alpha carbon and the shortest distance screens.

AUTHOR:-

Amanda Wilton 18/06/90

Computer Simulation of Liquid Crystals

A CCP5-sponsored discussion meeting was held at Bristol University on the afternoon of Wednesday 11 April, following the Annual Meeting of the British Liquid Crystal Society. The idea was to bring together those currently carrying out simulations of liquid crystals to discuss recent research and make future plans.

The meeting was attended by

M. P. Allen (Bristol)
D. J. Cleaver (Bristol)
J. W. Emsley (Southampton)
G. Jackson (Sheffield)
G. R. Luckhurst (Southampton)
A. J. Masters (Manchester)
W. Palke (Southampton)
D.J. Tildesley (Southampton)
M. Whittle (Manchester)
M. R. Wilson (Bristol)

George Jackson started by discussing recent simulations of hard dumbbells, formed from touching hard spheres (i.e. bond length $l = \sigma$, molecular end-to-end length-to-width ratio $L/D = 2$). The system size was $N = 250$ molecules. Conventional constant-pressure Monte Carlo techniques were used, with both the volume and the ratios of the sides of the cuboidal simulation box allowed to vary. The pressure was changed to give approximate increases in packing fraction of 0.02 between one run and the next. Typical run lengths were 1.2×10^7 configurations for equilibration and 10^7 configurations to accumulate the averages. The program calculated the equation of state, isothermal compressibility, the atomic (sphere–sphere) and molecular (centre–centre) radial pair distribution functions, the director, the order parameter $P_2(\cos\theta)$, and the orientational pair correlation function $g_2(r)$. On increasing the pressure of the system no evidence of orientational ordering before the freezing transition was found. The system forms an atomic close-packed structure with random bond orientational order. The equation of state for this system can be compared with theory for the isotropic fluid, and the theory can be extended to cover long flexible or rigid atomic chains. However, no information regarding the molecular g_2 correlations emerges from the theory.

Currently the work is being extended to examine trimers and longer chains, and there is interest in examining the influence of chain flexibility.

A separate side of the simulation work is a plan to examine more realistic liquid crystal models, using potentials of the Jorgensen type, linked to quantum mechanical *ab initio* calculations.

Martin Whittle described work undertaken in collaboration with Andy Masters involving constant-pressure MC simulations of hard-sphere linear chains of various lengths: a 6-atom chain with bond length $l = 0.5\sigma$ (end-to-end $L/D = 3.5$), an 8-atom chain also with $l = 0.5\sigma$ ($L/D = 4.5$), and an 8-atom chain with $l = 0.6\sigma$ ($L/D = 5.2$). (According to Veerman and Frenkel (preprint) $L/D = 3.5$ is the point at which a nematic branch begins to appear for spherocylinders.) Rather small systems ($N = 72$) but extremely long runs (750 000 MC sweeps for equilibration) were used. The most elongated systems were shown to form a nematic phase on compression, and there was some evidence of smectic ordering on further compression. The work is now being extended to larger systems ($N = 200$). The simulations produce site-site $g_{\alpha\beta}(r)$ functions for comparison with RISM theory, and also molecular $g(r, \Omega_1, \Omega_2)$ functions in the form of spherical harmonic expansions. The single-particle orientational distribution function about the director $f(\theta)$ in the nematic phase was also studied, and an attempt was made to measure the Frank elastic constants by the method of Allen and Frenkel. Results here are in the right ball-park but subject to large errors: use of a larger system size should reduce these. In the course of the work an assessment of different neighbour-list techniques was made, an atom-based one appearing to be the most efficient. The link-cell method seems to be more efficient than a simple Verlet neighbour list for $N > 150$.

Dominic Tildesley commented that he had simulated similar systems of linear Lennard-Jones tetramers and pentamers using constant-pressure molecular dynamics with typical runs of length 20 000 steps and had encountered forbidding timescale problems. Raising and then lowering the temperature could completely eliminate all trace of orientational ordering in an apparently stable nematic phase. Geoffrey Luckhurst reported that he and Ian McDonald had attempted a similar simulation using 4 Lennard-Jones atoms to give an overall $L/D = 3$, in an attempt to match simulations of the Gay-Berne system which is fitted to this very model. While the Gay-Berne system gives a nematic phase, the corresponding Lennard-Jones system apparently does not.

There followed some discussion of the differences between 'ellipsoidal' shapes and 'spherocylinder' shapes. It was generally agreed that it was not surprising that they behaved quite differently at these elongations, although at extreme elongations in the Onsager limit they should become similar. There is great interest in determining which shape is the most appropriate for

real mesogenic molecules. Further discussion concerned the similarities and differences between linear atomic chains and spherocylinders. Martin Whittle and Geoffrey Luckhurst both mentioned an interest in studying nonlinear 'kinked' molecules, rigid and flexible respectively.

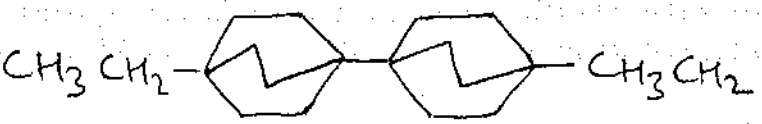
Mike Allen reported that the molecular dynamics simulations of hard ellipsoids of revolution, conducted over the last four years, are continuing, with more extreme shapes (axial ratios b/a=0.1,0.2,5,10) being studied. Thermodynamic, structural and dynamical properties (e.g. diffusion coefficients) in the nematic phase have been examined.

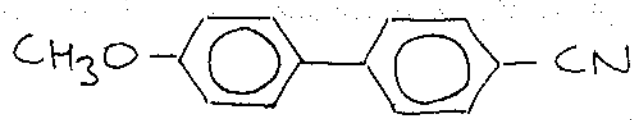
A more recent project has investigated hard ellipsoids with three distinct axes (a, b, c with $a = 1$, $c = 10$ and $1 \leq b \leq 10$). For this system at shapes intermediate between rod-like and plate-like, a biaxial phase intervenes between nematic and discotic. There is a crossover shape at which the system passes directly from isotropic to biaxial liquid crystal, at a bicritical point. An investigation of the phase diagram by Monte Carlo has shown the extent of this biaxial phase, and approximately located the bicritical point.

Other work involves the molecular dynamics simulation of linear rigid and flexible hard atomic chains, in collaboration with Mark Wilson. Part of the interest is in determining the effect of flexibility on the stability and properties of the nematic phase.

Mark Wilson suggested a simple six-sphere linear model of the relatively short molecule (a) below while Geoffrey Luckhurst suggested that compound (b), or alternatively perhaps p-terphenyl, would be worth modelling in this way.

Geoffrey Luckhurst briefly mentioned his work on the Lebwohl-Lasher

(a) 

(b) 

lattice model and its biaxial extension, which forms both uniaxial and biaxial nematic phases. These types of model were further discussed with Doug Cleaver and Mike Allen over tea, as they were not thought to be of general interest, although this situation will change with recent claims by experimentalists to have observed biaxial nematics. He then turned to the Gay-Berne potential, which is a phenomenological extension of the flawed Berne-Kushick-Pechukas potential. This is a 12-6 form with configuration-dependent well-depth and distance parameters. The shape is essentially that of a prolate ellipsoid of revolution. With a slightly modified version of the original potential, molecular dynamics simulations of an $N = 256$ system have produced, on cooling, nematic, smectic-A, and smectic-B phases before crystallization. Further work involves the linking together of Gay-Berne units into a flexible dimer, and the study of disc-like analogues which form a columnar phase. Much of the discussion centred around the choice of potential parameters, and in particular the ratio $\epsilon_{\parallel}/\epsilon_{\perp}$. Historically this has been taken to be 5, but an estimate based on site-site interactions for *p*-terphenyl suggests that $\epsilon_{\parallel}/\epsilon_{\perp} \approx 30$ is more realistic. However, in a simulation this value produces a slab-like configuration of molecules almost immediately. A general problem in estimating potential parameters of this kind is that nematogens are typically biaxial, and this biaxiality must be projected out of the potential.

Bill Palke then described his efforts to compute the thermodynamic parameter

$$\gamma = -\left(\frac{\partial \ln T}{\partial \ln V}\right)_{\overline{P_2}} = -\frac{(\partial \overline{P_2}/\partial \ln V)_T}{(\partial \overline{P_2}/\partial \ln T)_V}$$

by computer simulation. Simulated γ values can be compared with the experimental measurements of Jim Emsley and Geoffrey Luckhurst: values of $\gamma \approx 4$ are observed. The Gay-Berne potential was employed, $\overline{P_2}$ measured at various state points, and the required derivatives calculated from these measurements. Molecular-field theory suggests that γ is sensitive to the repulsive power of the potential: $\gamma \approx 4$ would imply $v(r) \propto r^{-12}$. In fact simulation gives $\gamma \approx 9$ from the above expression. However, the same simulation results give $\gamma \approx 0.5$ if the theoretically equivalent fluctuation expression (involving correlations of P_2 with the virial and the energy) is used. Simulations were also conducted using a modified Gay-Berne potential, obtained by replacing the repulsive part of the 12-6 Lennard-Jones form by an 18-6 form, smoothly

joined onto the attractive part of the 12-6 potential at the minimum. This dramatically raised the isotropic-nematic transition temperature, but seemed to have no effect on γ.

Dominic Tildesley then described simulations of Langmuir-Blodgett films using various models of stearic acid molecules. This system poses many of the same problems seen in simulations of liquid crystals: simulations are quite expensive, there are slow collective molecular motions, and orientational ordering is of interest. It was found that the representation of the chain using united CH_3 and CH_2 'atoms' was unrealistic. In studying tilt-angle transitions it was important to make the H atoms explicit. Typical system sizes in this work were $N = 64$ molecules per layer each of ~ 50 atoms, and run lengths of ~ 300 ps (consuming typically 40–60 hours on the CRAY) were needed. The point was made that some simulation 'packages', particularly those which used classical harmonic springs for bond stretching, were unsuitable for this kind of work.

Mark Wilson then described his work in which a realistic model of CCH5 was employed in a lengthy molecular dynamics simulation, attempting to establish a stable nematic phase. Run lengths of at least 200–500 ps seemed to be necessary, and this made the whole business very expensive. Looking from the chemist's viewpoint, the goal of rationalizing the large effect on nematic stability and properties which result from small changes in molecular structure was seen as quite a challenge. In the discussion it was recognized that the physical effect might be small (for example a shift in transition temperature) but the consequences for relative stability of two phases could easily be dramatic.

Following on from these discussions, it was decided that a workshop in this area would be very timely, and that the NATO Advanced Research Workshop format, involving typically ~ 30 participants from different countries, would be most suitable. The workshop could take place in 1991, at a venue to be decided, and it would be organized by Dominic Tildesley and Geoffrey Luckhurst. If funding from NATO was not forthcoming, CCP5 would be asked to consider sponsoring such a meeting.

MOLECULAR DYNAMICS ON PARALLEL COMPUTERS

The Molecular Modelling Transputer Applications Community Club (MMTACC) recently organised a one day seminar at the Rutherford Appleton Laboratory where five invited speakers described their work on molecular dynamics. The audience participated in a discussion on the aims of the club and future activities.

G.S.Pawley, gave an exciting paper describing his work at Edinburgh University on combining hetero architectures, using each where they were most appropriate on applications to simulation of a molecular lattice gas and the modelling of hydrodynamics of liquids using cellular automata. The DTI and the SERC are supporting a project at the Edinburgh Parallel Computer Centre to make a fast interface between two types of parallel computer, the AMT Distributed Array processor, and the Meiko Computing Surface. The use of the High Performance Parallel Interface, (HiPPI), means that the results will be applicable to a range of parallel hardware, not just to the two particular machines.

Monte Carlo methods are used in work on the Ising model. In the molecular lattice gas two atoms touch to form a molecule, a process favoured by the term in the Hamiltonian describing the system. When more than 2 atoms are joined, they form an aggregate, and this is discriminated against. There is a chemical potential which acts like pressure. Increasing it, forces the molecules together to form first crystallites, then aggregates. Generation of the configurations is an ideal operation for the DAP, but their subsequent analysis is better done on the Meiko Computing Surface.

Another project combines a lattice gas simulation of a polymer diffusing into a liquid modelled with cellular automata. The liquid is modelled on a hexagonal grid with automata which move between the grid nodes. This work is ideal for the DAP, to model the basic cellular automata operations for the liquid. However, the collisions of the polymer molecules with those of the liquid must obey the laws of conservation of energy and momentum. This calculation is better done on the transputers, since the energy and momentum have to be redistributed over the large molecule, which is not a local operation. There are problems of synchronisation of the two machines; these may be overcome by running two separate simulations concurrently, interleaving their usage of the two different machines.

P.Adams from the Department of Biochemistry, Edinburgh University, described work on molecular dynamics on the Meiko Computing Surface. He is studying proteins to try to find an effective inhibitor to the process which enables some bacteria to become resistant to penicillin. The substrate has been modelled into the active site using computer graphics, but energy minimisation is needed to determine the global substrate minimum. The FORTRAN source of the GROMOS87 program has been mounted on a transputer farm and energy minimisation run on 32 processors simultaneously but so far only local minima found. In another approach a parallel implementation of GROMOS has been made, using 2 rings of transputers, one for bonded, the other for non-bonded force calculations. He reported that programs which previously took 900 seconds for one time step on a VAX 11/750 now took only 22 seconds on the transputer system. He also mentioned EGO, the system built by Schulten et al. at the University of Illinois with special hardware containing a systolic ring of transputers for use on molecular dynamics problems.

A.Raine, from the NMR Group at Cambridge University, is working on methods of determining protein structures, where simulation is an important tool used with X-Ray and NMR methods of finding structures of biological macromolecules. SLS-PRO has been written in Occam II to run on a Meiko computing surface. A spherical distance cut off is imposed to reduce the amount of computing needed for each time step; adjacent residues are calculated on adjacent processors, which can introduce load balancing problems.

S.L.Fornili, University of Palermo, described his work on the hydrogen bond pathways which develop in liquids, for example in water containing ions such as ammonium or hydroxyl ions. These calculations were initially done on

computers such as a Vax 11/750 or a CRAY in Bologna, but the Vax was too slow and it was too difficult to get the data into the CRAY via the network, so they now use a more cost effective array of transputers hosted by an IBM PC-AT microcomputer with an Inmos B007 graphics board. The program has been written in Occam II to simulate the two dimensional spinodal phase separation of a large Lennard-Jones system with over 7000 particles. It uses geometric decomposition and includes a distributed dynamic load balancer. Plots of the state of the systems were shown at several time periods up to 450 pico seconds from the starting position. The execution time for a single time step (.01ps) on a Vax11/750 was 26seconds, on a single T800 transputer using sequential FORTRAN it was 14 seconds, but using parallel programming in Occam on 26 T800 transputers it was only 0.43 seconds.

The last speaker, U.C.Klump, Shell Thornton Research Labs, spoke on the simulation of organic liquids. He is interested in the elasto-hydrodynamic properties of lubricating oils between fast moving metal parts. These oils form thin films. Experimental measurements are exremely difficult so computer simulations are the best way to understand and and improve the lubricating action. He models the shear viscosity of the liquid, with sliding boundary conditions, on an array of 36 T800 transputers, with colour displays on an associated SUN workstation. A box of liquid containing 10,000 atoms is divided into columns, and each assigned to a transputer, which holds lists of all the atoms in the column and of their neighbours in the liquid. The forces between pairs of atoms in each column are calculated, the columns sheared, the lists updated and the forces recalculated. The bending and torsional stress on each atom are calculated and hence they find the parts of the molecule which contribute most to the stress. These are the parts which would need to be changed when new lubricants are designed able to withstand higher shear stress.

