MOLECULAR DYNAMICS SIMULATION UPGRADE - SOFTWARE USER'S MANUAL

Synectics Corporation
Lisa Kolek and Geraldine W. Rogers

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APPROVED:  
HERBERT F. HELBIG  
Project Engineer

FOR THE DIRECTOR:  
JOHN J. BART  
Acting Director, Reliability 
Electromagnetics & Reliability Directorate

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Lisa Kolek and Geraldine W. Rogers

Synectics Corporation
111 East Chestnut Street
Rome NY 13440-2831

Rome Laboratory/ERDR
525 Brooks Rd
Rome NY 1344-4505

Rome Laboratory Project Engineer: Herbert F. Helbig/ERDR/(315) 330-3495

Approved for public release; distribution unlimited.

The purpose of the MDEM simulation upgrade was to improve performance, enhance the "user-friendly" features and generally clean up the source code for the MDEM simulation software tool. Performance improvement was primarily focused on the attainment of MDEM processing speedup. This was achieved at a low level by examining the existing code structure, as well as at a high level by modifying the simulation algorithm. Enhancement of user-friendly features included the implementation of a prototype graphical user interface (GUI) and the creation of the user's guide for both the command-line and GUI versions of MDEM. Code cleanup involved deletion of unnecessary code and comments, and reorganization of variables. In addition to this, miscellaneous software engineering and development support was provided to Rome Laboratory on an "as required" basis.
# TABLE OF CONTENTS

## SECTION ONE GENERAL OVERVIEW

1.1 APPLICATION OVERVIEW ............................................ 1
1.2 OPERATIONAL ENVIRONMENT ....................................... 3
1.3 USER INTERACTION .................................................. 3
1.4 CONVENTIONS USED .................................................. 3
1.5 REFERENCED DOCUMENTS ............................................ 5
  1.5.1 Government Documents ....................................... 5
  1.5.2 Non–Government Documents ................................. 5
1.6 ASSISTANCE AND PROBLEM REPORTING ........................... 6
1.7 DOCUMENT OVERVIEW ............................................... 6

## SECTION TWO DATA REQUIREMENTS ................................... 8

2.1 INPUTS .................................................................. 8
  2.1.1 Rules and Conventions ....................................... 8
    2.1.1.1 System Parameters .................................... 8
    2.1.1.2 Atomic Data ........................................... 13
    2.1.1.3 Pinning Data ......................................... 14
  2.2 OUTPUTS ............................................................ 15
    2.2.1 Main Output File ........................................... 15
    2.2.2 Thermostat File ............................................. 15
    2.2.3 Screen Display ............................................. 16
    2.2.4 Use of Outputs .............................................. 18
      2.2.4.1 Line Graph .......................................... 18
      2.2.4.2 RasMol Output ........................................ 18

## SECTION THREE OPERATING INSTRUCTIONS ........................ 19

3.1 INSTALLING MDEM ................................................... 19
3.2 USING MDEM .......................................................... 21
  3.2.1 Command–Line Procedures ................................... 21
  3.2.2 Graphical User Interface Operation ....................... 23
    3.2.2.1 Functionality ......................................... 23
    3.2.2.2 Operating Instructions ............................... 25
3.3 RESOLVING ERRORS .................................................. 33

## SECTION FOUR FURTHER DEVELOPMENT OF MDEM ............ 36

4.1 SOFTWARE INVENTORY ............................................... 36
  4.1.1 Command–line Version ....................................... 38
  4.1.2 Graphical User Interface Version .......................... 38
4.2 ESTABLISHING COMPILER ENVIRONMENT ....................... 39
  4.2.1 Command–Line Compilers .................................... 39
4.2.2 Integrated Development Environment

APPENDIX A ACRONYMS

APPENDIX B SAMPLE FILES
B1. INPUT/OUTPUT FILE
B2. TM FILE
B3. PINNING POINT FILE
B4. OUTPUT FILE
B5. COMMAND-LINE SCREEN DISPLAY

APPENDIX C DJGPP
C1. GENERAL INFORMATION
C2. INSTALLATION
C3. COMPILER FLAGS USED

APPENDIX D MICROSOFT VISUAL C++
D1. GENERAL INFORMATION

APPENDIX E POSTPROCESSING VIEWER
List of Exhibits

Exhibit 1. Molecular Dynamics Simulation Using MDEM .................................................. 2
Exhibit 2. Data Explorer Header ...................................................................................... 9
Exhibit 3. Status Data ..................................................................................................... 9
Exhibit 4. Control Data .................................................................................................. 10
Exhibit 5. Pinning Point File ......................................................................................... 14
Exhibit 6. Thermostat File ............................................................................................. 15
Exhibit 7. Command-line Messages to Screen .............................................................. 16
Exhibit 8. GUI Messages to Screen .............................................................................. 17
Exhibit 9. Graph of Thermostat Data ........................................................................... 18
Exhibit 10. Copying Executable ..................................................................................... 19
Exhibit 11. File Management Options .......................................................................... 20
Exhibit 12. MDEM Main Screen ................................................................................... 26
Exhibit 13 Open Dialog Screen ...................................................................................... 26
Exhibit 14. MDEM Data Display .................................................................................. 27
Exhibit 15. Pinning Constants ....................................................................................... 28
Exhibit 16. Thermostat Data ........................................................................................ 29
Exhibit 17. Pinning Points .............................................................................................. 30
Exhibit 18. Atom Data .................................................................................................. 31
Exhibit 19. Save As ....................................................................................................... 31
Exhibit 20. MDEM Main Screen Showing Execution Time ........................................... 32
Exhibit B1. 13–Atom Input File ..................................................................................... B-1
Exhibit B2. TM File Listing ............................................................................................ B-3
Exhibit B3. TM File from 9,758 Atoms ........................................................................... B-3
Exhibit B4. Header Data for 9,758 Atom Data Set ......................................................... B-3
Exhibit B5. Pinning File ................................................................................................ B-5
Exhibit B6. 13–Atom Output File ................................................................................... B-5
Exhibit B7. Command–Line Screen Display ................................................................. B-7

List of Tables

Table 1. Conventions ...................................................................................................... 4
Table 2. System Parameters .......................................................................................... 10
Table 3. Input Rules ....................................................................................................... 12
Table 4. MDEM Error and Warning Messages ............................................................. 33
Table 5. Timing Examples ............................................................................................. 36
Table 6 Software Inventory ........................................................................................... 37
Table D1. Configuration Choices .................................................................................. D-1
Table E1. Pdb File Format .............................................................................................. E-1
This Software User's Manual (SUM) presents the information and instructions necessary for user interaction with the Molecular Dynamics Simulation of Electronic Materials program, "MDEM." The information contained herein will instruct the user about the procedures required to install and carry out the operation of the MDEM software.

This report satisfies the Contract Data Requirements List (CDRL) A003 according to DI–MISC–80711/T, Scientific and Technical Reports, which specifies the document's format be in accordance with ANSI Z39.18–1987, "Scientific and Technical Reports: Organization, Preparation, and Production."

1.1 APPLICATION OVERVIEW

Atomic motion reduces the useful life of microcircuits. Rome Laboratory's (Rome Lab's) approach was to develop simulation tools to investigate the three-dimensional atomic motion and structure. This solution uses molecular dynamics simulation to examine the growth and transport properties of polycrystalline structures at the molecular scale. The purpose of MDEM, therefore, is to reveal the atomic-level mechanisms that are responsible for the degradation of microelectronics components and interconnects.

The MDEM software reads in a user-supplied data set consisting of such input parameters as initial system temperature, number of integration steps, cutoff distance, x, y, and z coordinates and velocity components for the atoms, and a tag denoting each atom’s species, thermal, and grain properties. The user can supply an optional data set which describes the points to which atoms may be pinned by elastic forces. Data validation functions check for the presence of data, as well as checking to see that the values are within valid ranges. Next, MDEM performs the numerical integration of f=ma according to Stanley's STA\textsuperscript{1}. To efficiently perform the interatomic force calculations required by the integration, a grid of cells is overlaid on the atom data. This method of partitioning the data results in non-redundant pairing of atoms by examining the interaction between each cell and half of its adjacent neighbors. The data are written to file periodically, at a frequency set by the user in either the input file or from MDEM's graphical user interface (GUI).

\textsuperscript{1} Robert W. Stanley. "Numerical Methods in Calculation". American Journal of Physics, volume 52, number 6, p. 499 (June 1984)
The main output of the simulation is a data set, listing the atoms’ new coordinates, velocities, and the atoms’ tags. A secondary output file, optionally chosen by the user, is the thermostat file. The user can plot the thermostat data to determine changes in temperature.