The MMTACC is supported by the 'Transputer Initiative', which has joint funding from the UK Science and Engineering Research Council and the Department of Trade and Industry (DTI). It aims to provide better information for the community by organising seminars, a software library, a bibliography, a directory of members interests, an electronic bulletin board, demonstrators of molecular modelling for the 'Transputer Initiative', and better liaison with suppliers and other computing research activities in molecular modelling. The 'Transputer Initiative' publishes a monthly mailshot with details of new hardware, software, meetings etc. We welcome further contributions to our bibliography, please send them to the address below, from which a copy of the current bibliography can be obtained.

The next 'Transputer Initiative' meeting is planned for 21 November 1990 at the University of Edinburgh, on the topic, 'Graphics and Transputers'. This topic was suggested by members of MMTACC who have found it much more difficult to move the graphics than the molecular modelling. Speakers include Roger Hubbold, University of Manchester, on 'Graphics Standards and parallel computers', David White, University of Glasgow, who will describe his general graphics library, Terry Barnaby, Beam Ltd, describing 'An implementation of X-Windows for transputers' and we are hoping a speaker from the Edinburgh Parallel Computing Centre will describe 'Molecular graphics and the Illinois molecular modelling code on the Meiko computing Surface'. There will be an opportunity to visit the Edinburgh Parallel Computing Centre after the meeting. Will those interested please let the Chairman know (GSP@uk.ac.edinburgh), and indicate any particular interests they may have. Further details from the address below.

Membership of MTACC is free and open to anyone interested in molecular modelling, to join please contact: Mr T Mawby, Building R1, SERC/DTI Transputer Initiative, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX tel (0235) 445787 or e-mail MMTACC@uk.ac.rl.inf

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Molecular Modelling on Transputers References

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C-language Program for the Irregular Close Packing of Hard Spheres

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Abstract

The paper presents a C-language program for irregular close packing of equal hard spheres in a cubic box with periodic boundary conditions using Jodrey and Tory's algorithm [1,2,3]. For the nearest neighbour searching of a given sphere the link-cell method is applied. The program has been developed for microcomputers / workstations so that it incorporates the sequential algorithm optimized for computational time demands.

PROGRAM SUMMARY

Title of the program : NSCP3D

Computer : (a) IBM PC/AT clone with 80287 "FAST" (10MHz)
(b) DSI-020 board (MC68020/68881, 12.5MHz)
for IBM PC/XT-AT and clones (Definicon Systems, Inc.)
(c) AT 386 with 80387 (20MHz)
(d) Monoputer-2 board (T800, 20MHz)
for IBM PC/XT-AT and clones (MicroWay, Inc.)

Installation : Institute of Computer Science, AGH, Cracow, Poland

Operating system : (a) PC DOS v3.10
(b) PC DOS - DSI-020 Loader interface (v8.10-P)
(c) PC DOS v3.30
(d) PC DOS - Monoputer-2 Alien File Server (afserver) v1.3

Programming language used : C [1]

High speed storage required [2] : about 350 kB

Peripherals used : disk, lineprinter

No. of instructions in program and test deck : 5029 of program
58 of test data

[1] As defined in [4]

[2] For 4000 spheres and parameters of the test run

Keywords : irregular close packing, linked-list, chaining mesh.

Nature of physical problem
The program can be used to simulate the irregular close packing of equal hard spheres in a cubic box with periodic boundary conditions, starting from the ensemble of randomly distributed points taken as initial positions of the sphere centres.

Method of solution
The equal hard spheres are packed using Jodrey and Tory's algorithm [1,2,3]. Periodic boundary conditions are applied to make the system pseudo-infinite. In each iteration the worst overlap between spheres is eliminated by moving the spheres along a line joining their centres. Simultaneously the sphere diameters are modified according to actual system configuration. The linked-list structures [3,5] speed-up the nearest neighbour searching and the worst overlap determination. Final results as diameter of the spheres and related packing density as well as coordinates of the sphere centres are optionally saved for further analysis.

Restrictions on the complexity of the problem
The program is suitable for several thousand of spheres.

Typical running time
The overall program execution time obtained on different kinds of microcomputers is shown in Table 1. The presented timings correspond to the program runs in which the final packing density is about 0.62 and have been obtained using the following compilers
(a) Turbo C (v2.0)
(b) SVS C (v2.6)
(c) Turbo C (v2.0)
(d) 3L C (v2.0)

No. of	Program execution time [s]				Execution time per sphere [s]			
spheres	DSI-020	PC/AT	T800	AT 386	DSI-020	PC/AT	T800	AT 386
32	33	81	10	22	1.03	2.53	0.31	0.69
108	113	277	28	74	1.05	2.56	0.26	0.68
256	259	636	68	172	1.01	2.48	0.26	0.67
500	503	1221	135	337	1.01	2.44	0.27	0.67
864	866	2126	221	575	1.00	2.46	0.25	0.66
1372	1376	3374	362	921	1.00	2.46	0.26	0.67
2048	2073	5073	530	1373	1.01	2.48	0.26	0.67
2916	2977	7288	752	1964	1.02	2.50	0.26	0.67
4000	4164	10265	999	2727	1.04	2.57	0.25	0.68

Table 1: Typical timings for NSCP3D program.

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LONG WRITE-UP

1 Introduction

Irregular packing of hard spheres, also known as random close packing, has been extensively studied due to its importance as models for particulate systems in a wide variety of fields. The sphere packing problem is found in many domains of engineering, for example metallurgy, ceramics, soil science, physics, chemistry, etc. Equal, randomly packed spheres have also been suggested as models for liquid and glassy states [1,2].

The program NSCP3D (Neighbour Separation Close Packing in 3D) is designed for close irregular packing of equal hard spheres in a cubic box with periodic boundary conditions. The applied algorithm is described in the literature [2,3] and is based on the existing FORTRAN program of Jodrey and Tory [4]. However, contrary to the original code, our program is written according to specified methodology, close to that of the standard programming system OLYMPUS [5,6,7]. The standardization of the program structure, making it modular and mostly independent of the computer system speeds up the construction of the program and facilitates its further modifications. The program is provided with restart and on-line data saving facilities as well as with semigraphical lineprinter output and data control possibility. The overall program efficiency is increased due to careful optimisation of the most time-consuming procedure. The program is suitable for the PC/workstation environment thus is optimized for computational time demands. It is written in the C language as defined in [8].

The program determines final positions of the sphere centres as well as the final sphere diameter and corresponding packing density. Projections of final positions of the sphere centres as well as radial and angular distribution functions are calculated and plotted on the lineprinter.

2 Method description

2.1 Basic principles

The program generates the irregular close packing of N equal hard spheres in a cubic box of the volume $V = L^3$. The initial system configuration is a set of N randomly distributed points representing initial positions of the sphere centres. Each sphere has two diameters, inner and outer ones, which approach each other during the simulation. When the diameters attain equal values the program stops. The inner diameter d_{in}^n defines the actual packing density and is set after the n-th iteration to minimum center-to-center distance between any two spheres

$$d_{in}^n = \min r_{ij}^n, \quad i,j = 1,\ldots,N, \quad i \neq j \tag{1}$$

where $r_{ij}^n = |\vec{r}_i^{\,n} - \vec{r}_j^{\,n}|$ is the distance between spheres i and j. The outer diameter d_{out}^n is set initially to the value d_{out}^0, which yields a nominal packing density $\eta = 1$

$$d_{out}^0 = 2\,L\left(\frac{3\eta}{4\pi N}\right)^{1/3}. \tag{2}$$

In each iteration the outer diameter is reduced using a contraction rate τ

$$d_{out}^{n+1} = d_{out}^n - \left(\frac{1}{2}\right)^6 d_{out}^0/(N\tau), \tag{3}$$

$$\delta = \lfloor -\log_{10} \Delta\eta \rfloor, \tag{4}$$

where

d_{out}^n – outer diameter in the n-th iteration,

$\Delta\eta$ – difference between the nominal (based on the outer diameter) and actual (based on the inner diameter) packing densities,

τ – contraction rate of the outer diameter,

$\lfloor \cdot \rfloor$ – greatest integer function.

The outer spheres (contrary to the inner ones) can intersect each other. In each step the worst overlap between the spheres i and j is eliminated by moving their centres according to the following transformation

$$\vec{r}_i^{\,n+1} = \vec{r}_i^{\,n} + \frac{1}{2}\left(d_{out}^{n+1} - r_{ij}^n\right)\frac{\vec{r}_{ij}^{\,n}}{r_{ij}^n}, \tag{5}$$

$$\vec{r}_j^{\,n+1} = \vec{r}_j^{\,n} - \frac{1}{2}\left(d_{out}^{n+1} - r_{ij}^n\right)\frac{\vec{r}_{ij}^{\,n}}{r_{ij}^n}, \tag{6}$$

This ensures $r_{ij}^{n+1} = d_{out}^{n+1}$.

The system is made pseudo-infinite by application of classical periodic boundary conditions together with the minimum image technique [9].

2.2 Numerical scheme

In the program two lists are applied to speed-up the nearest neighbour searching and the worst overlap determination. The first one, sorted-list, keeps the spheres in increasing order of distances to their nearest neighbours. The first element of the sorted-list indicates the pair of the closest spheres in the ensemble, which is to be taken for processing in the current iteration. The second one, called linked-list, sorts the spheres according to the coordinates of their centres. It is used to locate the spheres with centres lying within a specified cutoff radius. Detailed description of the list structures is given below.

2.2.1 Nearest neighbours storage – the sorted-list

For intersecting pairs of outer spheres, (i,j), center-to-center distances, called "rods", are calculated. Due to the computational time savings the rods are stored in the sorted-list in order of increasing length of distances, up to the maximal value d_{max} corresponding to the packing density η_{max}

$$d_{max} = 2\,L\left(\frac{3\eta_{max}}{4\pi N}\right)^{1/3} \tag{7}$$

To ensure $d_{max} \geq r_{ij}$ for any neighbouring spheres i and j, the value of η_{max} should be greater than any attainable true value. Thus in the program η_{max} is equal to the maximal packing density in 3D, i.e. $\pi\sqrt{2}/6$ ($\simeq 0.7405$).

In order to speed up of the list processing the sorted-list is split into E parts, pointed by E separate entries. Each entry point indicates a list of rods from the related interval of distances.

The pair of spheres (i,j) separated by the distance r_{ij} belongs to the list indicated by the e-th entry point defined as follows

$$e = \left\lfloor E \frac{r_{ij}^2}{d_{max}^2} \right\rfloor \tag{8}$$

$SH(e)$ is the sorted-list table entry. A zero value of $SH(e)$ indicates that there are no rods from the related interval of distances, while another entry gives the number of the first sphere in the e-th list. The link coordinate of a sphere, $SL(i)$, either gives the number of the next sphere in the list or is equal to 0 to indicate the end of the list. Similarly the inverse link coordinate $SLI(i) > 0$ means the number of the previous sphere. If i is the first sphere in the list (i.e. $SH(e) = i$) then $SLI(i) \leq 0$ and its absolute value indicates the related entry point (i.e. $SLI(i) = -e$). Additionally the $NN(i)$ table entry contains the number of the i's nearest neighbour while the squared distance between i and $NN(i)$ is stored in $D(i)$. Under these assumptions the procedure for inserting the sphere i into the sorted-list together with its nearest neighbour $j = NN(i)$ can be summarized in the following steps

(a) determine the sorted-list entry point e according to (8)
(b) find the two subsequent spheres i_p and i_n
for which $SL(i_p) = i_n$ and $D(i_p) \leq r_{ij}^2 < D(i_n)$

```
i_n := SH(e)
i_p := -e
while (i_n > 0 and D(i_n) ≤ r_ij^2) do
    begin
    i_p := i_n
    i_n := SL(i_n)
    end
```
(9)

(c) place the sphere i between spheres i_p and i_n

```
if (i_n > 0) then SLI(i_n) := i
SLI(i) := i_p
if (i_p > 0) then SL(i_p) := i
else SH(e) := i
SL(i) := i_n
NN(i) := j;  NN(j) := -i
D(i) := r_ij^2
```

The method of sphere relocation may introduce new overlaps or may change or eliminate others. Thus a rod corresponding to the pair of spheres (i,j) is only placed in the sorted-list if the distance r_{ij} could not be changed by the elimination of a greater overlap (i.e. j has no closer neighbours than i),

$$(\forall k = 1,\ldots,N, k \neq i, k \neq j)(r_{kj} > r_{ij}). \tag{10}$$

Subject to this restriction rods are added to and removed from the sorted-list in each step of the simulation.

2.2.2 The nearest neighbour determination — the linked-list

The nearest neighbour of each sphere is searched only inside a specified cutoff radius r_{cut} which is initially set to the value

$$r_{cut} = 0.666 \cdot d^0_{out} \tag{11}$$

If the number of rods l queued for processing in the sorted-list is less than a specified value l_{min}, the cutoff radius is increased [4].

$$r_{cut} := r_{cut} \left(\frac{11\, l_{min}}{10\, l_{min} + l} \right)^{(d^n_{out} - d^n_{in})/d^n_{out}} . \tag{12}$$

For the nearest neighbour searching of a given sphere, the chaining mesh is introduced as a regular lattice of $M \times M \times M$ cells covering the computational box, together with the link-cell method [4,10,11]. Ranges of the computational box side lengths are $[0, M]$ in each direction (i.e. $L = M$), thus the cell indices calculation for the particular sphere is done by simple substitution of the sphere centre coordinates $r_{i\alpha}$ into the cell coordinates c_α. If $LH(c)$ is the head-of-chain table entry for chaining cell c and if $LL(i)$ and $LLI(i)$ are the forward and backward link coordinates for the sphere i then the procedure for inserting the sphere i to the linked-list with respect to the ranges of the computational box side lengths can be summarized as follows

$$\begin{aligned}
&c_\alpha := \lfloor r_{i\alpha} \rfloor \\
&c := M^2 \cdot c_x + M \cdot c_y + c_z \\
&i_f := LH(c) \\
&\underline{\text{if}}\ (i_f > 0)\ \underline{\text{then}}\ LLI(i_f) := i \\
&LL(i) := i_f \\
&LH(c) := i \\
&LLI(i) := -c
\end{aligned} \tag{13}$$

Tables for the list handling are set up to zero at the beginning of the algorithm. The linked-list is organized in the similar way to the sorted-list. Namely, a zero $LH(c)$ table entry indicates the empty cell c while $LL(i) = 0$ means the end of the list. For the first sphere in the list the $LLI(i)$ element is less than or equal to 0 and its absolute value points to the appropriate cell address in the LH table.