With molecular visualization packages, such as RasMol, which render molecular coordinates on the screen in a three-dimensional representation, the reformatted output from MDEM can be examined for density fluctuations due to shock or sound waves, reconstruction of a surface to achieve a lower energy configuration, and abrupt changes in regularity between regions of well-formed crystallinity. Exhibit 1 illustrates the functionality of MDEM in an end-to-end molecular dynamics simulation.

Exhibit 1. Molecular Dynamics Simulation Using MDEM

MDEM is a Rome Lab program, written and conceived by Rome Lab engineers and scientists. Synectics assisted Rome Lab in algorithm analysis and implementation, code cleanup, GUI design and implementation, and in preparing this SUM.
1.2 OPERATIONAL ENVIRONMENT

MDEM has two operational versions — command-line (CL) and graphical user interface (GUI). For both versions, the assumption is that MDEM resides locally. In its current format it is not intended for distributed processing.

The CL version is designed and coded to maximize the portability and flexibility of today’s high performance personal computers and workstations. It is written in ANSI C.

The GUI version is written for the 32-bit personal computer (PC). It was developed using Microsoft’s Visual C++, with calls to the Microsoft Foundation Classes (MFC).

The memory requirements for the executable code for both the CL and the GUI versions are under 300 KB. The amount of RAM and swap space depends upon the number of atoms in the data set.

1.3 USER INTERACTION

MDEM is designed to be an interactive system. However, while the CL version requires interaction, scripts can be written for automated operation of MDEM. The GUI version of MDEM uses the Windows Graphical User Interface to provide its look and feel. Use of a PC running a 32-bit operating system is required for the GUI version. For users unfamiliar with file transfer operations on the most common 32-bit PC operating system, “Windows 95,” a brief primer has been included in Section 3.1.

This manual introduces the user to the complete functionality of MDEM. It teaches the user how to implement these functions. The anticipated audience for the MDEM software are those familiar with molecular dynamics simulation. This manual, therefore, does not discuss how to analyze the results of the data.

1.4 CONVENTIONS USED

Certain conventions are used in this MDEM’s SUM to help the user understand the commands more easily. Table 1 describes these conventions.
<table>
<thead>
<tr>
<th><strong>DESCRIPTION</strong></th>
<th><strong>EXAMPLE</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>special font</td>
<td>C:\MDEM&gt;</td>
</tr>
<tr>
<td><strong>bold special font</strong></td>
<td>mdem4 06141555.25</td>
</tr>
<tr>
<td>italic special font</td>
<td>06141555.25</td>
</tr>
<tr>
<td><strong>SMALL CAPS BOLD FONT</strong></td>
<td>1. Enter a number in the <strong>TM FILE WRITE INTERVAL</strong> field.</td>
</tr>
<tr>
<td>type&gt;</td>
<td>1. type&gt;</td>
</tr>
<tr>
<td><img src="image" alt="Run MDEM" /></td>
<td>Select the <img src="image" alt="Run MDEM" /> button</td>
</tr>
<tr>
<td><img src="image" alt="Note" /></td>
<td><img src="image" alt="Note" /> The <img src="image" alt="Run MDEM" /> button is disabled during processing</td>
</tr>
<tr>
<td><img src="image" alt="Note" /></td>
<td><img src="image" alt="Note" /> The <img src="image" alt="Run MDEM" /> button is disabled during processing</td>
</tr>
<tr>
<td>1.</td>
<td>1. type&gt; mdem4 06141555.25</td>
</tr>
<tr>
<td>♦</td>
<td>♦ Or, use the “drag-and-drop” method to drop the input file 06141555.25 onto MDEM4.exe</td>
</tr>
<tr>
<td>⇒</td>
<td>⇒ displays the data file’s input parameters</td>
</tr>
<tr>
<td>&lt;CR&gt;</td>
<td>1. type&gt; mdem4 06141555.25 &lt;CR&gt;</td>
</tr>
</tbody>
</table>
The following instruction combines the conventions described in Table 1.

1. type `mdem4 data`

   ⇒ where `mdem4` is the name of the MDEM executable and `data` is the input data file name

   ⇒ displays the data file’s header information (list of parameters for the run)

   • Or, use the “drag–and–drop” method to drop the input file onto MDEM4.exe

1.5 REFERENCED DOCUMENTS

Government and non–Government documents used during the preparation of this document are referenced below.

1.5.1 GOVERNMENT DOCUMENTS

- DI–IPSC–81445 (Software Input/Output Manual — SIOM)
- DI–IPSC–81444 (Software Center Operator Manual — SCOM)
- DI–MCCR–80019A (Software User’s Manual — SUM)

1.5.2 NON–GOVERNMENT DOCUMENTS

- DJGPP Web Site, http://www.delorie.com/djgpp
1.6 ASSISTANCE AND PROBLEM REPORTING

Address MDEM inquiries to:

Herbert F. Helbig
Rome Laboratory/ERDR
525 Brooks Road
Rome, NY 13441-4505
e-mail: helbigh@rl.af.mil

1.7 DOCUMENT OVERVIEW

This manual is written for the most generic use of MDEM. It attempts to provide answers to questions which may arise, along with all information needed to use the MDEM software effectively.

Section 1 of this manual presents an overview of the MDEM application including its purpose, capabilities, operational environment, user interaction, the notational conventions used in this manual, and references.

Section 2 details the inputs required from the MDEM software as well as the expected outputs. Examples of each type of input and output are given.

Section 3 describes installation and operational procedures. It includes a brief primer on the Windows 95/NT file transfer techniques. Instructions are given for both the CL and the GUI versions of the MDEM software.

Section 4 contains information required for further development of the MDEM software, including a software inventory and instructions for setting up a project workspace for use with the Microsoft Visual C++ Development Studio.

Appendix A contains a list of commonly used acronyms.
Appendix B contains sample input files, main input file, and pinning point file.

Appendix C describes DJGPP, a freeware GNU C compiler, where to find DJGPP, and the flags used during compilation of the MDEM executable.

Appendix D contains notes on the various Microsoft Visual C++ code generation and optimization flags used during the development of MDEM.

Appendix E contains a brief description of RasMol, a molecular graphics viewer. Information is given on converting MDEM’s *.atm file into a file format suitable for viewing the molecular structure using the RasMol software.
SECTION TWO
DATA REQUIREMENTS

This section describes the input data required by the MDEM software as well as the results. Included are examples of each, in the form of screen shots. It must be noted that Microsoft WordPad was the editor used to display the text files in the examples. By no means is the user limited to the use of WordPad. Any text editor can be used for editing either the input or output files.

2.1 INPUTS

Section 2.1 covers the rules and convention for input files for the MDEM software. Examples are given in the form of screen shots. An example of the entire input data set is located in Appendix B.

2.1.1 RULES AND CONVENTIONS

MDEM requires at least one input data set consisting of the system parameters and the atomic coordinates, velocities, and tag value. Furthermore, a separate data set consisting of an identification number and x, y, and z coordinates which serve as pinning points can be input. Currently, all inputs are in text format. The only naming convention restriction for the input file (sometimes referred to as *.atm) is that the own_name parameter in the input file header must match the file's name.

2.1.1.1 SYSTEM PARAMETERS

The system parameters, or header data, are one per line, with the input value(s) following the parameter name (see Table 2). There are three sections to the header data: file structure information, status data, and control data. The structure information section shown in this SUM is generated by IBM’s “Data Explorer” software. It is not used by the MDEM software (Exhibit 2) except as part of the input data validation routines. Its presence facilitates viewing MDEM data with the “Data Explorer” software. Removal of this header will cause a data validation error ("Reached EOF too soon").
Exhibit 2.  Data Explorer Header

points = 5
format = ascii
header = marker "Start data\n"
field = locations, velocities, species
structure = 3-vector, 3-vector, scalar
type = float, float, int
dependency = positions, positions, positions
interleaving = field
end

The status data section contains a record for the previous MDEM run (Exhibit 3). From status data the user can determine the evolution of the current data set. In addition, system values for the current run are set by the final values from the last run of MDEM.