In an usual approach to the link-cell method the length of the elementary cell side of the chaining mesh is greater than or equal to the cutoff radius. As a consequence the only 26 neighboring cells of the current one are considered in the neighbours searching. Since in the algorithm the cutoff radius depends on the current arrangement of the spheres and can be changed from one step to another (Eq. 12) this assumption is no longer valid. Thus in this case another approach is proposed in which the numbers of cells taken into account are determined for each sphere separately. They form a minimal cuboid (with ranges $[c_{l\alpha}, c_{u\alpha}]$) containing all spheres with centres lying within r_{cut}. The values $c_{l\alpha}$ and $c_{u\alpha}$ for the sphere i are then calculated in the following way

$$\begin{aligned}
c_{l\alpha} &= \lfloor (r_{i\alpha} - r_{cut}) + L \rfloor, \\
c_{u\alpha} &= \lfloor (r_{i\alpha} + r_{cut}) + L \rfloor.
\end{aligned} \tag{14}$$

To transform the cell indices $c_\alpha \in [c_{l\alpha}, c_{u\alpha}]$ to the effective cell number c three tables, T_x, T_y, and T_z, are applied, set-up to the values

$$\begin{aligned} T_x(c_x) &= M^2 \cdot \mathrm{mod}\,(c_x, M), \\ T_x(c_y) &= M \cdot \mathrm{mod}\,(c_y, M), \\ T_x(c_z) &= \mathrm{mod}\,(c_z, M). \end{aligned} \tag{15}$$

Then the effective cell number c can be determined by the simple addition of the suitable elements of T_x, T_y, and T_z

$$c = T_x(c_x) + T_y(c_y) + T_z(c_z). \tag{16}$$

2.2.3 Optimization of the nearest neighbour searching

The periodic boundary condition (PBC) displacements are usually introduced using two conditional statements for each direction [4,9]. Contrary to the origin [4], in the presented program the PBC displacements are stored in the PBC table, which is set up to the following values

$$PBC(c_\alpha) = \begin{cases} L & \text{for} \quad c_\alpha \in [1,\ M-1], \\ 0 & \text{for} \quad c_\alpha \in [M,\ 2\,M-1], \\ -L & \text{for} \quad c_\alpha \in [2\,M,\ 3\,M-2]. \end{cases} \tag{17}$$

Knowing boundaries of the cells it is easy to check in what direction, if any, the PBC displacements should be introduced. It allows to specify eight kinds of the most time-consuming loop represented by subsequent program blocks

(a) determine the kind of the loop

$$\begin{aligned} &\underline{\text{if}}\ (T_\alpha(c_{u\alpha}) > T_\alpha(c_{l\alpha}))\ \underline{\text{then}}\ mic_\alpha := 0 \\ &\underline{\text{else}}\ mic_\alpha := 1 \\ &mic := 4\,mic_x + 2\,mic_y + mic_z \end{aligned}$$

(b) perform the appropriate loop resulting from mic

```
case mic of                                   (18)
    0 : loop with no PBC
    1 : loop with PBC in z direction
    2 : loop with PBC in y direction
    3 : loop with PBC in y and z directions
    4 : loop with PBC in x direction
    5 : loop with PBC in x and z directions
    6 : loop with PBC in x and y directions
    7 : loop with PBC in x, y, and z directions
```

The loop for finding the nearest neighbour j of a sphere i (Eq. 19) is executed over all cells determined by the values of $c_{l\alpha}$ and $c_{u\alpha}$. The addition of the $PBC(c_\alpha)$ table element enclosed in square brackets ([ ], Eq. 19) is optional and depends on the particular loop kind (see Eq. 18). In such an approach consisting of the eight kinds of the loop and the PBC displacements storage, significant (about 30%) increase of the overall program efficiency is achieved [12] as compared with the single loop and conditional statements application as in [4].

```
r²_min := r²_cut;  j := 0
for c_x = c_lx to c_ux do
    for c_y = c_ly to c_uy do
        for c_z = c_lz to c_uz do
            begin
            c := Σ_α T_α(c_α)
            k := LH(c)
            while (k > 0) do
                begin
                r_ikα := r_iα − r_kα [+PBC(c_α)]                    (19)
                r²_ik := Σ_α r²_ikα
                if (r²_ik < r²_min) then
                    begin
                    r²_min := r²_ik
                    j := k
                    end
                k := LL(k)
                end
            end
```

2.2.4 Summary of one iteration step

One iteration step of the program can be summarized in the following way :

1. Determine the pair of the closest spheres i, j in the ensemble, i.e. take the first element from the sorted-list.
2. Reduce the outer diameter d_{out} (Eqs. 3-4).
3. Remove the spheres i and j from the sorted- and linked-lists.
4. Check the number of rods l in the sorted-list and, if necessary, modify the cutoff radius according to (12).
5. For spheres i and j do :
   (a) relocate the sphere according to (5,6),
   (b) find the nearest neighbour of the sphere, (Eqs. 18,19),
   (c) place the sphere into the linked-list as in (13),
   (d) if the nearest neighbour of the sphere is found fulfiling the condition (10) place the sphere into the appropriate position of the sorted-list according to (9).

If in any step the sorted-list is exhausted (i.e. if $l = 0$) or if the inner diameter exceeds the outer one, a new calculation cycle is performed. At the beginning of each cycle the sorted- and linked-lists are rebuilt in respect to actual system configuration. While this procedure leads to the convergence criterion of the algorithm, i.e.

$$d_{out}^n \leq d_{in}^n, \tag{20}$$

the program stops and the value of d_{in} determines the final packing density.

2.3 Projections of the sphere centres

Graphical representation of the three-dimensional structures is made by drawing projections on the $(x-y)$, $(x-z)$, and $(y-z)$ planes of all spheres whose centres are contained within a given range of z, y, and x respectively. Two kinds of projections are also available :

1. characters on the projection plane $(0,1,2,\ldots,J,K)$ correspond to relative sphere heights in the selected layer (thickness of the layer should be less than the sphere diameter to avoid the sphere centres overlaps on the projection).

2. characters on the projection plane represent the numbers of spheres with coordinates from the corresponding interval (in this case all spheres from the computational box may be considered),

2.4 Radial distribution function

The program can calculate and plot on the lineprinter the radial distribution function on a basis of the final positions of sphere centres. Consider a typical central sphere. Let $N(r,\Delta r)$ be the average number of spheres with centres at a distance between $r-\frac{1}{2}\Delta r$ and $r+\frac{1}{2}\Delta r$. The radial distribution function $g(r)$ is then defined by

$$g(r) = \frac{V}{N}\cdot\frac{N(r,\Delta r)}{4\pi r^2\Delta r}, \tag{21}$$

and is determined for $0 \le r \le \frac{1}{2}L$.

2.5 Distribution of angles between spheres

The distribution of angles between final positions of the sphere centres can also be calculated and plotted together with the rdf. Let i be the chosen central sphere. Then we calculate the angles between all pairs of vectors $\vec{r}_{ij}$, $\vec{r}_{ik}$ for which

$$r_{ij} < \gamma\, d_{out},\quad r_{ik} < \gamma\, d_{out}, \tag{22}$$

where $\gamma > 1$ is an arbitrary chosen coefficient.

If $N(\beta,\Delta\beta)$ is a number of angles between $\beta-\frac{1}{2}\Delta\beta$ and $\beta+\frac{1}{2}\Delta\beta$, we can define the angular distribution function $a(\beta)$

$$a(\beta) = \frac{N(\beta,\Delta\beta)}{N}, \tag{23}$$

for $0 \le \beta \le \pi$.

3 Structure of the program

3.1 Introduction and top level procedures

The structure of the program in the sense of procedure calls is similar to the OLYMPUS system standard [5,6,7], with slight modifications resulting from unique properties of the program.

The full index of the procedures (together with their brief functional description) and external variables of the program (listed in external blocks and alphabetically) is given in the program comments.

The main program < 0.0 > contains descriptive comments and controls the calculations by calling appropriate functions (< 0.1 >–< 0.3 >). Procedure < 0.1 > *basic* initializes the basic program data defining the program operation mode and output form, while the < 0.2 > *modify* changes those presumed values if necessary according to the user-prepared data input file. The procedure < 0.3 > *control* controls the run by calling functions from the rest of classes (1-4) subject to the new or restart run.

3.2 Initialization procedures

The first class of procedures is the initialization one and is devoted to establishing the system configuration and parameters. In the procedure < 1.1 > *label_run* some run identification labels are introduced. Procedure < 1.2 > *preset* initializes program external variables needed to specify the run conditions. They can be modified in the < 1.3 > *data* procedure.

On the basis of the established program parameters the auxiliary values are calculated in the < 1.4 > *auxiliary_val*. In the procedure the tables T_α for cell indices transformation and the PBC table containing PBC displacements are allocated and filled. In a case of the new run the remaining program arrays are also allocated.

In each new run the < 1.5 > *initial* function is invoked to set up the initial system configuration. It is done either by using the < *U*.10 > *ran* utility function for random numbers generation (section 1.1), or by reading the system configuration from the user-prepared external file (section 1.2). While the restart run is assumed the < 1.6 > *resume* procedure is involved (instead of < 1.5 > *initial*), to restore the sphere configuration and other program parameters from the external file. The procedure < 1.7 > *start* builds up the initial versions of the sorted- and linked-lists according to the actual system configuration (section 2). In section 3 it also determines initial values of the inner diameter and related packing density.

3.3 Step on the calculation

The < 2.1 > *stepon* function is executed once in each simulation step. Its section 1 determines the two nearest spheres in the ensemble while the section 2 separates them according to Eqs. (5,6). While sphere coordinates modification the periodic boundary conditions are applied (sections 2.6.1 and 2.6.2). Then *stepon* calls < 2.2 > *min_separation* for both of the spheres separately (see sections 2.6.1 and 2.6.2) and determines their nearest neighbours. In sections 2.7-2.9 the actual and nominal packing densities are calculated as well as the final packing density estimated.

Procedure < 2.2 > *min_separation* in its section 2 finds the nearest neighbour of the particular sphere according to the scheme presented in Eqs. (18,19). In section 3 the sphere is placed into the linked-list as given in Eq. (13) while in the section 6 the sphere is inserted to the appropriate place in the sorted-list together with its nearest neighbour (according to (9)).

3.4 Output of the program and utility procedures

The < 3.1 > *output* function handles the main output of the program and it is called at different points as necessary, providing initialization, cycle, periodic and final output. Its additional feature is to make intermediate and final savings of program results to external files. Semigraphical lineprinter output is provided for projection drawing, arranged by < 3.2 > *projection* together with < 3.3 > *proj_draw* procedures, as well as radial and angular distribution functions control

(< 3.4 > *sphere_distrib*) computing (< 3.5 > *distrib_calcul*) and plotting (< 3.6 > *plot*). Some examples of projections as well as rdf and adf graphs produced by the program are presented in Figures 1-3 respectively.

The procedure < 4.1 > *test_end* tests the program convergence criterion (20), while < 4.2 > *end_run* closes program external files and frees allocated memory.

Procedures marked with "U" are utilities used for simple input/output, debugging, system date and time determination, pseudo-random numbers generation, etc.

The detailed description of the program external files, data input formats and methods for dealing with the program is given in the Manual.

4 Acknowledgements

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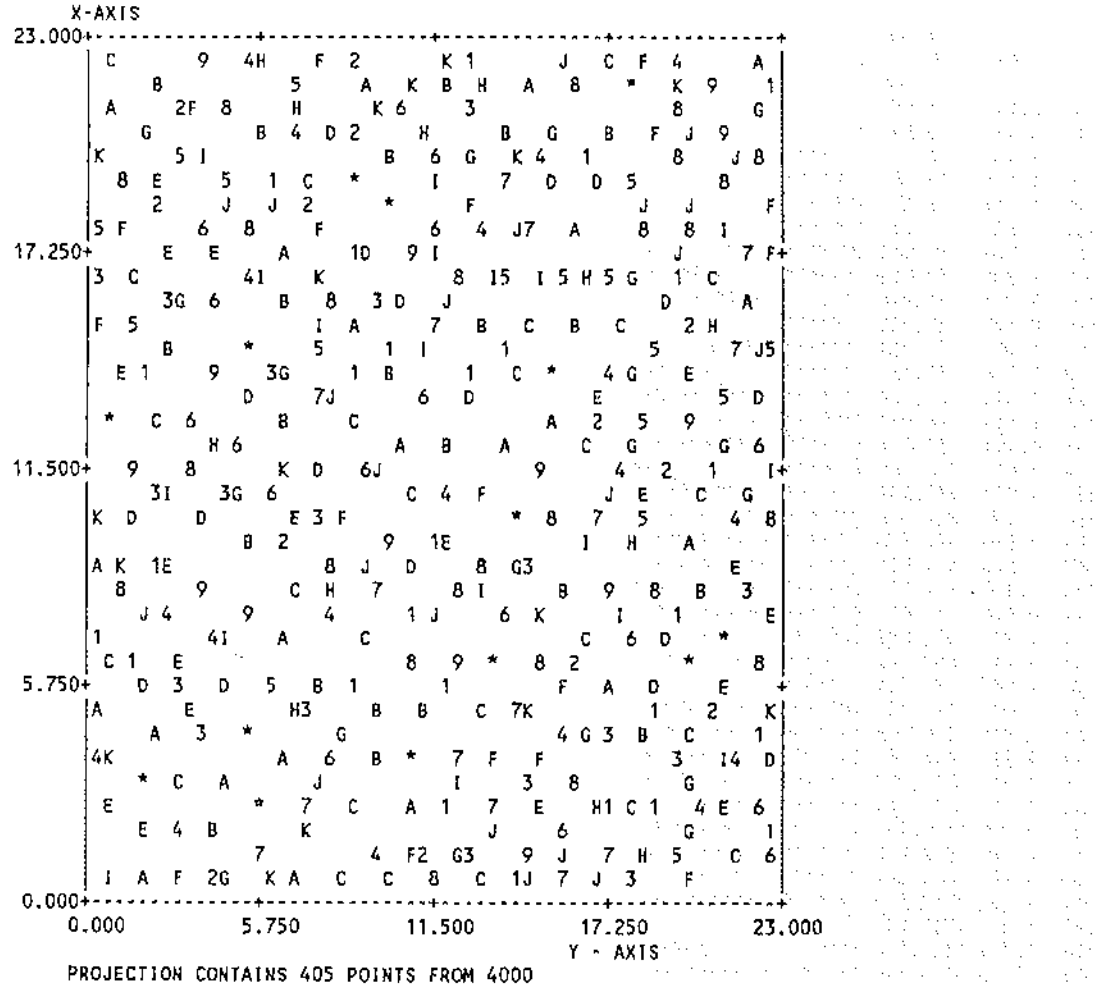

Fig.1. Sample projection of the sphere centres in z direction; characters on the projection means the relative sphere centres heights in the selected layer; thickness of the layer $= 0.1L$.

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RADIAL DISTRIBUTION FUNCTION

R	RDF	INT RDF	0 1 2 3 4
0.144	0.000	0.000	*
0.431	0.000	0.000	*
0.719	0.000	0.000	*
1.006	0.000	0.000	*
1.294	0.000	0.000	*
1.581	3.074	4.564	**********
1.869	0.625	10.424	**********
2.156	0.526	13.172	**********
2.444	0.788	17.418	**********
2.731	1.298	25.962	**********
3.019	1.320	38.852	**********
3.306	0.770	50.992	**********
3.594	0.808	62.188	**********
3.881	1.067	77.931	**********
4.169	1.152	99.368	**********
4.456	1.011	123.179	**********
4.744	0.885	146.931	**********
5.031	0.961	173.212	**********
5.319	1.076	205.738	**********
5.606	1.042	243.268	**********
5.894	0.964	282.606	**********
6.181	0.956	324.176	**********
6.469	1.013	371.048	**********
6.756	1.037	424.357	**********
7.044	0.998	481.881	**********
7.331	0.977	542.482	**********
7.619	0.989	607.782	**********
7.906	1.020	679.741	**********
8.194	1.007	757.753	**********
8.481	0.996	840.468	**********
8.769	0.988	928.132	**********
9.056	1.001	1021.993	**********
9.344	1.011	1123.154	**********
9.631	0.999	1230.596	**********
9.919	0.996	1343.845	**********
10.206	0.996	1463.644	**********
10.494	1.004	1590.862	**********
10.781	1.004	1725.807	**********
11.069	0.998	1867.714	**********
11.356	1.00	2016.864	**********

Fig.2. Example of the RDF calculated and plotted by the program.