Exhibit 3.  Status Data

- Status Data -

date_time 970602191228
this_filename five.atm
last_filename five.atm
first_filename five.atm
t=0_filename arm010.atm

#_of_atoms 5
evolution_time 0.0000000000E+000
cut_off 5.8340000E-010

kin_energy 2.221899E-016
current_temperature 0.0000000000E+000
t_stat_work 1 -9.881646E-015
t_stat_work 2 0.0000000000E+000
t_stat_work 3 0.0000000000E+000
t_stat_work 4 0.0000000000E+000

The control data section (Exhibit 4) consists of input values which bound the data run, such as the number of integration steps for the current run and how often to increase the system temperature.
Exhibit 4. Control Data

- Control Data -

integration_steps_this_run 10
write_data_every 2000

time_step 2.00000E-015

value_of_xi 1 7.617050706E+011
desired_temperature 1 1.100000E+003
temp_step 1 0.000000E+000
pin_const 1 1.000000E-001 1.000000E-001 1.000000E-001

value_of_xi 2 0.00000000000E+000
desired_temperature 2 -1.000000E+000
temp_step 2 0.000000E+000
pin_const 2 1.000000E-001 1.000000E-001 1.000000E-001

value_of_xi 3 0.00000000000E+000
desired_temperature 3 -1.000000E+000
temp_step 3 0.000000E+000
pin_const 3 1.000000E-001 1.000000E-001 1.000000E-001

value_of_xi 4 0.00000000000E+000
desired_temperature 4 -1.000000E+000
temp_step 4 0.000000E+000
pin_const 4 1.000000E-001 1.000000E-001 1.000000E-001
pin_pt_filename
t-stat_time_const_tau 1.00000E-014

The input file requires a keyword identifier followed by the numerical value. These keywords are similar to, but not identical to, the source code's variables. Table 2 maps each keyword with the source code parameter; a one line description of each is also included.

Table 2. System Parameters

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>KEYWORD</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Status Data</td>
<td></td>
<td></td>
</tr>
<tr>
<td>hdr_date_time</td>
<td>date_time</td>
<td>creation date–time stamp for data set</td>
</tr>
<tr>
<td>own_name</td>
<td>this_filename</td>
<td>birth (file) name of data set</td>
</tr>
<tr>
<td>last_file</td>
<td>last_filename</td>
<td>data set from which this file was created</td>
</tr>
<tr>
<td>PARAMETER</td>
<td>KEYWORD</td>
<td>DESCRIPTION</td>
</tr>
<tr>
<td>-----------</td>
<td>-----------------------</td>
<td>-------------------------------------------------------</td>
</tr>
<tr>
<td>frst_file</td>
<td>frst_filename</td>
<td>first file of run</td>
</tr>
<tr>
<td>eve_file</td>
<td>t=0_filename</td>
<td>record of earliest file (*.atm) in evolution</td>
</tr>
<tr>
<td>numatoms</td>
<td>#_of_atoms</td>
<td>number of atoms</td>
</tr>
<tr>
<td>elapsed_time</td>
<td>evolution_time</td>
<td>system evolution time of the last run in seconds</td>
</tr>
<tr>
<td>cut_off</td>
<td>cut_off</td>
<td>the force cutoff length in meters of the last run</td>
</tr>
<tr>
<td>ke</td>
<td>kin_energy</td>
<td>system kinetic energy of the last run in Joules</td>
</tr>
<tr>
<td>temp</td>
<td>current_temperature</td>
<td>system temperature in Kelvins</td>
</tr>
<tr>
<td>WTCum</td>
<td>t_stat_work</td>
<td>accumulated energy delivered by the thermostats per integration step in Joules</td>
</tr>
</tbody>
</table>

**Control Data**

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>KEYWORD</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>nsteps</td>
<td>integration_steps_this_run</td>
<td>number of integration steps to be done</td>
</tr>
<tr>
<td>write_intrvl</td>
<td>write_data_every</td>
<td>frequency of writing out data to file</td>
</tr>
<tr>
<td>del_t</td>
<td>time_step</td>
<td>integration time step in seconds</td>
</tr>
<tr>
<td>xi0</td>
<td>value_of_xi</td>
<td>initial thermostat function value in (seconds)^-1</td>
</tr>
<tr>
<td>temp_step</td>
<td>temp_step</td>
<td>change in temp_ref per time step in Kelvins</td>
</tr>
<tr>
<td>temp_ref</td>
<td>desired_temperature</td>
<td>desired system temperature in Kelvins</td>
</tr>
<tr>
<td>pin_const</td>
<td>pin_const</td>
<td>array of pinning force constants in Newtons/meter</td>
</tr>
<tr>
<td>pin_file_name</td>
<td>pin_pt_filename</td>
<td>name of external pinning points file</td>
</tr>
<tr>
<td>tau</td>
<td>t_stat_time_const_tau</td>
<td>thermostat time constant in seconds</td>
</tr>
</tbody>
</table>

Most inputs have only one value. The exceptions are the pinning point constants (pin_const) and the thermostat related data items, including xi, t_stat_work, and temp_step. There can be a maximum of seven thermostat values used. For example, the data corresponding to thermostat 2 resides in array element 2 of all thermostat data arrays.

Table 3 presents the input “rules” — input length for character arrays, format conventions, sequencing of the data, punctuation, etc.
## Table 3. Input Rules

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DATA TYPE</th>
<th>INPUT LENGTH</th>
<th>MIN. VALUE</th>
<th>MAX. VALUE</th>
<th>RESTRICTIONS</th>
<th>REQ'D</th>
</tr>
</thead>
<tbody>
<tr>
<td>hdr_date_time</td>
<td>char</td>
<td>[12]</td>
<td>n/a</td>
<td>n/a</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>own_name</td>
<td>char</td>
<td>[13]</td>
<td>n/a</td>
<td>n/a</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>last_file</td>
<td>char</td>
<td>[15]</td>
<td>n/a</td>
<td>n/a</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>frst_file</td>
<td>char</td>
<td>[13]</td>
<td>n/a</td>
<td>n/a</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>eve_file</td>
<td>char</td>
<td>[13]</td>
<td>n/a</td>
<td>n/a</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>numatoms</td>
<td>ul²</td>
<td>*³</td>
<td>1</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>elapsed_time</td>
<td>double</td>
<td>*</td>
<td>none</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>cut_off</td>
<td>double</td>
<td>*</td>
<td>none</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>ke</td>
<td>double</td>
<td>*</td>
<td>none</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>temp</td>
<td>double</td>
<td>*</td>
<td>none</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>WTCum</td>
<td>double</td>
<td>[8]</td>
<td>none</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
</tbody>
</table>

### Status Data

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>DATA TYPE</th>
<th>INPUT LENGTH</th>
<th>MIN. VALUE</th>
<th>MAX. VALUE</th>
<th>RESTRICTIONS</th>
<th>REQ'D</th>
</tr>
</thead>
<tbody>
<tr>
<td>nsteps</td>
<td>ul</td>
<td>*</td>
<td>1</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>write_intervl</td>
<td>ul</td>
<td>*</td>
<td>0</td>
<td>none</td>
<td>must be &gt;= 0</td>
<td>✓</td>
</tr>
<tr>
<td>del_t</td>
<td>double</td>
<td>*</td>
<td>none</td>
<td>none</td>
<td>not equal 0</td>
<td>✓</td>
</tr>
<tr>
<td>xi0</td>
<td>double</td>
<td>[8]</td>
<td>none</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>temp_step</td>
<td>double</td>
<td>[8]</td>
<td>none</td>
<td>none</td>
<td></td>
<td>✓</td>
</tr>
<tr>
<td>temp_ref⁴</td>
<td>double</td>
<td>[8]</td>
<td>none</td>
<td>none</td>
<td>not equal 0</td>
<td>✓</td>
</tr>
<tr>
<td>pin_const</td>
<td>double</td>
<td>[8]</td>
<td>none</td>
<td>none</td>
<td>not equal 0</td>
<td>✓</td>
</tr>
<tr>
<td>pin_file_name</td>
<td>char</td>
<td>[20]</td>
<td>n/a</td>
<td>n/a</td>
<td></td>
<td>✓⁵</td>
</tr>
<tr>
<td>tau</td>
<td>double</td>
<td>*</td>
<td>none</td>
<td>none</td>
<td>not equal 0</td>
<td>✓</td>
</tr>
</tbody>
</table>

### Control Data

² ul — unsigned long integer
³ * — depends upon the target system’s definition of the variable (integer, double, etc).
⁴ temp_ref[] — holds the thermostat values. Atoms without thermostat tags will be assigned temp_ref[0] which should be negative. That forces their xi[0] to hold constant at xi[0]=0 so no thermostat force is applied in move_atoms().
⁵ pin_file_name — identifies the name of the pinning point file optionally supplied by the user. The keyword is required but an associated file name is not. If a pinning point file name is not supplied, the system does not pin the atoms.
2.1.1.2 Atomic Data

The atomic data follows the "Start Data" indicator in the input file. The atomic coordinates, velocities, and tag values are in seven columns by number of atoms format. Two spaces separate each column, including the one column reserved for the negative sign. The atom tag is left-justified within its column.

The x, y, and z coordinates and velocities are read into MDEM as double precision floats. The atom tag is an integer value.

The atom tags are the encoded numbers representing information on each atom, such as species or atomic number, grain, pinning status, and thermostat number. A bitwise mask and shift of the atom tag is used to extract these properties. For example, when atom_tag[i] is masked with PIN_MASK and shifted by PIN_SHIFT, a value of one (1) indicates that the atom is pinned. A value of zero (0) indicates that it is not pinned.

The following masks and shifts, taken from "Mdemutl.h" are ANDed with atoms_tag[i] to extract information about atom i:

- SPECIES_MASK — isolates atomic numbers, integers up to 127, that are used to enter a lookup table of atomic masses which is in moveAtoms() in mdemutl.c

- GRAIN_MASK — marks atoms according to their initial location so that visualization software can color them and reveal migrations. Eight possibilities are available by adding the various combinations of 0, 128, 256, 512 to atoms_tag[]. The combination 128 + 256 + 512 = 896 will tag an atom to be excluded from the system KE (and temperature) calculation. This is useful for deposition studies where the incoming atoms should not contribute to the substrate temperature until they become part of it. This interpretation is enforced in move_atoms. In Mdemutl.h, the GRAIN_MASK is defined as "896." GRAIN_SHIFT = 7.

- PIN_MASK — marks atoms that are pinned or immobilized in some way. Add 1,024 to atoms_tag[i] to pin atom i. In Mdemutl.h, the PIN_MASK is defined as "1024." PIN_SHIFT = 10.

- THERM_MASK — marks atom i as a thermostat set at one of 7 temperatures by adding combinations of 2,048, 4,096 and 8,192 to atoms_tag[]. THERM_SHIFT is the number of bits of right shift that will make the masked data equal to 0, 1, 2, ..., 7. Mdemutl.h defines the THERM_MASK as 14336 and the THERM_SHIFT as 11.

Note: Not all elements in the periodic table are supported by MDEM. Edit the arrays mass[] and rm_u0[] in mdemutl.c to add elements.
2.1.1.3 Pinning Data

This section discusses the pinning point data file, an optional input to MDEM. If a pinning point file name is listed after the keyword "pin_file_name", MDEM attempts to locate and open this file. The pinning point file consists of four columns, each separated by two spaces. The first column contains integers that correspond to the atom’s position in the main input file (i.e., the number 1 identifies the first atom in the main file, and so.). The values in the first column must be right-justified. The remaining three columns hold the x, y, and z coordinates used to pin atom[i]. These coordinates are double precision floats. The file can contain as many pinning points as desired as long as the number of atoms in the main input file are not exceeded. Exhibit 5 is an example of a pinning point file.

Exhibit 5. Pinning Point File

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1.375325E-08</td>
<td>-6.978250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-1.375325E-08</td>
<td>-6.436250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>-1.375325E-08</td>
<td>-5.894250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>-1.375325E-08</td>
<td>-5.352250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>-1.375325E-08</td>
<td>-4.810250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>-1.375325E-08</td>
<td>-4.268250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>-1.375325E-08</td>
<td>-3.726250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>-1.375325E-08</td>
<td>-3.184250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>-1.375325E-08</td>
<td>-2.642250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>-1.375325E-08</td>
<td>-2.100250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>-1.375325E-08</td>
<td>-1.558250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>-1.375325E-08</td>
<td>-1.016250E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>-1.375325E-08</td>
<td>-4.742500E-10</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>-1.375325E-08</td>
<td>6.774978E-11</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>-1.375325E-08</td>
<td>6.097496E-10</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>-1.375325E-08</td>
<td>1.151750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>-1.375325E-08</td>
<td>1.693750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>-1.375325E-08</td>
<td>2.235750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>-1.375325E-08</td>
<td>2.777750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>-1.375325E-08</td>
<td>3.319750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>-1.375325E-08</td>
<td>3.861750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>-1.375325E-08</td>
<td>4.403750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>-1.375325E-08</td>
<td>4.945750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>-1.375325E-08</td>
<td>5.487750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>-1.375325E-08</td>
<td>6.029750E-09</td>
<td>0.000000E+00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

* The above pinning point file is a valid example of a pinning point file. However, it does not correspond to the main input file shown as an example.
2.2 OUTPUTS

MDEM produces two types of output — information written to file and information displayed to the screen. MDEM writes a main output file automatically; the user must specifically request the thermostat file.

MDEM writes the main output file and the thermostat file to the same directory as the MDEM executable for both the CL and GUI versions. However, using the "Properties" feature of Windows 95/NT to specify the full path, the location of the output files can be changed.

2.2.1 MAIN OUTPUT FILE

The main output is the *.atm file which is written at a user specified frequency (write_data_every). As the output file can be used for an input file the same layout, rules and conventions apply. See Section 2.1 for a detailed discussion and Appendix B for an example.

2.2.2 THERMOSTAT FILE

A secondary output is the thermostat (*.tm) file (Exhibit 6) which is also user specified, both in whether to create and in what frequency to write the thermostat data. The values for the last integration step are also written to file. This file consists of several columns of numbers — the integration step number followed by the system temperature (temp), and the accumulated work done by the thermostats (WTcum[i]) at that integration step for each thermostat. The value for the accumulated work only writes to file if it is not equal to zero (0). The integration step is a unsigned long integer and ke and WTcum are double precision floats.

Exhibit 6. Thermostat File

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0001</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0002</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0003</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0004</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0005</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0006</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0007</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0008</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0009</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0010</td>
<td>+6.04949e+002</td>
<td>-9.88165e-015</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
2.2.3 Screen Display

Information is displayed to the screen both in the CL version as well as in the GUI version. The CL version writes to screen a summary of the input parameters, number and type of atoms, thermostat and accumulated energy after each integration, and time to execute the integration. Knowing the expected user responses during the run, the user can pipe the output to a file for viewing at a later time. In this example (Exhibit 7), the user elected to write a thermostat file every integration step.

Exhibit 7. Command-line Messages to Screen

PLEASE REVIEW THE FOLLOWING DATA.

Edit the header of the seed file 13rica.atm if they are incorrect.

There are 13 atoms in the system. The have evolved for 0.000000E+000 seconds, originally from the file 13RIC.atm

System ke and temperature are 0.000000E+000 J and 0.000000E+000 kelvins

Recall that Tstat<0 implies xi=constant=xi0.

Thermostat 1 is set for -5.000000E-008 kelvins and will change at temp_step 1 = 0.000000E+000 kelvins per step.

xi0 1 = 0.000000E+000 N s/m

Thermostat 2 is set for -1.000000E+000 kelvins and will change at temp_step 2 = 0.000000E+000 kelvins per step.

xi0 2 = 0.000000E+000 N s/m

Thermostat 3 is set for -1.000000E+000 kelvins and will change at temp_step 3 = 0.000000E+000 kelvins per step.

xi0 3 = 0.000000E+000 N s/m

Thermostat 4 is set for -1.000000E+000 kelvins and will change at temp_step 4 = 0.000000E+000 kelvins per step.

xi0 4 = 0.000000E+000 N s/m

The Tstat time constant is 1.000000E-014 seconds

10 integration time steps are scheduled each step of length 1.000000E-015 seconds

A *.atm file will be saved every 2000000 steps.

The force cut off length is 9.000000E-010 meters.

To modify these conditions, quit now and change the seed file.

The interatomic force model is called several times in move_atoms() by a name that should start with "force_". Both move_atoms() and force_* are in the file mdeemnul.c; look there for details.

-----------------------------------------------------------------------------------

-16-
Do you want to create a separate temperature output file?
Enter either a 'Y' or 'N'.
Enter the interval to use when writing a *.tm file.
Enter a 1 (one) to update after every step, or
a 5 for every fifth step, etc.

------------------------------------
Choose 'continue' if data are correct.
c -continue; q -quit

The atom data have loaded successfully.

There are 13 Ar atoms in this data set.

------------------------------------
Choose 'continue' if data are correct.
c -continue; q -quit

00001 +2.134e-013K +5.746e-035J
00002 +8.536e-013K +2.298e-034J
00003 +1.921e-012K +5.171e-034J
00004 +3.414e-012K +9.192e-034J
00005 +5.334e-012K +1.436e-033J
00006 +7.680e-012K +2.068e-033J
00007 +1.045e-011K +2.814e-033J
00008 +1.365e-011K +3.675e-033J
00009 +1.727e-011K +4.650e-033J
00010 +2.132e-011K +5.740e-033J
stop time: 165724
start time: 165724
Execution time = 0.00 seconds
Mean compute time per 1.000e-015 sec of simulation time
for a system of 13 atoms
was 0.000e+000 sec

mdem done

The GUI version of MDEM displays messages to the user in the bottom pane of the interface screen called the “Status Area” (Exhibit 8). These messages range from noting errors to updating the progress of the integration run.