File: cpcfig3 Printed Sun Sep 09 23:04:57 1990 Page: 1

ANGLE DISTRIBUTION FUNCTION

ANG	ADF	COSINE	0 1 2 3 4 5 6 7
0.039	0.000	0.999	*
0.118	0.000	0.993	*
0.196	0.000	0.981	*
0.275	0.000	0.962	*
0.353	0.000	0.938	*
0.432	0.000	0.908	*
0.511	0.000	0.872	*
0.589	0.000	0.831	*
0.668	0.000	0.785	*
0.746	0.000	0.734	*
0.825	0.000	0.679	*
0.903	0.000	0.619	*
0.982	2.277	0.556	**********
1.060	6.529	0.489	**********
1.139	1.590	0.419	**********
1.217	1.173	0.346	**********
1.296	1.083	0.271	**********
1.374	0.952	0.195	**********
1.453	0.951	0.118	**********
1.532	1.014	0.039	**********
1.610	1.098	-0.039	**********
1.689	1.145	-0.118	**********
1.767	1.351	-0.195	**********
1.846	1.552	-0.271	**********
1.924	1.756	-0.346	**********
2.003	2.058	-0.419	**********
2.081	2.078	-0.489	**********
2.160	1.300	-0.556	**********
2.238	1.069	-0.619	**********
2.317	0.944	-0.679	**********
2.395	0.823	-0.734	**********
2.474	0.779	-0.785	**********
2.553	0.718	-0.831	**********
2.631	0.659	-0.872	**********
2.710	0.601	-0.908	**********
2.788	0.531	-0.938	**********
2.867	0.472	-0.962	**********
2.945	0.384	-0.981	**********
3.024	0.254	-0.993	**********
3.102	0.099	-0.999	**********

Fig.3. Example of the ADF calculated and plotted by the program.

C-language Molecular Dynamics Program for the Simulation of Lennard–Jones Particles

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Abstract

The paper presents a Molecular Dynamics C-language program suitable for mixtures of monoatomic molecules of different types included in a cuboid box with periodic boundary conditions. The molecules mutually interact with the short range Lennard-Jones potential. To solve the Newtonian equations of motion the leapfrog scheme is applied. Neighbors of a particular molecule are searched using the link-cell method. The program has been developed for microcomputers/workstations so that it incorporates the sequential algorithm optimized in respect with CPU-time.

Program Summary

Title of the program : MD3DLJ

Computer : (a) IBM PC/AT clone with 80287 (10MHz)
(b) DSI-020 board (MC68020/68881, 12.5MHz)
for IBM PC/XT-AT and clones (Definicon Systems, Inc.)
(c) AT 386 with 80387 (20MHz)
(d) Monoputer-2 board (T800, 20MHz)
for IBM PC/XT-AT and clones (MicroWay, Inc.)

Installation : Institute of Computer Science, AGH, Cracow, Poland

Operating system : (a) PC DOS v3.10
(b) PC DOS – DSI-020 Loader interface (v8.10-P)
(c) PC DOS v3.30
(d) PC DOS – Monoputer-2 Alien File Server (afserver) v1.3

Programming language used : C [1]

High speed storage required : about 500 kB [2]

Peripherals used : disk, lineprinter

No. of instructions in program and test deck : 6402 of program
79 of test data

[1] As defined in [1]

[2] For 2916 molecules and parameters of the test run

Keywords : molecular dynamics, monoatomic molecule mixture, Lennard-Jones fluid, link-cell method, leapfrog algorithm.

Nature of physical problem
The program can be used to simulate conventional constant energy/constant volume monoatomic molecule mixtures in 3 dimensions with short range interactions.

Method of solution
A system of monoatomic molecule mixtures of a few thousand of molecules is simulated. The Newtonian equations of motion are solved in a series of timesteps using the leapfrog algorithm [2,3]. At each timestep the force acting on each molecule is found according to Lennard-Jones short range interaction. To achieve computational time savings the link-cell method [4] is introduced together with other techniques [5] making the method of forces calculation more efficient. Periodic boundary conditions are applied to make the system pseudo-infinite. When the system is in thermal equilibrium, thermodynamic measurements are made by averaging over time. The system parameters such as coordinates and momenta of the molecules may be stored in chosen timesteps for further analysis.

Restrictions on the complexity of the problem
The program is suitable for several thousand of molecules.

Typical running time
The execution time per MD timestep of the simulation obtained on different kinds of microcomputers, is presented in Table 1. The timings have been obtained using the following compilers :
(a) Microsoft C (v3.0)
(b) SVS C (v2.6)
(c) Turbo C (v2.0)
(d) 3L C (v2.0)

No. of	MD timestep [s]				MD timestep per particle [s]			
particles	DSI-020	PC/AT	T800	AT 386	DSI-020	PC/AT	T800	AT 386
6912	145.0		23.05		0.021		0.0033	
5324	114.7		18.57		0.022		0.0035	
4000	89.4		14.82	51.68	0.022		0.0037	0.013
2916	61.2	203.4	9.74	34.32	0.021	0.070	0.0033	0.012
2048	44.7	149.7	7.30	25.32	0.022	0.073	0.0036	0.013
1372	31.7	107.8	5.40	18.30	0.023	0.079	0.0039	0.013
864	18.2	60.3	2.90	10.92	0.021	0.070	0.0033	0.013
500	11.2	37.7	1.88	6.85	0.022	0.075	0.0038	0.014
256	6.7	23.1	1.23	4.25	0.026	0.090	0.0048	0.017

Table 1: Timings for MD3DLJ program with *cube technique* (average values for first 100 steps of simulation).

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LONG WRITE-UP

1 Introduction

The current molecular dynamics simulation activity is FORTRAN oriented and emphasized on vector and parallel processing on large supercomputers. Due to large technological development however, a modest but reasonable simulation work can be done in other than FORTRAN languages and in microcomputer world evolving fast toward several MFLOPs on the desk.

With wide availability of personal computers and workstations C language becomes more and more popular. C is also the main language in large scientific projects in parallel processing like Caltech/JPL Concurrent Computational Projects [1].

MD3DLJ (Molecular Dynamics in 3D using Lennard-Jones potentials) is a program which applies the method of conventional constant energy/constant volume dynamics simulation to monoatomic molecule mixtures in which trajectories of the individual molecules are determined by numerical integration of the Newtonian equations of motion. Interactions between the molecules are described using the short range Lennard-Jones pair potential. Quantities calculated by MD3DLJ include the potential, kinetic and total energy, temperature and pressure of the system supported with their R.M.S. fluctuations, the radial distribution functions and the mean square displacements of the molecules. For further analysis it is possible to store the appropriate quantities (i.e. molecules coordinates and momenta) at successive time steps. The program is provided with restart and on-line save-data facilities improving reliability of calculations. The program is suitable for the PC/workstation environment thus is optimized for computational time demands. It is written in the C language as defined in [2].

2 Method description

2.1 Basic principles

The program simulates a system of N monoatomic molecules in a cuboidal box of volume V. The ensemble may consist of a number of species S (i.e. number of molecule kinds). Each species is characterized by the atomic mass, m_s, number of molecules, N_s, and kind of interaction with other molecules. Thus $N = N_0 + N_1 + \ldots + N_s + \ldots + N_{S-1}$. The molecules interact via a pair potential $u_k(r)$, where $r = |\vec{r}|$ is a distance between interacting molecules (i,j), $\vec{r} = \vec{r}_i - \vec{r}_j$, and k indicates a kind of potential depending on kinds of interacting molecules ($k = 0, \ldots, M-1$). Number of different kinds of the pair potential is $M = S(S+1)/2$. Each timestep of the simulation commences with calculation of the individual pair forces

$$\vec{f}_{ij} = -\frac{du_k}{dr}\,\frac{\vec{r}}{r}. \tag{1}$$

Simultaneously the potential energy Φ and virial Ψ of the system are evaluated.

$$\Phi = \sum_i \sum_{j>i} u_k(r), \tag{2}$$

$$\Psi = -\sum_i \sum_{j>i} \vec{r} \cdot \vec{f}_{ij}. \tag{3}$$

The Newtonian equations of motion to be solved for each molecule i of the species s are as follows

$$\frac{d\vec{r}_i}{dt} = \frac{\vec{p}_i}{m_s}, \tag{4}$$

$$\frac{d\vec{p}_i}{dt} = \vec{F}_i, \tag{5}$$

where $\vec{F}_i$ is a force acting on the particle i derived from neighboring particles and $\vec{p}_i$ represents the particle momentum. The set of equations (4)-(5) is integrated over the time interval $[n\Delta t, (n+1)\Delta t]$ using the well known leapfrog algorithm [3,4]

$$\vec{p}_i^{\,n+1/2} = \vec{p}_i^{\,n-1/2} + \Delta t \vec{F}_i^{\,n}, \tag{6}$$

$$\vec{r}_i^{\,n+1} = \vec{r}_i^{\,n} + \Delta t \vec{p}_i^{\,n+1/2}/m_s. \tag{7}$$

The momenta

$$\vec{p}_i^{\,n} = \frac{1}{2}(\vec{p}_i^{\,n+1/2} + \vec{p}_i^{\,n-1/2}), \tag{8}$$

are used for calculating the kinetic energy at step n

$$K = \frac{1}{2}\sum_i |\vec{p}_i^{\,n}|^2/m_s. \tag{9}$$

At each step we calculate the instantaneous total energy E

$$E = \Phi + K, \tag{10}$$

which is a conserved quantity and is used to verify the validity of the numerical algorithm.

The leapfrog algorithm requires a starting configuration. Thus initial positions and momenta of the molecules have to be specified at the beginning of the simulation. Two common methods for positions determination are adopted in the program. The first one is to arrange N molecules on a face-centered cubic lattice [5] (what implies $N = 4\ n^3$ where n is integer). In the second method initial coordinates of the molecules are read from an external file. The initial momenta are assigned randomly and modified in order to eliminate bulk momentum and to suit to the desired temperature of the system.

2.2 Thermodynamic quantities

The instantaneous pressure P and temperature T are calculated using the kinetic energy, K, and virial, Ψ

$$P = (\frac{2}{3}\,K - \frac{1}{3}\,\Psi)/V_m, \tag{11}$$

$$T = \frac{2\,K}{3\,N_A\,k_B}, \tag{12}$$

are also found in the conventional way. Here V_m is the molar volume of the system and N_A and k_B mean the Avogadro's and Boltzmann's constants.

Temperature of the system can be adjusted roughly at the beginning of simulation. Having known the desired temperature T_d of the system we calculate for the species s [5]

$$\kappa_s = 2\sqrt{m_s\,k_B\,T_d}, \tag{13}$$

and for every molecule i

$$p_{i\alpha} = \kappa_s \, x_R, \tag{14}$$

where $\alpha \in \{x, y, z\}$ and x_R is a pseudo-random number of uniform distribution from the interval $(-1, 1)$. Then the bulk motion is removed

$$p_{i\alpha} := p_{i\alpha} - < p_{i\alpha} >, \tag{15}$$

and the obtained momenta are scaled to suit the desired temperature [5]

$$p_{i\alpha} := \frac{1}{2} p_{i\alpha} \, \kappa_s / \sqrt{< \vec{p}_i \cdot \vec{p}_i > /3}. \tag{16}$$

When the simulation is in progress first several hundred or thousand steps is used to reaching the thermal equilibrium. During that stage the temperature scaling

$$p_{i\alpha} := p_{i\alpha} \sqrt{T_d / < T >}, \tag{17}$$

may be applied every multiple of the timestep, where $< T >$ is the average value of the temperature from the last scaling.

2.3 The Lennard-Jones interaction

The empirical force law representing the intermolecule interaction of the k-th kind is generally derived from a two body potential energy function such as the Lennard-Jones one [3,5]

$$u_k(r) = 4 \, \varepsilon_k \left[\left(\frac{\sigma_k}{r} \right)^{12} - \left(\frac{\sigma_k}{r} \right)^{6} \right]. \tag{18}$$

The individual pair forces (Eq. 1) are accumulated to give the total force on each molecule. In this evaluation the interaction between a pair of molecules is ignored if their separation r is greater than a chosen cutoff radius r_c. To avoid long range corrections compensating the interactions for $r \geq r_c$, the shifted form of the Lennard-Jones function [6] (for which $u_k(r) = 0$ for $r \geq r_c$) is used in the program. Thus the values of $u_k(r)$ are shifted by $u_k^0 = u_k(r_c)$

2.4 Radial distribution function

The program can calculate and plot on a lineprinter the radial distribution functions. Consider a typical central molecule of a species s. Let $N_{s'}(r, \Delta r)$ be the average number of molecules of a species s' at a distance between $r - \frac{1}{2}\Delta r$ and $r + \frac{1}{2}\Delta r$. The radial distribution function (rdf) is defined by [3]

$$g_{ss'}(r) = \frac{V}{N_{s'}} \frac{N_{s'}(r, \Delta r)}{4\pi r^2 \Delta r}, \tag{19}$$

The range of the rdfs is restricted to r_c $(0 < r < r_c)$. The rdfs are averaged over timestep intervals defined by the user.

2.5 Mean-square displacement

The mean-square displacements are calculated within timestep intervals defined by the user. Assume that n_1 and n_2 are beginning and end timesteps of the interval. Then for molecules of a species s [3]

$$msd_s = \frac{1}{N_s}\sum_{i\in s}(\vec{r}_i^{\,n2} - \vec{r}_i^{\,n1})^2 = \frac{1}{N_s}(\Delta t)^2 \sum_{i\in s}(\sum_{k=n_1}^{n_2-1} \vec{p}_i^{\,k+1/2}/m_s)^2. \tag{20}$$

The mid-step quantities $\vec{p}_i^{\,k+1/2}/m_s$ are accumulated for each molecule over timesteps so the msds can be found as functions of time.

2.6 Numerical scheme

2.6.1 Program units

The program employs the dimensionless positions, time, mass and energy using the program units. Since for forces calculations the *link-cell* method is adopted [8,9] (see section 2.6.4) thus the program unit of length $\mathcal{L}$ is equal to the length of the cell side (for the reason explained below)

$$\mathcal{L} = \left[\frac{V_m\, N}{N_A\,(NC_x \cdot NC_y \cdot NC_z)}\right]^{1/3}, \tag{21}$$

where NC_α is the number of cells in α direction. The method for NC_α determination is shown in section 2.6.4 of the paper. The unit of time $\mathcal{T}$ is equal to the simulation timestep

$$\mathcal{T} = \Delta t, \tag{22}$$

while the unit of mass is equal to the mass of species 0

$$\mathcal{M} = m_0. \tag{23}$$

The unit of energy $\mathcal{E}$ is defined on the basis of the mass of species 0 [5]

$$\mathcal{E} = m_0\,(\mathcal{L}/\mathcal{T})^2. \tag{24}$$

2.6.2 Boundary conditions

The system is made pseudo-infinite by the application of periodic boundary conditions in the three Cartesian coordinates [3,7] using the transformation

$$\begin{aligned} r_{i\alpha} &:= r_{i\alpha} - L_\alpha \quad \text{if} \quad r_{i\alpha} > L_\alpha, \\ r_{i\alpha} &:= r_{i\alpha} + L_\alpha \quad \text{if} \quad r_{i\alpha} < 0, \end{aligned} \tag{25}$$

where L_α are lengths of the sides of the computational box , thus $r_{i\alpha} \in [0, L_\alpha]$.