**Exhibit 8. GUI Messages to Screen**
2.2.4 USE OF OUTPUTS

One use of computer simulations is to assist the user in the calculation of complex equations. Another use is the visual aspect — one cannot obtain an intuitive notion of either the starting data or the output data from a list of coordinates. One solution, therefore, is to employ a software package which represents the atom coordinates in three dimensions. With a graphic, spatial patterns are more obvious. Hence the use of packages, such as RasMol which is available free for download from the Internet.

2.2.4.1 LINE GRAPH

Using the data from the thermostat file, a plot can be graphed. A smooth curve more accurately reflects changes in the data. Exhibit 9 is a plot of the thermostat data from a data set consisting of 9,758 atoms over 20 integrations. The plot was created using Microsoft Excel.

Exhibit 9. Graph of Thermostat Data

2.2.4.2 RasMol OUTPUT

RasMol renders the three–dimensional coordinates for a molecule using the pdb file format. This format is not supported by MDEM, although MDEM’s molecular coordinates can be stripped from the main output file and reformatted appropriately. Appendix E contains more information on the postprocessing required to move from the *.atm to a *.pdb format.
SECTION THREE
OPERATING INSTRUCTIONS

Section 3 contains the operating instructions for MDEM, from installation, to operation of either version of MDEM, to error resolution.

3.1 INSTALLING MDEM

Installing and executing MDEM depends upon the platform and operating system in use. The directions presented here apply to installing both the executable and the source code. Since the target platform for MDEM is the PC, the instructions here are specific to machines running either Windows™ 95 or Windows™ NT (version 4.0) and will work for either the CL version or GUI version of MDEM.

Basically, there are three methods of moving files in Windows 95.

- (MS-Prompt) Command-line — use the copy command to copy a file from one location to another. For example, use the MS-DOS command-line to copy MDEM\gui.exe from a floppy disk in drive A to a folder called MDEM\FOLDER,

1. type> copy a:\Mdem\gui.exe \MDEM\FOLDER <CR>

   ⇒ displays the message: 1 file(s) copied
   ⇒ see Exhibit 10

Exhibit 10. Copying Executable
“Drag-and-drop”

1. Using the mouse, click on the target icon.

2. Keeping the mouse button depressed, “drag” the icon to the intended destination.

“Copy-paste”

1. Click on the icon with the right mouse button.
   ⇒ displays a popup menu of editing/file management options (Exhibit 11)

2. Move the mouse pointer to the command **copy** and release the button.
   ⇒ creates a copy of the file in memory

3. Click the right mouse button on the intended target directory.

4. Click the right mouse button.
   ⇒ displays the popup menu

5. Select the **paste** command.
   ⇒ creates a copy of the file in the selected directory

**Exhibit 11. File Management Options**

To install MDEM on a workstation, consult the system operator and/or system administration guidelines for the instructions specific to the particular environment.
3.2 USING MDEM

MDEM has two operational modes, CL and GUI. Sections 3.2.1 lists the procedures for using the CL version, while Section 3.2.2 details capabilities and procedures for using the GUI version.

3.2.1 COMMAND–LINE PROCEDURES

The following instructions describe and illustrate the process for executing the CL version of MDEM, by either using the MS–DOS prompt window or using the “drag–and–drop” execution method.

If a pinning point file is specified in the main input file, it must be located in the same directory as the MDEM executable.

1. type> mdem4 data

⇒ where mdem4 is the name of the MDEM executable and data is the name of the input data file

∗ Or, use the “drag–and–drop” method to drop the input file onto mdem4.exe

⇒ displays a review of the data contained in the header information

PLEASE REVIEW THE FOLLOWING DATA.

Edit the header of the seed file five.atm if they are incorrect.

There are 5 atoms in the system.
They have evolved for 0.000000E+000 seconds,
originally from the file armo10.atm

System ke and temperature are 2.221899E-016 J and 2.145732E+006 kelvins

Recall that Tstat<0 implies xi=constant=x0.

Thermostat 1 is set for 1.100000E+003 kelvins
and will change at temp_step 1 = 0.000000E+000 kelvins per step.
x10 1 = 7.617051E+011 N s/m
Thermostat 2 is set for -1.000000E+000 kelvins
and will change at temp_step 2 = 0.000000E+000 kelvins per step.
x10 2 = 0.000000E+000 N s/m
Thermostat 3 is set for -1.000000E+000 kelvins
and will change at temp_step 3 = 0.000000E+000 kelvins per step.
x10 3 = 0.000000E+000 N s/m
Thermostat 4 is set for -1.000000E+000 kelvins
and will change at temp_step 4 = 0.000000E+000 kelvins per step.
x10 4 = 0.000000E+000 N s/m

The Tstat time constant is 1.000000E-014 seconds
15 integration time steps are scheduled
each step of length 2.000000E-015 seconds
A *.atm file will be saved every 2000 steps.

The force cut off length is 5.834000E-010 meters.
To modify these conditions, quit now and change the seed file.
The interatomic force model is called several times in move_atoms() by a name that should start with "force_". Both move_atoms() and force_ are in the file mdemutl.c; look there for details.

⇒ displays the input parameters to the screen

⇒ displays message allowing the user to create a "separate temperature output file"

Do you want to create a separate temperature output file? Enter either a 'Y' or 'N'.

2. type> Y

⇒ requests that the user enter the number for the write frequency

Enter the interval to use when writing a *.tm file. Enter a 1 (one) to update after every step, or a 5 for every fifth step, etc.

3. type> 1

⇒ "1" writes to file the thermostat information after every step

Choose 'continue' if data are correct.
C -continue; Q -quit

4. type> C

⇒ loads the atom data

⇒ displays the "successful load" message

The atom data have loaded successfully.

⇒ displays the number of atoms by type.

There are 5 Ni atoms in this data set.

⇒ displays message to continue if input parameters are correct, or to quit if not correct (enter "c" to continue or "q" to quit)

Choose 'continue' if data are correct.
C -continue; Q -quit

5. type> C

⇒ starts execution

⇒ writes to file a record of the run

⇒ displays summary of data to screen for each integration step
Daemon displays the time to manipulate the atoms

```
stop time: 220106
start time: 220106
Execution time = 0.05 seconds
Mean compute time per 2.000e-015 sec of simulation time
for a system of 5 atoms
was 3.333e-003 sec
```

⇒ displays the message, “mdem done”

```
mdem done
```

Using “drag–and–drop” to start MDEM spawns a MS–DOS prompt window which will disappear as soon as the “mdem done” message has displayed.

⇒ returns to the command–line prompt

To interrupt MDEM at any point during the integration, while holding down <CTRL>, press <C>.

Refer to Section 3.3 for instructions on resolving any errors.

### 3.2.2 Graphical User Interface Operation

The GUI version of Mdem contains all of the functional capabilities of the CL version in addition to features that allow the user to interactively correct invalid data and create new data sets with new input parameters.

#### 3.2.2.1 Functionality

The enhanced capabilities of the GUI version are:
Main functions

- Load Data — loads the data from any *.atm file; uses the Windows’ standard Open dialog, allowing the user to traverse the machine’s directory.
- Save Data — saves to a new file the inputs as seen on the interface along with the original atom data loaded; uses the Window’s standard Save As dialog.
- Reset Data — restores the original values for the current data set; Once the data has been saved as a new input file, the new input values are the “original.”
- Run Mdem — processes the integration; if any changes to the original values are detected, the Save As dialog automatically displays. To not save the changes (if already saved, for example), click on the Save As dialog’s “Cancel” button.
- Cancel Mdem — cancels the current operation; if the integration is in progress, Mdem finishes the current integration step and writes out the last step to the output file.
- Exit Mdem — exits the program
- Help — displays minimal information on the program

View Atoms — displays the number of atoms by type comprising the data set

View Thermostat Data 1–7 — displays the values for the seven initial thermostats in a popup window for:
  - xi0 — initial thermostat values
  - temp_ref — desired system temperature
  - temp_step — change in temp_ref per time step
  - total work — accumulated energy delivered by the thermostats per integration step
  - temp_stat — signals that thermostat x is active if the value equals one (1)

Pinning

- Change Pinning File — displays the name of the pinning file associated with the loaded data set, if any; user can use this button to display the OPEN dialog, for selecting or changing a pinning file
- View Pinning Points — displays the x, y, and z pinning points (coordinates) in a popup window
- View Pinning Constants — displays the x, y, and z pinning force constants in a popup window
Status Area

- Processing Messages — displays processing messages such as, detection of invalid data during the load process, the current integration step number, and the mean compute time per sec of simulation time for a system of n-atoms.
- Processing Meter — visual confirmation that the system is still working.

The values of all fields on the interface, except the Execution, System Initial Temperature, and Pinning file name fields, can be changed directly on the interface. This provides the flexibility of running integrations with minor to major variations in the system parameters while saving the changes as new files.

3.2.2.2 Operating Instructions

The following instructions list and illustrate the procedures for using the GUI version of MDEM.

Tip: If a pinning point file is specified in the main input file, it must be located in the same directory as the MDEM executable. With the GUI version, the pinning point file can be changed via the Change Pinning File button after the initial data load is complete.

1. Start MDEM4_GUI.exe from the (graphical) directory structure, by one of the following methods:
   - Double-click the left mouse button on MDEM4_GUI.exe
   - Or, from the MS-DOS command line, type `mdem4_gui`

⇒ displays the MDEM main dialog (Exhibit 12)
2. Select **Load Data** button

⇒ displays the **OPEN** dialog (Exhibit 13)
Select the desired input file by either of the following actions

- Double-click on the file name in the listing, or
- Type the file name into the **FILE NAME** field on the dialog and then click on the **Open** button

⇒ retrieves and displays the data in the appropriate fields (Exhibit 14)

**Exhibit 14. MDEM Data Display**

3. Enter a number in the **TM FILE WRITE INTERVAL** field
   
   ⇒ determines how often to write to file the thermostat information
   ⇒ default equals 1 (one), writing data after each integration step
   ⇒ change to 0 (zero) to not write a separate thermostat file

4. Enter changes to the input parameters directly on the interface

   ⇒ **DO NOT** hit “Enter” on the keyboard
5. Select button to make changes to pinning points

⇒ displays the PINNING CONSTANTS dialog, with values from the input file (Exhibit 15)

**Exhibit 15. Pinning Constants**

- Click on the desired field to make a change
- Enter the new value
- Select the button

6. Select button to make changes to the thermostat data

⇒ displays the THERMOSTAT DATA dialog, with values specified in the input file (Exhibit 16)
Exhibit 16. Thermostat Data

- Click on the desired field to make a change
- Enter the new value
- Select the **OK** button
  - removes the dialog and updates the values in the system

7. Select the **View Pinning Points** button to view the pinning points

  - displays the **PINNING POINTS** dialog (read-only) from the pinning file shown in the pinning file read-only field (Exhibit 17)
    - column one: atom number
    - column two: x coordinate
    - column three: y coordinate
    - column four: z coordinate
Exhibit 17. Pinning Points

- Click the [Change Pinning File] button to select another pinning file
  ⇒ displays the OPEN dialog
- Select desired input file by doing either of the following.
  - double-click on the desired file name in the list, or
  - type the file name into the FILE NAME field and then click on the Open button
  ⇒ displays the selected file name in the pinning file read-only field
- Reselect the [View Pinning Points] button to view the new pinning points

8. Select [View Atoms] button to view information on the atom types
  ⇒ displays the ATOM DATA dialog (read-only) which lists the types of atoms comprising the data set and the number of each type (Exhibit 18)
9. Select the **Save Data** button to save any changes for a new input file
   
   ⇒ displays the **SAVE AS** dialog (Exhibit 19)
   
   ♦ Enter a file name in the **SAVE AS** dialog **FILE NAME** field to save changes
   
   • Select the **Save** button

**Exhibit 19. Save As**

⇒ writes a new file as a record of the input parameters

⇒ can select at any time

⇒ optional
10. Select the **Build MDEM** button

⇒ displays the **SAVE AS** dialog if any changes to the original inputs are detected

♦ Enter a file name in the **SAVE AS** dialog **FILE NAME** field to save changes
  
  • Select the **Save** button

♦ Or, select **Cancel** if changes were saved using **Save Data** button or to not save the changes

⇒ executes the integration

⇒ writes a new file as a record of the input parameters executes the program

⇒ writes the TM file during execution

⇒ writes the output file

⇒ displays the time required to integrate the data set in the **EXECUTION TIME** field

(Exhibit 20)

**Exhibit 20. MDEM Main Screen Showing Execution Time**
11. Select the **Cancel MDEM** button to halt the integration process

⇒ cancels the integration step
⇒ disables all buttons, except **Load Data** and **Res MDEM**.

♦ Select **Load Data** to load another data set

12. Select **Exit MDEM** button

⇒ exits the program

---

Clicking the X-box in the top right corner of the dialog, on the title bar, kills the program, losing any data not written to file.

---

### 3.3 RESOLVING ERRORS

MDEM generates the following error and warning messages when confronted with incorrect or missing data (Table 4).

#### Table 4. MDEM Error and Warning Messages

<table>
<thead>
<tr>
<th>MESSAGE</th>
<th>RESOLUTION</th>
</tr>
</thead>
</table>
| Must enter filename on command line; quit & restart | ♦ Enter Q to quit MDEM  
♦ Use the MS-DOS command line to enter: mdem data, or drag the data icon onto the executable icon |
| 'this_filename' in input file disagrees with command line argument | ♦ CL — Quit MDEM  
♦ Edit data file's header to match the file names  
♦ GUI — Correct the file name in the **FILE NAME** field |
| write_intrvl must be >= 1                   | ♦ CL — Quit MDEM  
♦ Edit data file's header  
♦ GUI — Correct the value in the **ATM FILE WRITE INTERVAL** field |
| del_t must not be 0.0                        | ♦ CL — Quit MDEM  
♦ Edit data file's header  
♦ GUI — Correct value in the **TIME INTERVAL** field |
<table>
<thead>
<tr>
<th>MESSAGE</th>
<th>RESOLUTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>tau must not be 0.0</td>
<td>✧ t_stat_time_const_tau value cannot equal zero (0)</td>
</tr>
<tr>
<td></td>
<td>✧ CL — Quit MDEM</td>
</tr>
<tr>
<td></td>
<td>◦ Edit data file’s header</td>
</tr>
<tr>
<td></td>
<td>✧ GUI — Correct the value in the THERMOSTAT TIME CONSTANT field</td>
</tr>
<tr>
<td>atom is pinned w/o supporting data</td>
<td>✧ pin_const[t_stat] == 0.0</td>
</tr>
<tr>
<td></td>
<td>✧ CL — Quit MDEM</td>
</tr>
<tr>
<td></td>
<td>◦ Edit data file</td>
</tr>
<tr>
<td></td>
<td>◦ Restart MDEM</td>
</tr>
<tr>
<td></td>
<td>✧ GUI — Edit *.atm file in text editor</td>
</tr>
<tr>
<td></td>
<td>◦ Reload data file</td>
</tr>
<tr>
<td>atom is pinned but no pinning point is specified</td>
<td>✧ CL — Quit MDEM</td>
</tr>
<tr>
<td></td>
<td>◦ Edit pinning point file</td>
</tr>
<tr>
<td></td>
<td>✧ GUI — Edit pinning point file using text editor</td>
</tr>
<tr>
<td></td>
<td>◦ Save changes</td>
</tr>
<tr>
<td></td>
<td>◦ Reload pinning point file via the [Change Pinning Point File] button</td>
</tr>
<tr>
<td>reached EOF too soon looking for end could not open file</td>
<td>✧ File does not contain the correct number of lines</td>
</tr>
<tr>
<td></td>
<td>✧ CL — Quit MDEM</td>
</tr>
<tr>
<td></td>
<td>◦ Edit *.atm file in text editor and save changes</td>
</tr>
<tr>
<td></td>
<td>✧ GUI — Edit *.atm file in text editor and save changes</td>
</tr>
<tr>
<td></td>
<td>◦ Reload data file</td>
</tr>
<tr>
<td>desired temperature cannot be zero</td>
<td>✧ temp_ref values cannot equal zero (0)</td>
</tr>
<tr>
<td></td>
<td>✧ CL — Quit MDEM</td>
</tr>
<tr>
<td></td>
<td>◦ Edit data file’s header to change temp_ref values and save changes</td>
</tr>
<tr>
<td></td>
<td>◦ Restart MDEM</td>
</tr>
<tr>
<td></td>
<td>✧ GUI — Correct value in the TEMP REF fields on the THERMOSTAT dialog</td>
</tr>
<tr>
<td>t_stat_time_const cannot be zero</td>
<td>✧ t_stat_time_const_tau value cannot equal zero (0)</td>
</tr>
<tr>
<td></td>
<td>✧ CL — Quit MDEM</td>
</tr>
<tr>
<td></td>
<td>◦ Edit data file’s header</td>
</tr>
<tr>
<td></td>
<td>✧ GUI — Correct the value in the THERMOSTAT TIME CONSTANT field</td>
</tr>
<tr>
<td>MESSAGE</td>
<td>RESOLUTION</td>
</tr>
<tr>
<td>---------</td>
<td>------------</td>
</tr>
</tbody>
</table>
| pin_const.(x,y,z) = 0.0; this will have no effect on the system. Unless you change pin_const in the header, pin_const.(x,y,z) will be removed from future *.atm files. | ♦ pin_const.(x,y,z) = 0.0  
♦ CL — Quit MDEM  
♦ Edit data file’s header to change pin_const values and save changes  
♦ Restart MDEM  
♦ GUI — Correct values in the PINNING FORCE CONSTANT fields on the PINNING CONSTANTS dialog |
| reached EOF too soon after dx header | ♦ Data file is incomplete  
♦ CL — Quit MDEM  
♦ Edit *.atm file in text editor and save changes  
♦ GUI — Edit *.atm file in text editor and save changes  
♦ Reload data file |
| could not open pinning point file | ♦ Specified pinning point file does not exist in the directory being searched |

The CL version displays the error message or warning to the screen and then prompts the user to quit, edit the data file, and then restart MDEM.