2.6.3 Representation of species and kinds of interactions

The program investigates dynamics of the system containing molecules of S species. Every molecule is marked by its species kind. For computational time savings a matrix of molecule kinds $\Xi = \{\Xi_i\}$ is introduced. Thus for particular i molecule, its kind is represented by

$$s = \Xi_i, \quad i = 0, \ldots, N-1, \tag{26}$$

where s means the kind of molecule i. The array Ξ is initialized subsequently

```
i := 0
for s := 0 to S − 1 do
    for n_s := 0 to N_s − 1 do
        begin
        Ξ_i := s
        i := i + 1
        end
```
(27)

and next randomized using a pseudo-random generator producing numbers $x_R \in (0,1)$

```
for determined number of random shifts do
    begin
    i := N · x_R
    j := N · x_R
    s := Ξ_i
    Ξ_i := Ξ_j
    Ξ_j := s
    end
```
(28)

The kind k of the intermolecule interaction is represented by the two dimensional array $\mathcal{X} = \{\mathcal{X}_{ss'}\}$, which is determined as follows

```
l := 0
for i := 0 to N − 1 do
    for j := 0 to N − 1 do
        begin
        X_ij := l
        X_ji := l
        l := l + 1
        end
```
(29)

Thus for a pair of molecules of kinds s and s', the kind of their interaction is obtained with

$$k = \mathcal{X}_{ss'} \qquad s = 0, \ldots, S-1, \; s' = 0, \ldots, s. \tag{30}$$

2.6.4 Calculation of the forces

The Lennard-Jones parameters ε_k and σ_k of the interaction between two molecules of kinds s and s' while given ε_s, $\varepsilon_{s'}$, σ_s and $\sigma_{s'}$ are calculated [5]

$$\varepsilon_{ss'} = (\varepsilon_s \cdot \varepsilon_{s'})^{1/2}, \qquad s = 0, \ldots, S-1,\ s' = 0, \ldots, s, \tag{31}$$

$$\sigma_{ss'} = (\sigma_s + \sigma_{s'})/2, \qquad s = 0, \ldots, S-1,\ s' = 0, \ldots, s. \tag{32}$$

Due to computational time savings, values of the pair potentials vs. the squared intermolecule distance are stored in U_k arrays, $k = 0, \ldots, M-1$. The number of elements in every array, ν, is a parameter of the program. The distance interval covered by the grid starts from the square of potential "hard-core" ρ_k^2

$$\rho_k = \beta\, \sigma_{ss'}, \tag{33}$$

where index k is given by Eq. (30) and β is a parameter ($\beta < 1$). The end of the distance interval is equal to square of the cutoff radius, r_c^2

$$r_c = \gamma \cdot \max_s \sigma_s, \quad s = 0, \ldots, S-1. \tag{34}$$

γ reflects the range of interaction (usually $\gamma = 2.5 \div 3.0$).

The values of potential are tabulated at uniform intervals Δr^2 to avoid square root computation while using the tables elements

$$\Delta r^2 = (r_c^2 - \min_k \rho_k^2)/(\nu - 1). \tag{35}$$

For the k-th kind of the intermolecule interaction the elements of the table $U_k = \{u_{kl}\}$ contain

$$u_{kl} = 2\, u_k(r_l^2)/\Delta r^2 - u_k^0, \quad l = 1, \ldots, \nu, \tag{36}$$

while

$$r_0^2 = \rho_k^2, \quad r_{l+1}^2 = r_l^2 + \Delta r^2. \tag{37}$$

The individual pair force (Eq. 1) is determined for the k-th type of interaction

$$f_{ij\alpha} = -(u_{kl+1} - u_{kl})\,(r_{i\alpha} - r_{j\alpha}), \tag{38}$$

where

$$l = \lfloor (r^2 - \rho_k^2)/\Delta r^2 \rfloor, \tag{39}$$

and $\lfloor \cdot \rfloor$ means the greatest integer function. Then

$$F_{i\alpha} = \sum_{j=0}^{J-1} f_{ij\alpha}, \tag{40}$$

where J is a number of the i-th molecule neighbors for which $r < r_c$ and $J \ll N$ due to short range of the interactions.

To determine neighboring molecules to the current one the *link-cell* method is applied [8,9]. For further reduction of the computer time two techniques are applied. The *cube technique* [10] concept differs from the original *linked list* method in some additional conditions limiting the number of i-th particle neighbours to those confined in the cube of centre at $\vec{r}_i$ and side length

equal to $2\,r_c$. Thus the squared distance between two particles i and j is not evaluated unless differences in particles coordinates fulfil $|r_{i\alpha} - r_{j\alpha}| < r_c$. In the second technique [10] tiny cells of side lengths less than r_c are introduced in contradiction to the conventional approach in which the lengths of the chaining mesh cell sides are always greater than or equal to the r_c. Obviously, more neighboring cells in each direction have to be taken into account. In the program each of the previously defined cells is divided into SCR (side cell ratio, $SCR = 1,2,\ldots$) parts along each side defining tiny cells. In this case the number of neighboring molecules is diminished. Assume for example that every side of 27 neighboring cells is divided into 2 parts, then 125 out of 216 cells is taken into consideration only. In that case the *tiny cell technique* should consume 0.58 of the time spent on calculations with classical cells. In practice advantage of the method is not so high according to more computational time spent for cells searching.

Let NC_α be the number of cells in α direction respectively. It is obtained with the input data

$$NC_\alpha = \left[\frac{V_m\, N}{N_A\,(Q_x \cdot Q_y \cdot Q_z)}\right]^{1/3} \frac{Q_\alpha \cdot SCR}{r_c}, \tag{41}$$

where Q_α reflects the side lengths of the computational box and r_c is given in physical units. Using the fcc starting configuration, Q_α means also a number of the fcc cells in α direction. The ratio of side lengths of the computational box should fulfil $Q_x : Q_y : Q_z = k : kl : klm$, where k, l, m are integers. The overall number of program cells is

$$NC = \prod_\alpha NC_\alpha. \tag{42}$$

To apply the link cell method [8,9], let $HOC(c)$ be a head of chain table entry for cell c and let LL_i be the link coordinate for the molecule i. Then (in respect to the program unit of length) the procedure for filling the HOC and LL tables is summarized by [8,9]

```
for c := 0 to NC − 1 do
    HOC(c) := −1
for i := 0 to N − 1 do
    begin
    c_α := ⌊r_iα⌋                                   (43)
    c := c_x + NC_x · (c_y + NC_y · c_z)
    LL_i := HOC(c)
    HOC(c) := i
    end
```

A (-1) entry in $HOC(c)$ indicates that there are no molecules in cell the c. Another entry gives the address of the coordinates of the first molecule in the list. Similarly, the link coordinate of a molecule either gives the address of the coordinates of the next molecule in the list or is equal to (-1) to indicate the end of the list.

For computer time savings several auxiliary tables are introduced.

Periodic boundary conditions are used with help of the tables $MIC_\alpha(c_\alpha)$. Due to the computational box dimensions

$$MIC_\alpha(c_\alpha) = \begin{cases} -NC_\alpha & \text{for} \quad -SCR < c_\alpha < 0, \\ 0 & \text{for} \quad 0 \le c_\alpha < NC_\alpha, \\ NC_\alpha & \text{for} \quad NC_\alpha \le c_\alpha < NC_\alpha + SCR. \end{cases} \tag{44}$$

The cell index c is usually computed using the equation

$$c = c_x + NC_x \cdot (c_y + NC_y \cdot c_z). \tag{45}$$

In the most time consuming parts of the program Eq.(45) is replaced by

$$c = NCB_x(c_x) + NCB_y(c_y) + NCB_z(c_z), \tag{46}$$

where number of operations is reduced and NCB_α are auxiliary tables conserving the meaning of Eq. (45).

For the molecule i lying in cell c_i the neighboring particles are those from cell c_i and $NNC = (2 \cdot SCR + 1)^3 - 1$ neighboring cells. Due to the Newtonian law only half of the neighboring cells is taken into account. In the program the neighbors lying above the current cell and half cells from the same level are investigated. Parameter SCR states how many neighboring cells is taken into considerations in one direction. Then numbers of neighboring cells in particular layers are

a) along every coordinate : $m = 2 \cdot SCR + 1$,

b) lying above the current cell : $m_1 = m^2 \cdot SCR$,

c) lying on the same level as the current cell : $m_2 = (m + 1) \cdot SCR$,

Adding m_1 and m_2 we get the number of neighboring cells considered $NNC2 = m_1 + m_2 = (m^3 - 1)/2$. In order to determine coordinates of the jc-th neighboring cell ($jc = 0, \ldots, NNC2 - 1$) the tables NH_α are introduced. The value of $NH_\alpha(jc)$ means the shift of the jc neighboring cell in α direction relative to the current cell. Thus

$$c_{j\alpha} = c_{i\alpha} + NH_\alpha(jc), \tag{47}$$

where $c_j = (c_{jx}, c_{jy}, c_{jz})$ is a neighbor of c_i. NH_α tables are set up as follows. Let $i_\alpha \in [-SCR,\ SCR]$, then

$$\begin{array}{l} jc := 0 \\ \text{for all combinations of } i_x, i_y, i_z \text{ for which} \\ (i_z > 0) \text{ or } (i_z = 0, i_y < 0) \text{ or } (i_x = i_y = 0, i_x \leq 0) \\ \quad \underline{\text{begin}} \\ \quad NH_\alpha(jc) := i_\alpha \\ \quad jc := jc + 1 \\ \quad \underline{\text{end}} \end{array} \tag{48}$$

The forces calculations are performed within two loops using the tables U_k (Eq. 36). The primary loop is organized over all cells of the computational box. Calculations of the individual particle forces are done within the secondary loop. In order to increase the overall efficiency, the simple secondary loop is replaced by its three different types, represented by program blocks [10]

```
for c_i := 0 to NC − 1 do
    begin
    block_one
    for jc := 0 to m_1 − 1 do { cells with NH_z(jc) > 0 }
        block_two
    for jc := m_1 to NNC2 − 1 do { cells with NH_z(jc) = 0 }
        block_three
    end
```
(49)

The first type of the secondary loop (**block_one**) determines forces derived from the molecules belonging to the same cell as the current molecule. The second type (**block_two**) takes into account interactions with molecules belonging to the cells with z-coordinates greater than the current cell (only molecules from cells lying above the current one are examined). The third type of the secondary loop (**block_three**) reflects interactions derived from the molecules belonging to the cells lying on the same level as the current cell (with the same z-coordinate) and also half of them is considered only. Thus subsequent program blocks are as follows

```
block_one
    begin
    i := HOC(c_i)
    while (i > −1) do
        begin
        j := LL_i
        s := Ξ_i
        while (j > −1) do
            begin
            r_α := r_iα − r_jα
            r^2 := Σ_α r_α^2
            if (r^2 < r_c^2) then block_common
            j := LL_j
            end
        i := LL_i
        end
    end
```
(50)

block_two

```
begin
c_jα := c_iα + NH_α(jc) { for α ∈ {x,y,z}}
mic_α := MIC_α(c_jα) { for α ∈ {x,y,z}}
c_j := NCB_x(c_jx) + NCB_y(c_jy) + NCB_z(c_jz)
i := HOC(c_i)
j := HOC(c_j)
while (i > −1) do
      begin
      s := Ξ_i
      r_iα := r_iα − mic_α                                              (51)
      while (j > −1) do
            begin
            if (r_jx < r_c + r_ix and r_jx > r_ix − r_c and
                r_jy < r_c + r_iy and r_jy > r_iy − r_c and
                r_jz < r_c + r_iz and Σ_α r_α^2 < r_c^2) then block_common
            j := LL_j
            end
      j := HOC(c_j)
      i := LL_i
      end
end
```

block_three

```
begin
c_jα := c_iα + NH_α(jc) { for α ∈ {x,y}}
mic_α := MIC_α(c_jα) { for α ∈ {x,y}}
c_j := NCB_x(c_jx) + NCB_y(c_jy) + NCB_z(c_iz)
i := HOC(c_i)
j := HOC(c_j)
while (i > −1) do
      begin
      s := Ξ_i
      r_iα := r_iα − mic_α (for α ∈ {x,y})                              (52)
      while (j > −1) do
            begin
            if (r_jx > r_ix − r_c and r_jy < r_c + r_iy and
                Σ_α r_α^2 < r_c^2)then block_common
            j := LL_j
            end
      j := HOC(c_j)
      i := LL_i
      end
end
```

Within every type of the secondary loop the following **block_common** is used to calculate the

forces (see Eqs. 30–40)

block_common
begin
$s' := \Xi_j$
$k := \mathcal{X}_{ss'}$
$l := \lfloor (r^2 - \rho_k^2)/\Delta r^2 \rfloor$
$\Delta u_k := u_{kl+1} - u_{kl}$
$f_{ij\alpha} := -\Delta u_k \, (r_{i\alpha} - r_{j\alpha})$
$F_{i\alpha} := F_{i\alpha} + f_{ij\alpha}$
$F_{j\alpha} := F_{j\alpha} - f_{ij\alpha}$
$\Phi^* := \Phi^* + (u_{kl+1} + u_{kl})$
$\Psi := \Psi - r^2 \, \Delta u_k$
end (53)

Potential energy is equal to $\Phi = \Phi^*/2$.

Splitting of the secondary loop reduces the computational time since in every type the necessary operations are performed only in respect to reciprocal cells orientation. The application of the *cube technique* can be seen in conditional statements of Eqs. (51)–(52) with proper order of conditions verification reducing the computer time.

To verify efficiency of the algorithm some comparisons have been performed with the non-split secondary loop [9] (neglecting the *cube* and the *tiny cell* techniques), see Figure 1. For consistency, potential tables and tables with kinds of interaction as well as with kinds of molecules have been applied in the reference loop. Using the approach presented above (without the *cube technique* however), the computational time savings of 20% have been obtained in comparison with the non-splitting secondary loop. With the *tiny cell technique*, but still without the *cube* one the savings increase to 35% for $SCR = 2$. Applying the *cube technique* but without the *tiny cell* one gets the maximal savings of 45%. Mixing the *cube* and *tiny cell* techniques together is not useful because in that case savings decrease monotonically with SCR increase. Another feature of the *cube technique* is the weak dependence of computational time for a single timestep per particle on proper determination of the cutoff radius with reference to the cell side.

3 Description of the program

3.1 Introduction and top level procedures

The structure and conventions adopted in the program are based on and similar to those of the standard programming system OLYMPUS designed for FORTRAN programs [11,12,13].

The full index of the program procedures and external variables (listed in external blocks and alphabetically) is given in program comments. References appearing in the form $< c.m >$ refer to the decimal numbering of procedures.

The main program $< 0.0 >$ contains descriptive comments and controls the calculations by calling appropriate functions ($< 0.1 >$–$< 0.3 >$). Procedure $< 0.1 >$ *basic* initialises the basic program data defining the program operation mode and output form, while the $< 0.2 >$ *modify* routine changes those presumed values if necessary, according to the user-prepared input data

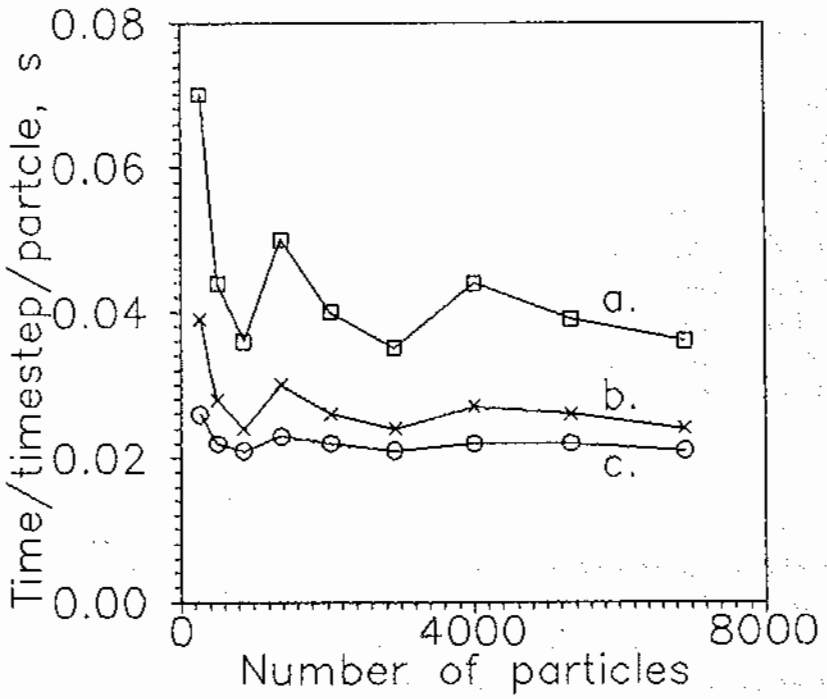

Figure 1: Execution time for MD timestep per particle (on DSI-020 board) for various *Forces* procedures, $R_{cut} = 2.5\sigma$. a) non-split secondary loop based on [9] coded in C language, b) secondary loop split into three types with *tiny cell technique*, c) secondary loop split into three types with *cube technique*. Average values for first 100 timesteps.

file. The procedure $<0.3>$ *control* controls the run by calling functions from the rest of groups (1–4) subject to new or restart run. Procedures from the class $<0.m>$ involve also some utility procedures from the class $<U.m>$.