The GUI version of MDEM flags the same warnings, which display in the Status Area on the MDEM dialog. In addition to errors detected during the loading process, the GUI version automatically flags the entry of wrong data types entered on the MDEM dialog (i.e., user entered a float in a field requiring an integer). These messages are displayed in a popup box which can be dismissed by clicking the dialog’s “Ok” button.
SECTION FOUR
FURTHER DEVELOPMENT OF MDEM

The MDEM program provides information on the forces interacting between atoms, thereby providing a vehicle for predicting a substance’s static and dynamic properties. In doing so the performance of the MDEM software varies significantly based on compiler, mode, platform, number of atoms, and number of integration steps. Table 5 provides the user with a comparison of the various compilers, their representative compilation/optimization flags, and the experienced execution times for a box about 70 x 106 x 140 angstroms filled with 112423 FCC Nickel atoms. The tags have 2,048 added to them to activate thermostat #1. The atoms were integrated for 20 steps.

A more detailed table can be found in Volume I, Scientific and Final Technical Reports (FINAL).

Table 5. Timing Examples

<table>
<thead>
<tr>
<th>OPERATIONAL MODE</th>
<th>OPTIMIZATION</th>
<th>TOTAL EXECUTION TIME (Seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pentium (75 MZ, 24 MB RAM, Windows 95)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CL</td>
<td>–O1</td>
<td>insufficient memory</td>
</tr>
<tr>
<td>CL</td>
<td>–O2</td>
<td>insufficient memory</td>
</tr>
<tr>
<td>MVCC</td>
<td>Blend, Global</td>
<td>1037.82</td>
</tr>
<tr>
<td>GUI</td>
<td>Blend, Global</td>
<td>1169</td>
</tr>
<tr>
<td>Pentium Pro (200 MZ, 64 MB RAM, Windows NT)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>CL</td>
<td>–O1</td>
<td>396.70</td>
</tr>
<tr>
<td>CL</td>
<td>–O2</td>
<td>286.81</td>
</tr>
<tr>
<td>MVCC</td>
<td>Blend, Global</td>
<td>191.64</td>
</tr>
<tr>
<td>GUI</td>
<td>Blend, Global</td>
<td>275</td>
</tr>
</tbody>
</table>

4.1 SOFTWARE INVENTORY

This section contains information on the software files required for further development of the MDEM software as well as the name of the executable required. Table 6 lists the files required
for compilation for the two versions. The CL version requires 8 files, while the GUI created using Microsoft Visual C++ (version 5.0) includes the same 8 files plus another 29 files.

<table>
<thead>
<tr>
<th>FILE</th>
<th>CL</th>
<th>GUI</th>
</tr>
</thead>
<tbody>
<tr>
<td>AfxDlg.rtf</td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td>MakeHelp.bat</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdem.c</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdemo.c</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdemmem.c</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdemutil.c</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdem.h</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdemo.h</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdemmem.h</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>Mdemutil.h</td>
<td>✔</td>
<td>✔</td>
</tr>
<tr>
<td>PinConstDlg.cpp</td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td>PinConstDlg.h</td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td>PinPointsDlg.cpp</td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td>PinPointsDlg.h</td>
<td>✔</td>
<td></td>
</tr>
<tr>
<td>resource.h</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>StdAfx.cpp</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>StdAfx.h</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.ico</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.rc2</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.cnt</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.hm</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.hpj</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.ph</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.aps</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.bak</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.cpp</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.dsp</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.dsw</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.h</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.mak</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.ncb</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.opt</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.plg</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1.rc</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1Dlg.cpp</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>test1Dlg.h</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>ThermDlg.cpp</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>ThermDlg.h</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>ViewAtomsDlg.cpp</td>
<td></td>
<td>✔</td>
</tr>
<tr>
<td>ViewAtomsDlg.h</td>
<td></td>
<td>✔</td>
</tr>
</tbody>
</table>
4.1.1 COMMAND–LINE VERSION

To run the CL version of MDEM, the executable MDEM4.exe is required. Consult Table 6 for the exact files required to compile the CL version of MDEM.

4.1.2 GRAPHICAL USER INTERFACE VERSION

The GUI version requires the executable MDEM4_gui.exe. Consult Table 6 for a complete listing of the files required to compile the GUI version of MDEM.

The Microsoft Visual C++ programming environment requires the creation of a project workspace. In version 5.0, this file has the extension of *.dsw. The following is a description of each file created by Microsoft Visual C++, as described in the file “ReadMe.txt”:

- test1.h — This is the main header file for the application. It includes other project specific headers (including Resource.h) and declares the CTest1App application class.

- test1.cpp — This is the main application source file that contains the application class CTest1App.

- test1.rc — This is a listing of all of the Microsoft Windows resources that the program uses. It includes the icons, bitmaps, and cursors that are stored in the RES subdirectory. This file can be directly edited in Microsoft Developer Studio.

- res\test1.ico — This is an icon file, which is used as the application’s icon. This icon is included by the main resource file test1.rc.

- res\test1.rc2 — This file contains resources that are not edited by Microsoft Developer Studio. Place all resources not editable by the resource editor in this file.

- test1.clw — This file contains information used by ClassWizard to edit existing classes or add new classes. ClassWizard also uses this file to store information needed to create and edit message maps and dialog data maps, and to create prototype member functions.

- test1Dlg.h, test1Dlg.cpp (the dialog) — These files contain your CTest1Dlg class. This class defines the behavior of the application’s main dialog. The dialog’s template is in test1.rc, which can be edited in Microsoft Developer Studio.

- MakeHelp.bat — Use this batch file to create the application’s Help file, test1.hLP.
test1.hpj — This file is the Help Project file used by the Help compiler to create the application's Help file.

hlp\*.bmp — These are bitmap files required by the standard Help file topics for Microsoft Foundation Class (MFC) Library standard commands.

hlp\*.rtf — This file contains the standard help topics for standard MFC commands and screen objects.

StdAfx.h, StdAfx.cpp — These files are used to build a precompiled header (PCH) file named test1.pch and a precompiled types file named StdAfx.obj.

Resource.h — This is the standard header file, which defines new resource IDs. Microsoft Developer Studio reads and updates this file.

These files are required in order to continue development on the current implementation of the GUI version of MDEM.

Code written using Microsoft Visual C++ is not necessarily downward compatible.

4.2 ESTABLISHING COMPILER ENVIRONMENT

Setting up the programming environment depends upon the platform and compiler being used. Regardless of using a command-line compiler or a graphical programming environment/compiler, following the compiler's instructions will most efficiently establish the programming environment.

4.2.1 Command-Line Compilers

While the compiler may not require the source code to be located in a specific directory, setting certain environment variables may be necessary. Follow the directions of the compiler being used regarding where to place source code and which environment variables to set.

4.2.2 Integrated Development Environment

Graphical programming environments, such as Watcom™ C/C++ 10.0, Borland™ C++, and Microsoft™ Visual C++ may have specific requirements for the location of all or certain source files. As with the command-line compilers, certain environment variables may need to be set.
In addition to the source code files, the modern compilers create a "project" or a "workspace," with very specific files required. Use the compiler's instructions in conjunction with the appropriate files, shown in Table 6, to set up the programming environment.

For example, to further develop the GUI version of MDEM, using Microsoft Visual C++ (version 5.0), in the Microsoft Visual C++ default workspace directory, use the following steps.