3.2 Initialisation procedures

The first class of procedures is the initialisation one. It is devoted to establishing the system configuration and parameters. In the procedure $<1.1>$ *label_run* some headings of the program are introduced, procedure $<1.2>$ *preset* initialises those external variables needed to specify the run conditions. They can be changed next in the $<1.3>$ *data* procedure.

3.2.1 Auxiliary parameters

On the basis of the established program parameters the auxiliary values are calculated in $<1.4>$ *auxiliary_val*. In the section 2 of $<1.4>$, procedure $<1.15>$ *convert_si* is invoked which converts physical quantities of the system into SI units if necessary. Then (sections 3, 4.2 and 7 of $<1.4>$) some tables used within the program are allocated. Section 4.1 of $<1.4>$ involves procedure $<1.8>$ *scale_proc* which calculates the number of cells, NC_α, in x, y and z directions, the total number of cells, NC (section 1 of $<1.8>$ (Eqs. 41–42), the program units $\mathcal{L}$, $\mathcal{T}$, $\mathcal{M}$ and $\mathcal{E}$ (section 2 of $<1.8>$, Eqs. 21–24), the Lennard-Jones parameters ε_k and σ_k (sections 4–5 of

< 1.8 >, Eqs. 31–32), the potential "hard-core" ρ_k and the cutoff radius r_c (Eqs. 33–34).

Section 5 of < 1.4 > involves procedure < 1.9 > *neigh_cells_matrices*, which purpose is to calculate neighboring cells coordinates NH_α.

Section 6 of < 1.4 > invokes < 1.11 > *potential_init* which purpose is to fill the potential tables U_k (Eq. 36). Potential values shifted by u_k^0 are put into every potential table at the uniform interval Δr^2 (see < 1.12 > *potential*, Eqs. 35, 37 and 39). Last of all, section 7 of < 1.4 > allocates memory for tables containing the periodic boundary displacements and involves < 1.16 > *boundary_cond* to fill the tables.

3.2.2 Initial system configuration

In each new run < 1.5 > *initial* function is invoked to set up the initial system configuration. It allocates also (section 1 of < 1.5 >) most of program tables, including molecules positions, momenta, forces, etc. The initial configuration of the system can be generated within the program in a form of the fcc lattice (using procedure < 1.13 > *partcls_coord* involved in section 2.1). The configuration can also be read from the user prepared external file (see section 2.2 of < 1.5 >). Section 3 of < 1.5 > involves procedure < 1.10 > *kind_arrays* in order to define the matrix of molecules kinds Ξ (Eqs. 26–28). Section 2 of < 1.10 > determines the matrix of kinds of the molecules interactions $\mathcal{X}$ (Eq. 30).

Section 4 of < 1.5 > sets up and scales starting momenta of molecules (< 1.13 > *momentum*, Eqs. 13–17), in order to remove the bulk motion of the system and to achieve the desired temperature.

While the restart run is assumed the procedure < 1.6 > *resume* is involved (instead of < 1.5 > *initial*), the purpose of which is to restore the molecules configuration and momenta as well as other physical and numerical parameters from the external file. In that case the computer memory for most of the program arrays is allocated in < 1.6 >. Procedure < 1.7 > *start* starts the calculations within the time loop.

3.3 Step on the calculations

The < 2.1 > *stepon* procedure is executed once in every simulation step. In its section 1 the procedures for forces calculations, namely < 2.2 > *forces* or < 2.5 > *forces_with_rdf* are invoked depending whether the rdfs are to be determined for the current timestep. The rdfs are calculated within and averaged over user defined time intervals. In the case of rdf calculations procedure < 3.4 > *rdf* (Eq. 19) is also invoked in this section.

3.3.1 Force calculation

Procedures < 2.2 > *forces* and < 2.5 > *forces_with_rdf* apply the algorithm described in section 2.4.5 of the paper.

3.3.2 Calculate molecules motion and rdfs

Procedure < 2.3 > *motion* (called in section 2 of < 2.1 >) solves the set of equations of motion (Eqs. 4–5) using the leapfrog algorithm (Eqs. 6–7). Displacements of molecules are used in msds calculations also (Eq. 20). Section 2 computes the kinetic energy, K, of the system (Eqs. 8–9). In section 3 the < 3.7 > *msd* procedure is invoked for mean square displacement calculations

(Eq. 20) within user-defined time intervals (called msd windows). Sample examples of rdf and msd graphs are presented in Figure 2 and Figure 3 respectively.

3.3.3 Timestep quantities

Timestep quantities representing properties of the system in every timestep are computed within the procedure $< 2.4 >$ *values_total* (invoked in section 3 of $< 2.1 >$). Section 1 computes molar step quantities, i.e. potential energy (Eq. 2), kinetic energy (Eq. 9), virial (Eq. 3), total energy (Eq. 10), pressure (Eq. 11), and temperature (Eq. 12). Then the rolling averages (in section 3) and average values together with R.M.S. fluctuations (in section 4 of $< 2.4 >$) are determined. Section 5 of $< 2.4 >$ performs classical temperature scaling [5] (see Eq. 17), applied every multiple of timestep.

3.4 Output of the program and utility procedures

Output of the program is organized with the procedure $< 3.1 >$ *output* which provides initialisation, periodic and final output (supported with auxiliary procedures $< 3.2 >$ *out_mat* and $< 3.3 >$ *out_scale*). Its additional feature is to make intermediate and final savings of program results on external files. Semigraphical output is provided for rdfs and msds drawing on the lineprinter, which is arranged with procedures $< 3.5 >$ *rdf_output* and $< 3.8 >$ *msd_output*.

Class $< U.m >$ represents utility procedures used for simple input and output, debugging, system date and time determination, pseudo-random numbers generation, etc. Procedure $< U.10 >$ *error* prints execution error messages causing abnormal program termination.

The detailed description of program external files, data input formats and methods for dealing with the program is given in the Program Manual.

4 Acknowledgments

We are grateful to Professor Jerzy Kapelewski for arranging partial financial support under the project number CPBP 01.08 D4.3. We are also grateful to Dr. Marian Bubak from the Institute of Computer Science AGH, Cracow, for comments on the manuscript.

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RADIAL DISTRIBUTION FUNCTION
OF (1 , 1) SPECIES

WINDOW NO 1 STEP INTERVAL (2801 TO 3000) FOR DT = 1.00000e-14

R	RDF	INT RDF
0.012	0.000	0.0
0.037	0.000	0.0
0.062	0.000	0.0
0.087	0.000	0.0
0.111	0.000	0.0
0.136	0.000	0.0
0.161	0.000	0.0
0.186	0.000	0.0
0.211	0.000	0.0
0.235	0.000	0.0
0.260	0.000	0.0
0.285	0.000	0.0
0.310	0.000	0.0
0.334	0.013	0.0
0.359	0.583	0.1
0.384	2.076	0.5
0.409	2.529	1.2
0.434	2.041	2.1
0.458	1.539	2.8
0.483	1.168	3.5
0.508	0.935	4.0
0.533	0.787	4.5
0.557	0.714	5.0
0.582	0.682	5.4
0.607	0.703	6.0
0.632	0.711	6.5
0.657	0.787	7.2
0.681	0.876	8.0
0.706	0.991	8.9
0.731	1.077	10.0
0.756	1.149	11.3
0.780	1.184	12.8
0.805	1.207	14.4
0.830	1.157	16.0
0.855	1.110	17.7
0.880	1.031	19.4
0.904	0.963	21.1
0.929	0.921	22.7
0.954	0.893	24.4
0.979	0.895	26.2

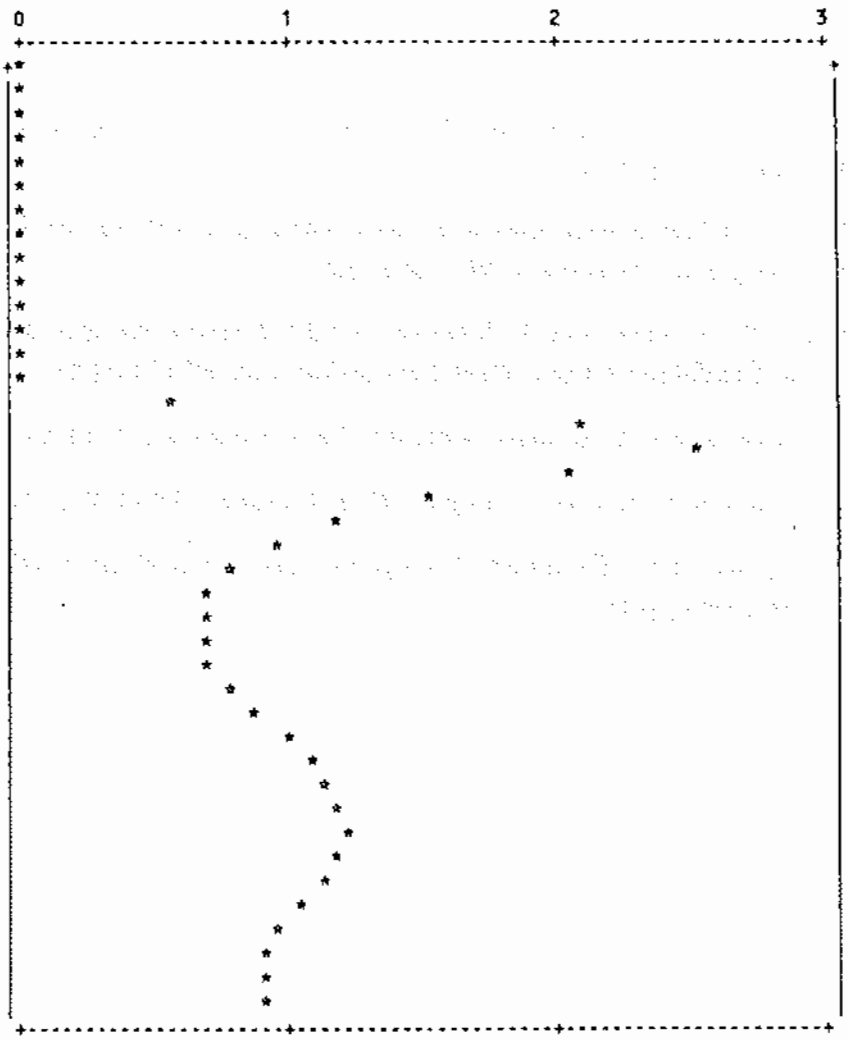

Figure 2: Example of the RDF function calculated and plotted by the program.

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MEAN SQUARE DISPLACEMENT
OF 1 SPECIE

WINDOW NO 1 STEP INTERVAL (2801 TO 3000) FOR DT = 1.00000e-14

TIME	MSD
2.5e-14	7.8e-23
7.5e-14	4.6e-22
1.2e-13	1.1e-21
1.8e-13	2.1e-21
2.3e-13	3.1e-21
2.7e-13	4.3e-21
3.2e-13	5.4e-21
3.7e-13	6.7e-21
4.2e-13	7.9e-21
4.7e-13	9.1e-21
5.2e-13	1.0e-20
5.7e-13	1.2e-20
6.2e-13	1.3e-20
6.7e-13	1.4e-20
7.2e-13	1.5e-20
7.7e-13	1.6e-20
8.2e-13	1.7e-20
8.7e-13	1.8e-20
9.2e-13	1.9e-20
9.7e-13	2.0e-20
1.0e-12	2.1e-20
1.1e-12	2.2e-20
1.1e-12	2.3e-20
1.2e-12	2.4e-20
1.2e-12	2.5e-20
1.3e-12	2.6e-20
1.3e-12	2.7e-20
1.4e-12	2.8e-20
1.4e-12	2.9e-20
1.5e-12	3.0e-20
1.5e-12	3.1e-20
1.6e-12	3.2e-20
1.6e-12	3.3e-20
1.7e-12	3.4e-20
1.7e-12	3.5e-20
1.8e-12	3.6e-20
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1.9e-12	3.8e-20
1.9e-12	3.9e-20
2.0e-12	4.0e-20

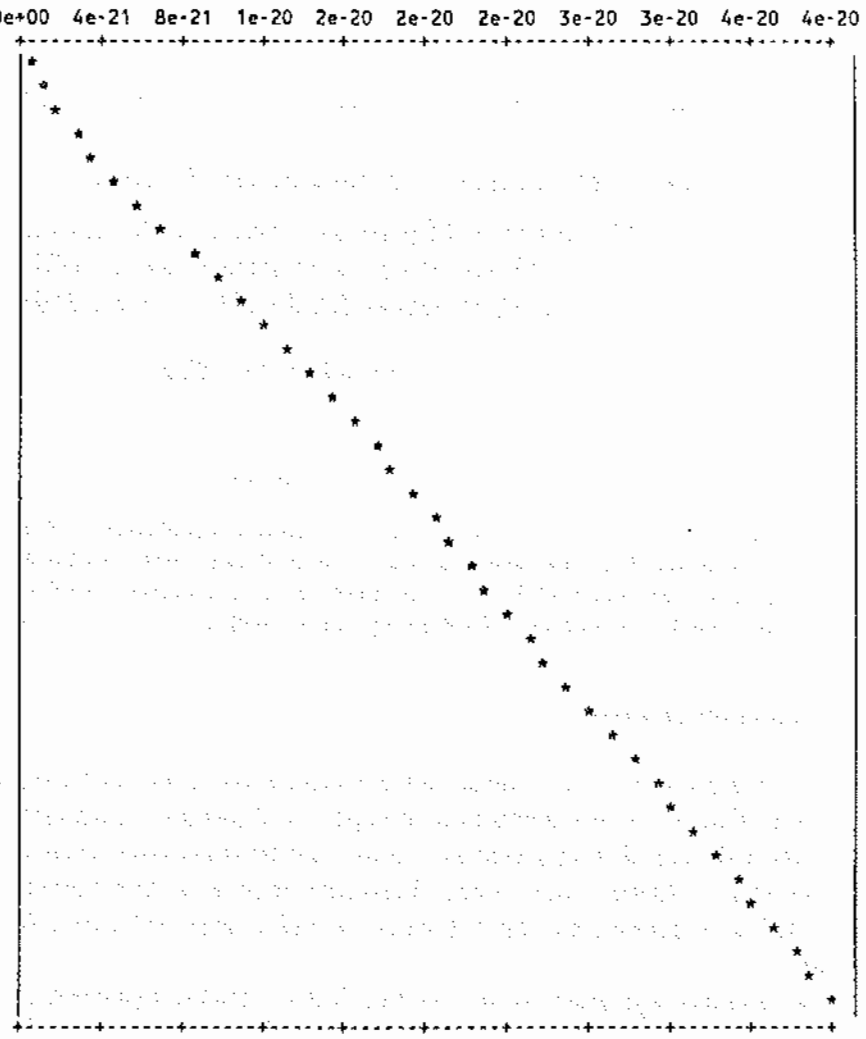

Figure 3: Example of the MSD function calculated and plotted by the program.

Microscale hydrodynamics on microcomputers

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October 20, 1990

Abstract

In the paper we report about microcomputer simulation of formation and shedding of vortices using 2-D molecular dynamics. It is shown that results of limited, but reasonable scope could be obtained for a system made up of a moderate number of particles ($N \sim 5000$) using a moderate number of time-steps ($n \sim 10000$).

1 Introduction

Computer simulation is a popular and powerful method for understanding chemical and physical processes. One of the main subjects of super– and parallel computers challenge is fluid dynamics due to its wide practical applications. Since it is primary concerned with macroscopic phenomena in fluids (e.g. diffusion, convection, laminary flows and fully developed turbulence), the theory is not based in general on the behaviour of individual molecules, but rather on their collective motions.

The popular approach is to use the *Navier–Stokes* equations, which has been applied by many researches to obtain the flow field of different characteristics (e.g. [1]–[4]). This kind of equations is usually difficult to be solved in general and some simplifying assumptions and limitations have to be introduced prior to numerical solution.

Another approach to simulation of fluid dynamics are applications of the *cellular automata* (*lattice gas*) [5]. Their wide spread applications are at least partially based on their inherent computational simplicity, although the results seem to be valuable and interesting [6]–[7]. This feature is also a drawback of the lattice gas because there is no explicit continuous modelling of forces acting in the fluid.

In engineering applications the most of flow studies concern dynamics at high Reynolds numbers, for example $Re \approx 10000$. However, in order to understand the stability and transient properties during formation of vortices – it is profitable to start investigations at low Reynolds numbers.

Since the work is in progress, in the paper we present some preliminary results obtained from computer experiments using the *Molecular Dynamics* (*MD*) approach to model fluid flow around an obstacle. Although similar results have been reported in the literature ([8], [9], [10]), in Conclusions we point out some items among which use of microcomputers for such a kind of simulation might be of interest.

2 Flow modelling

Conventionally, the model consists of a finite number of particles, N, with mass, m, enclosed into the 2-D computational box. The periodic boundary conditions are introduced in both x and y directions.

One of the approaches to investigations of formation of vortices is to divide the computational box into two *zones* of different properties: a thin thermal zone outside the obstacle, which purpose is to "close" the flow, and the rest of the box in which the constant acceleration field is introduced [8], [9].

In the paper we propose other partitions of the box into *zones* [11]:

- thin acceleration zone outside the obstacle in which the constant acceleration field is introduced (the "pump" concept); the flow of the particles evaluates free in the rest of the box,
- thin acceleration zone (with constant acceleration field) and the thin thermal zone to maintain the constant total energy.

There are also several methods for introducing the obstacle (or a wall) into the system of particles:

- "thermal" obstacle (or the wall) [8]–[9], [12], which simulates roughness of the surface; this is equivalent to randomizing the velocity of a particle at its closest approach to the boundary, while keeping the kinetic energy unchanged,
- "steady" particles (creating the obstacle or/and the wall), for which the equations of motion are not solved – thus the particles forming the obstacle remain in their initial positions during the simulation [13],
- "heavy" particles, with the mass $\sim 10^{10}m$, which are simulated in the same way as the rest of the particles of the system [10].

Due to simplicity of the algorithm, in the paper the last approch is used.

For our study constant volume model in two-dimensional (2-D) geometry is adopted. The computer experiments are accomplished using the short-range 12/6 Lennard–Jones (L-J) interactions between the particles. Parameters for Argon are adopted.

Due to computational time savings, values of the pair potential versus the squared interparticle distance are stored in an array. They are tabulated at uniform intervals Δr^2 to avoid square root computation while using the table elements.

The most time consuming part of every *MD* program is forces evaluation. In the reported algorithm the *link-cell* method [14] is applied to determine neighbour particles of the current one.

The set of Newtonian equations of motion is solved using the well known *leapfrog* algorithm.

More details of the simulation program are presented in Appendix B.

3 Results

In the paper results of two computer experiments are reported. They have been carried out using an AT-386/387 (20 MHz) microcomputer and the 32-bit SVS FORTRAN-386 compiler (see Appendix B for timings). For the both the "pump" concept for the flow modelling with the

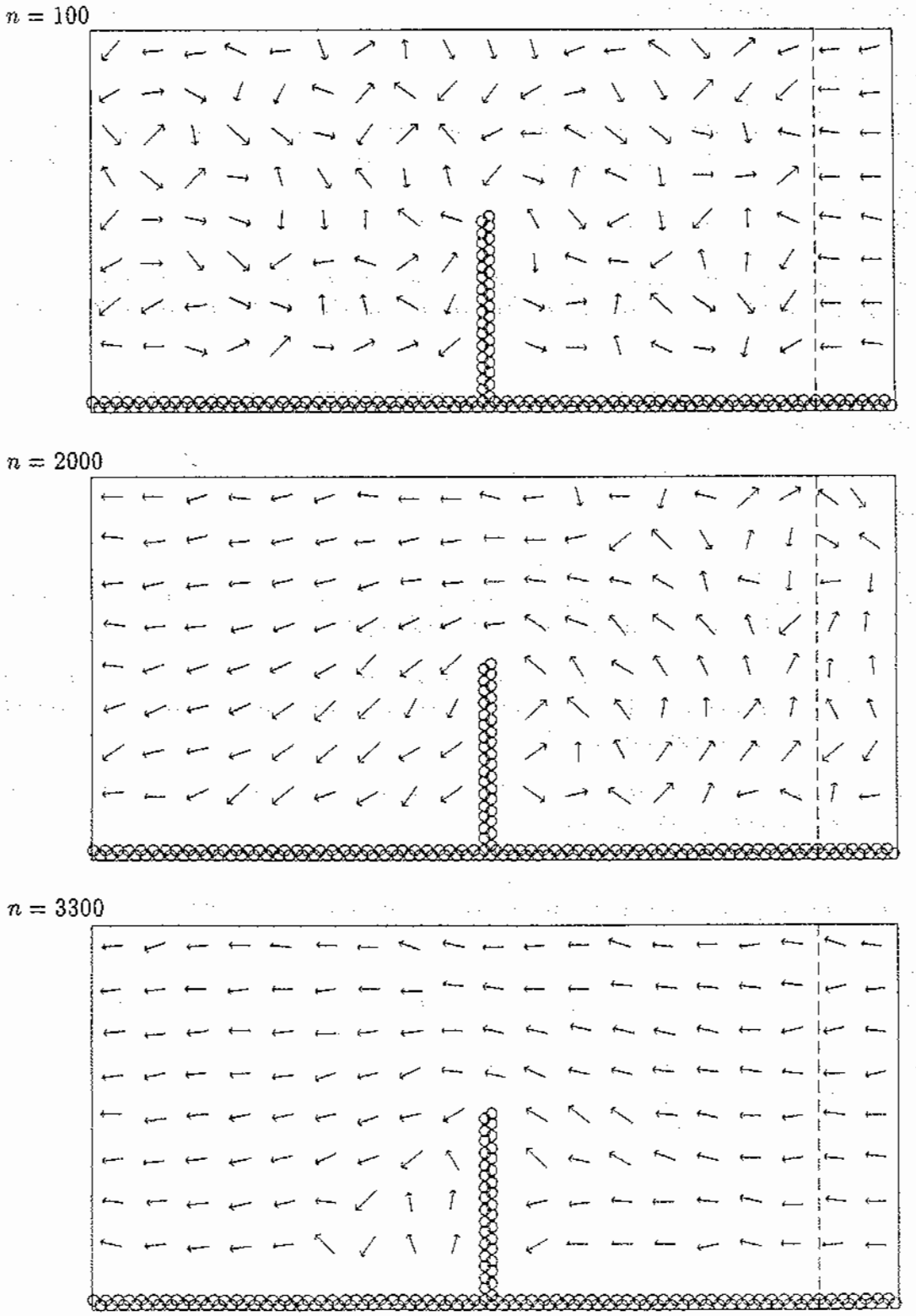
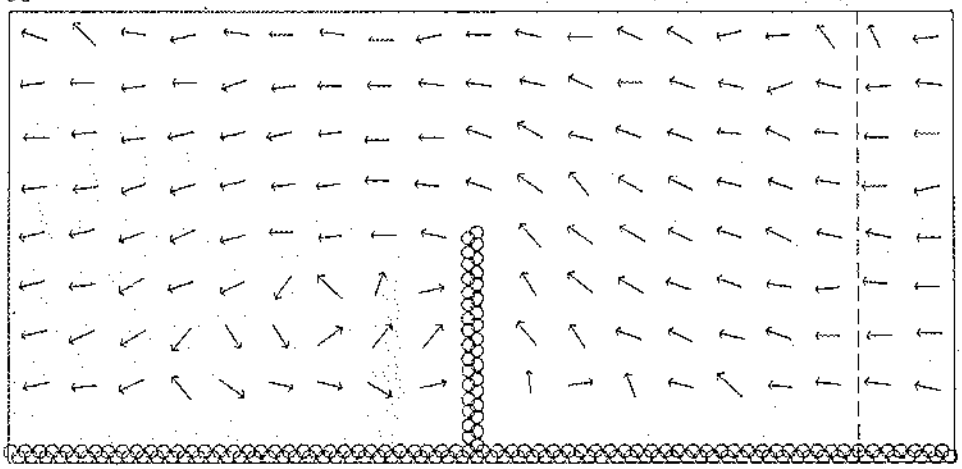
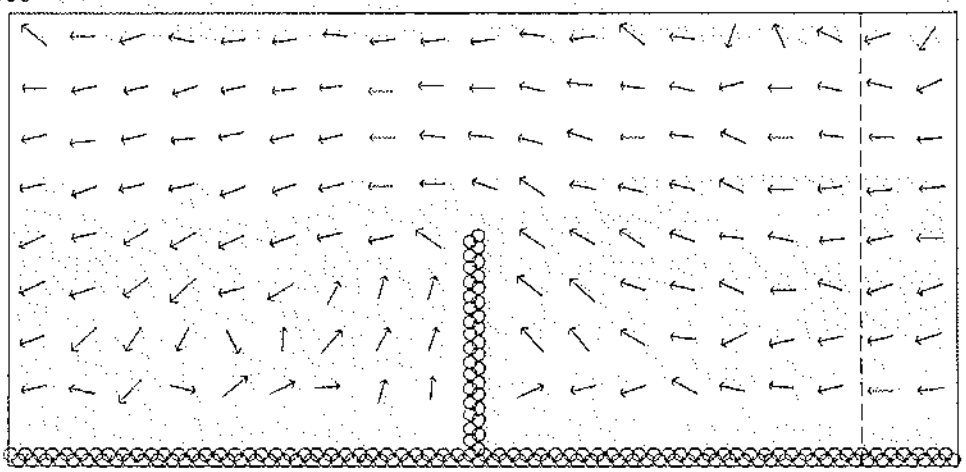


Figure 1: Particles velocity distributions for time-steps: $n = 100, 2000, 3300$.

$n = 5600$



$n = 6100$



$n = 7000$

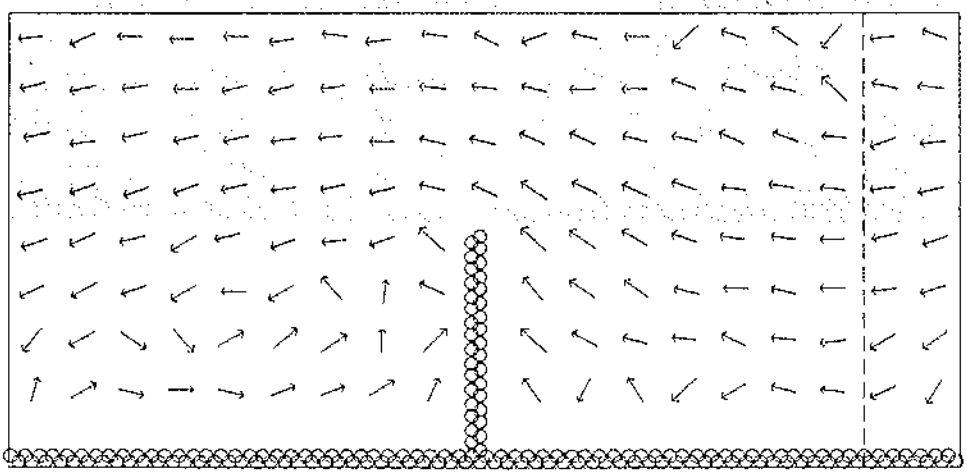
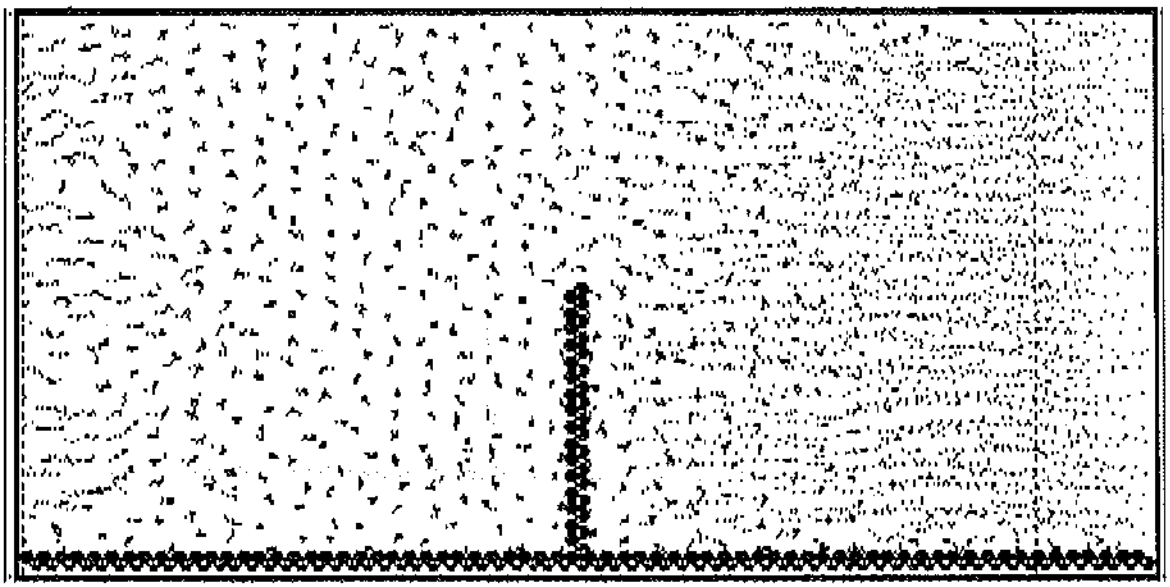


Figure 1 (cont.): Particles velocity distributions for time-steps: $n = 5600, 6100, 7000$.

$n = 100 \div 1000$



$n = 5000 \div 6500$

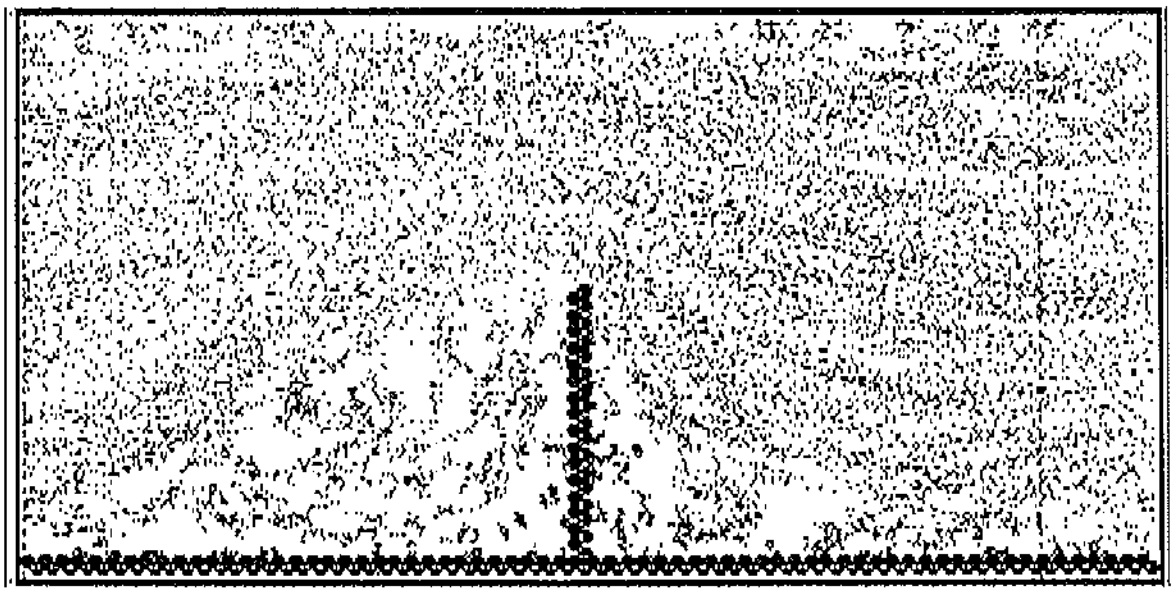


Figure 2: Particles trajectories for time-steps: $n = 100 \div 1000$ and $n = 5000 \div 6500$.

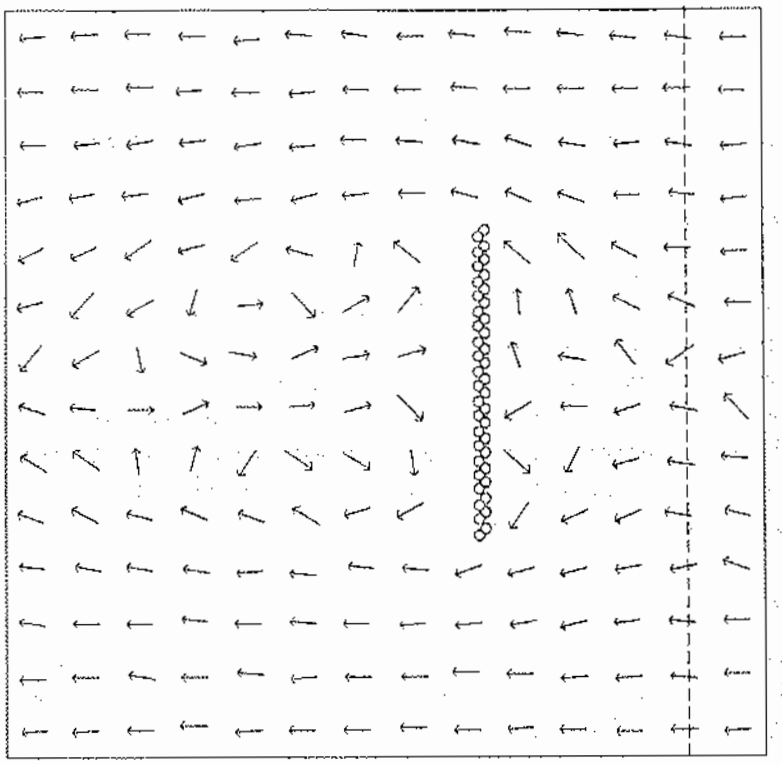


Figure 3: Particles velocity distribution for time-step $n = 5600$.

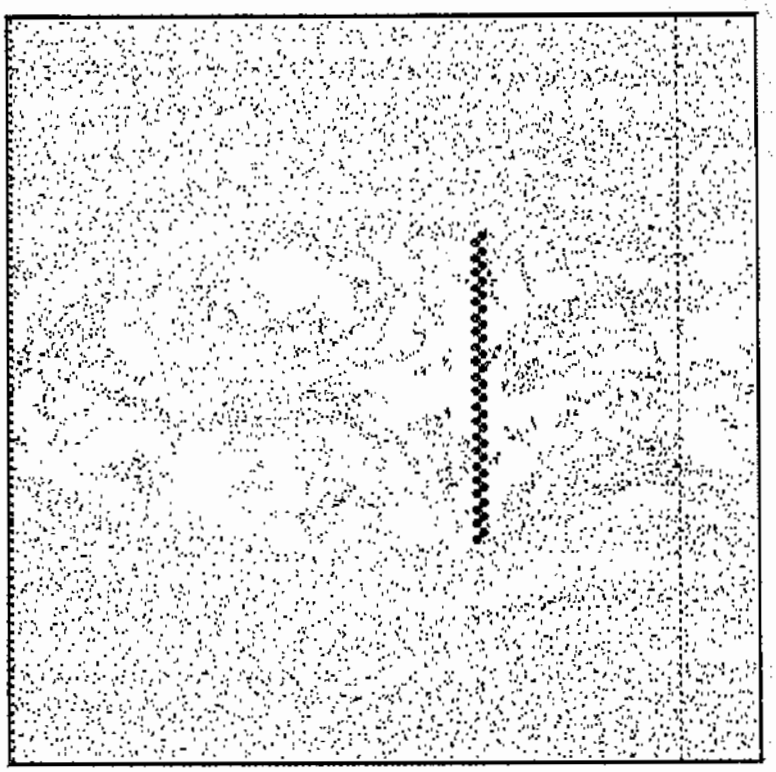


Figure 4: Particles trajectories for time-steps $n = 6100 \div 7300$.

constant acceleration field ($a = 2.5 \times 10^{14} m/s^2$) and the potential cutoff $R_C = 2.5\sigma$ (σ is a L-J parameter) is used. The acceleration field acts only in 0.1 part of the box.

In the both experiments the average system velocity increases with the simulated time remaining below the sound speed for Argon at its triple point ($864 m/s$).

3.1 Experiment 1

In the first experiment the ratio of computational box dimensions is equal to $x/y = 2$ and the total number of particles $N = 4624$. The "heavy" particles ($N_H = 169$) form the obstacle and "close" the system in y direction.

In Figure 1 particles velocity distributions in the sample time-steps are shown. The velocity vectors represent direction of motion only, they do not amount to velocity values. They concern averages, which are determined on a base of computational box partition into sub-cells.

In Figure 2 sample particles trajectories are presented. Analyzing the figures, the formation and shedding of the vortex can be seen.

3.2 Experiment 2

In the second experiment the cubic computational box with no boundary of the "heavy" particles in y direction is adopted ($N = 5000$, $N_H = 42$). The obstacle is located centrally in the box. Particles velocity distribution in a chosen time-step and sample particles trajectories are presented in Figures 3 and 4. The formation of the vortices can be seen as well, with strong symmetry along the flow.

4 Conclusions

From the presented results it follows that the molecular dynamics approach to microscale hydrodynamics could be used (at limited scope at present) for simulation of hydrodynamical phenomena. Some items might be of interest:

- use of microcomputers – the results presented in the literature have been carried out using a coupled array of 4 × FPS-264 processors of the IBM Center at Kingston (U.S.A.) – [8], [9], or a CRAY XMP-12 [10],
- use of a relatively small number of particles, $N \approx 5 \times 10^3$, against $N \approx 1.6 \times 10^5$ in [8]–[9]; in [10] however, a small number of particles ($N \approx 3 \times 10^3$) has been used as well,
- use of a relatively small number of time-steps, $n < 10^4$ against $n \approx 1.2 \times 10^5$ in [8]–[9] and $n \approx 3 \times 10^4$ in [10]; in every case $\Delta t \approx 10^{-14}$s,
- use of the shifted form of the L-J potential function with $R_C = 2.5\,\sigma$, whereas in [8]–[9] the attractive tail of L-J function is eliminated, leaving only a repulsive core.

5 Acknowledgments

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A Presentation manager program EDSIMP

The program EDSIMP is a graphic shell for molecular dynamics (2-D) programs [11]. It can be used for input data modifications and for graphical editing of initial positions of the particles. It offers many options for graphical presentation of the simulation results, namely: the particles positions in subsequent time-steps, the particles trajectories, the particles momenta distributions and 3-D grid of the local particles density.

The program is written in TURBO PASCAL (v4.0) for INTEL 8088 – 80486 based microcomputers with EGA or Hercules graphic adapters.

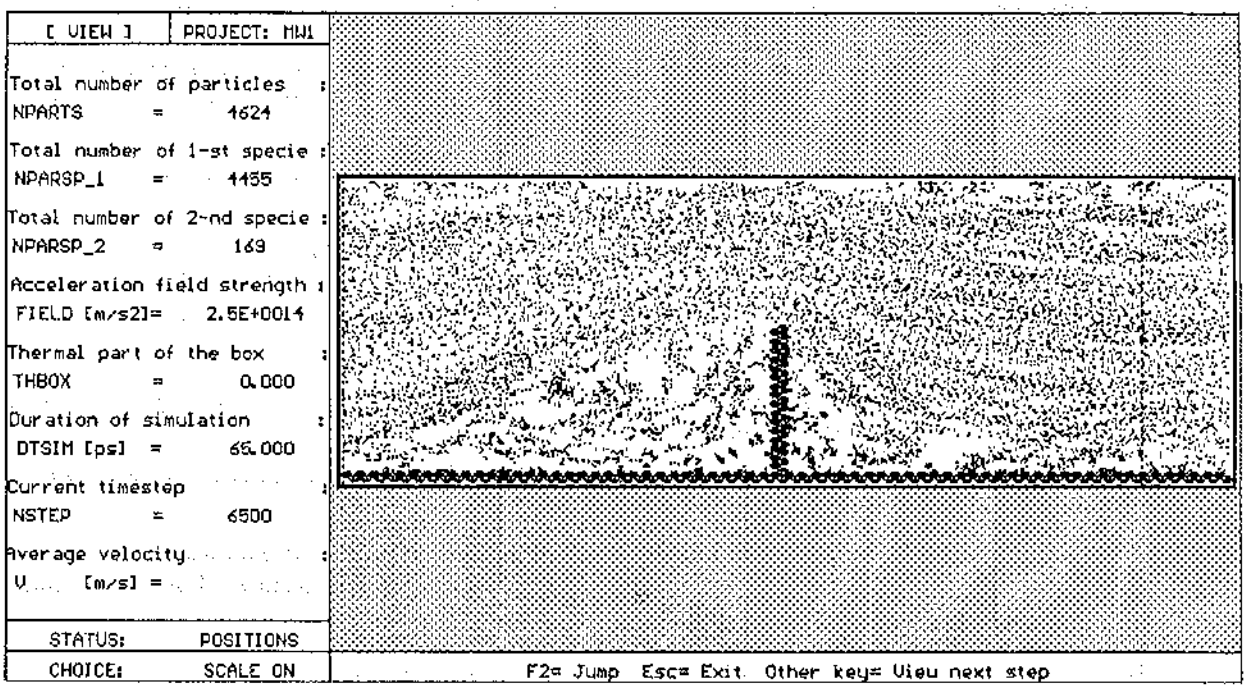


Figure A.1: Sample program screen.

The options are chosen from pull-down menus. *Help* option is at disposal for a novice. In Figure A.1 a sample screen of the program is presented.

B Simulation program HMD-MD2DLJ

The program ([11]) is written in FORTRAN 77 using the Olympus convention [15]–[17].

Timings for PC/XT (10 MHz) and for AT-386 (20 MHz) microcomputers (with coprocessors) have been obtained with RM/Fortran 77 (16-bit) and SVS Fortran 77 (32-bit) compilers.

No. of particles	MD time-step [s]		MD time-step per particle [s]	
	PC/XT	AT-386	PC/XT	AT-386
242	5.87	0.67	0.024	0.0028
512	8.72	1.15	0.017	0.0022
1152	15.37	2.26	0.013	0.0020
5000	59.89	8.87	0.012	0.0018

Table 1: Timings for HMD-MD2LJ program (average values for first 100 steps of simulation).

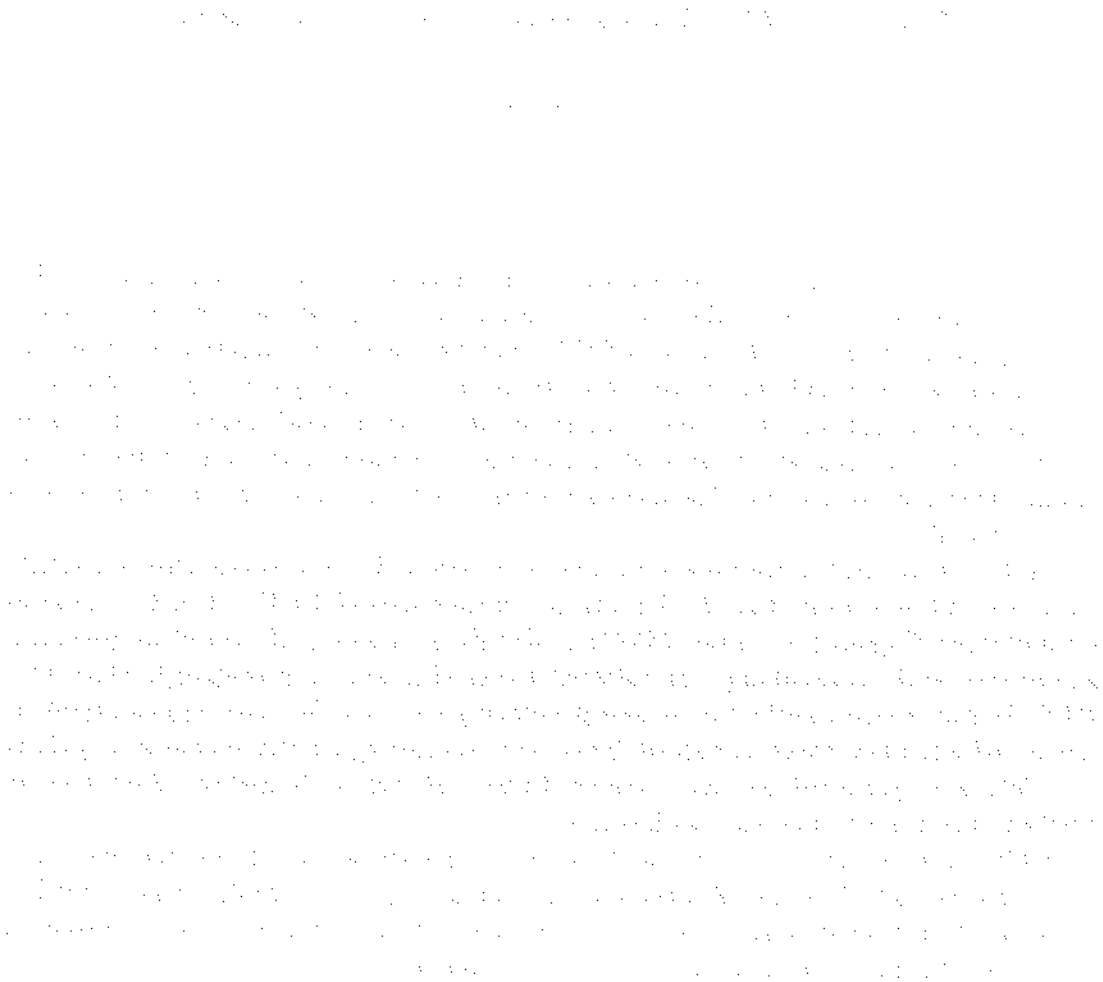
The CCP5 Literature Survey 1989

W. Smith

In the following pages we present the CCP5 Literature Survey for 1989. As in previous years, we note that the references included form only a fraction of all the possible papers relevant to the work of CCP5, but because of our limited resources, we have deliberately adapted our search profile to produce a manageable subset. We know this sometimes disappoints our readers, especially those whose work has been overlooked, but we repeat our promise to carry an addendum in a later newsletter, including any relevant references sent to us. Meanwhile we hope that the survey produced here is of value to you all.

 We are grateful to Mr. Geoff Jones, Head of Selective Services at INSPEC for his advice and assistance.

Finally, it is a pleasure to thank Mrs. C.M. Smith for proof reading the pages presented here and Miss A.P. Haskayne of the Daresbury Reprographic Service for her sterling work in typing it all. Since the CCP5 editors did precious little, it stands to reason they should be blamed for any errors that remain.



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