1. Locate the Microsoft Visual C++ Developer's Studio.

   \Rightarrow C:\Program Files\DevStudio\MyProjects

2. Create a working directory \texttt{Mdem}

3. Create the subdirectory \texttt{hlp}

4. Place the following files into:

   \texttt{Program Files\DevStudio\MyProjects\Mdem\hlp}

   - \texttt{AfxDlg.rtf}
   - \texttt{test1.cnt}
   - \texttt{test1.hm}
   - \texttt{test1.hpj}
   - \texttt{test1.ph}

5. Create the subdirectory \texttt{res}

6. Place the following files into:

   \texttt{Program Files\DevStudio\MyProjects\Mdem\res}

   - \texttt{test1.ico}
   - \texttt{test1.rc2}

Place all other source files into the working directory \texttt{Mdem}
<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DJGPP</td>
<td>D.J.'s Gnu C++ (compiler)</td>
</tr>
<tr>
<td>FAQ</td>
<td>Frequently Asked Questions</td>
</tr>
<tr>
<td>IUPAC</td>
<td>International Union of Pure and Applied Chemistry</td>
</tr>
<tr>
<td>MFC</td>
<td>Microsoft Foundation Class</td>
</tr>
<tr>
<td>MVCC</td>
<td>Microsoft Visual C++</td>
</tr>
</tbody>
</table>
APPENDIX B
SAMPLE FILES

B1. INPUT/OUTPUT FILE

Exhibit B1 is a 13–atom data set consisting of a regular icosahedron tagged and scaled for Argon. The velocities (current_temperature and ke) are zero. The coordinates are ideal and correspond to minimal potential energy.

Exhibit B1. 13–Atom Input File

```
points = 13
format = ascii
header = marker "Start data
field = locations, velocities, species
structure = 3-vector, 3-vector, scalar
    type = float, float, int
dependency = positions, positions, positions
interleaving = field
end

This is a 13-atom regular icosahedron tagged and scaled for Argon.
The velocities (temperature and ke) are zero.
The coordinates are ideal and correspond to minimal PE.

- Status Data -

date_time 960820

this_filename 13RIC.atm
last_filename 13RIC.atm
frst_filename 13RIC.atm
t=0___filename 13RIC.atm

#_of_atoms 13
evolution_time 0.000000000
    cut_off 9.00E-10

kin_energy 0.000000000E+00
current_temperature 0.000000000E+00
t_stat_work 1 0.000000000E+00
t_stat_work 2 0.000000000E+00
t_stat_work 3 0.000000000E+00
t_stat_work 4 0.000000000E+00
```
- Control Data -

integration_steps_this_run 10
write_data_every 2000000

time_step 1.00000E-15

value_of_xi 1 0.000000000E+00
desired_temperature 1 -5.000000E-08
temp_step 1 0.000000000E+00
pin_const 1 .1 .1 .1

value_of_xi 2 0.00000000000E+00
desired_temperature 2 -1.000000E+00
temp_step 2 0.000000000E+00
pin_const 2 .1 .1 .1

value_of_xi 3 0.00000000000E+00
desired_temperature 3 -1.000000E+00
temp_step 3 0.000000000E+00
pin_const 3 .1 .1 .1

value_of_xi 4 0.00000000000E+00
desired_temperature 4 -1.000000E+00
temp_step 4 0.000000000E+00
pin_const 4 .1 .1 .1

pin_pt_filename
t-stat_time_const_tau 1.00000E-14

Start data
0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
3.29477756E-10 0.00000000E+00 1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
1.0181461E-10 3.1335182E-10 1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
-2.6655297E-10 1.9366227E-10 1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
1.0181461E-10 -3.1335182E-10 1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
-2.6655297E-10 -1.9366227E-10 1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
-1.0181461E-10 3.1335182E-10 -1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
-3.29477756E-10 0.00000000E+00 -1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
-1.0181461E-10 -3.1335182E-10 -1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
2.6655297E-10 -1.9366227E-10 -1.6473973E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066
0.00000000E+00 0.00000000E+00 -3.6836752E-10 0.00000000E+00 0.00000000E+00 0.00000000E+00 2066

B2. TM FILE

The TM file listing in Exhibit B2 was produced from the sample input file shown in Exhibit B1. The data set contains 13 atoms and had 10 integration steps. The accumulated work column is blank as the values equaled 0.
**Exhibit B2. TM File Listing**

<table>
<thead>
<tr>
<th>Index</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>00001</td>
<td>+2.13411e-013</td>
</tr>
<tr>
<td>00002</td>
<td>+8.53616e-013</td>
</tr>
<tr>
<td>00003</td>
<td>+1.92053e-012</td>
</tr>
<tr>
<td>00004</td>
<td>+3.41403e-012</td>
</tr>
<tr>
<td>00005</td>
<td>+5.33390e-012</td>
</tr>
<tr>
<td>00006</td>
<td>+7.67992e-012</td>
</tr>
<tr>
<td>00007</td>
<td>+1.04518e-011</td>
</tr>
<tr>
<td>00008</td>
<td>+1.36491e-011</td>
</tr>
<tr>
<td>00009</td>
<td>+1.72716e-011</td>
</tr>
<tr>
<td>00010</td>
<td>+2.13186e-011</td>
</tr>
</tbody>
</table>

The TM file listing in Exhibit B3 was produced from a data set of 9,758 atoms. Exhibit B4 contains the header data for this sample.

**Exhibit B3. TM File from 9,758 Atoms**

<table>
<thead>
<tr>
<th>Index</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>00001</td>
<td>+1.13225e+003 -9.88165e-015</td>
</tr>
<tr>
<td>00002</td>
<td>+1.15961e+003 -9.88164e-015</td>
</tr>
<tr>
<td>00003</td>
<td>+1.17657e+003 -9.88164e-015</td>
</tr>
<tr>
<td>00004</td>
<td>+1.17903e+003 -9.88162e-015</td>
</tr>
<tr>
<td>00005</td>
<td>+1.16635e+003 -9.88160e-015</td>
</tr>
<tr>
<td>00006</td>
<td>+1.14131e+003 -9.88156e-015</td>
</tr>
<tr>
<td>00007</td>
<td>+1.10924e+003 -9.88151e-015</td>
</tr>
<tr>
<td>00008</td>
<td>+1.07651e+003 -9.88147e-015</td>
</tr>
<tr>
<td>00009</td>
<td>+1.04903e+003 -9.88142e-015</td>
</tr>
<tr>
<td>00010</td>
<td>+1.03097e+003 -9.88139e-015</td>
</tr>
<tr>
<td>00011</td>
<td>+1.02417e+003 -9.88138e-015</td>
</tr>
<tr>
<td>00012</td>
<td>+1.02804e+003 -9.88137e-015</td>
</tr>
<tr>
<td>00013</td>
<td>+1.04009e+003 -9.88136e-015</td>
</tr>
<tr>
<td>00014</td>
<td>+1.05666e+003 -9.88136e-015</td>
</tr>
<tr>
<td>00015</td>
<td>+1.07381e+003 -9.88136e-015</td>
</tr>
<tr>
<td>00016</td>
<td>+1.08816e+003 -9.88136e-015</td>
</tr>
<tr>
<td>00017</td>
<td>+1.09744e+003 -9.88136e-015</td>
</tr>
<tr>
<td>00018</td>
<td>+1.10082e+003 -9.88136e-015</td>
</tr>
<tr>
<td>00019</td>
<td>+1.09876e+003 -9.88136e-015</td>
</tr>
<tr>
<td>00020</td>
<td>+1.09264e+003 -9.88136e-015</td>
</tr>
</tbody>
</table>

**Exhibit B4. Header Data for 9,758 Atom Data Set**

```plaintext
points = 9758
format = ascii
header = marker "Start data\n"
field = locations, velocities, species
structure = 3-vector, 3-vector, scalar
type = float, float, int
dependency = positions, positions, positions
interleaving = field
end
```

B-3
- Status Data -

date_time 961107014110
this_filename 11070141.atm
last_filename 10291002.atm
frst_filename 10291002.atm
t=0_filename armoll0.atm

#:of_atoms 9758
evolution_time 1.4300000004E-10
cut_off 5.8340000E-10

kin_energy 2.221899E-16
current_temperature 1.099473E+03
t_stat_work 1 -9.881646E-15
t_stat_work 2 0.000000E+00
t_stat_work 3 0.000000E+00
t_stat_work 4 0.000000E+00

- Control Data -

integration_steps_this_run 20
write_data_every 2000

time_step 2.000000E-15

value_of_xi 1 7.617050706E+11
desired_temperature 1 1.10000000E+03
temp_step 1 0.00000000E+00
pin_const 1 1.1.1.1

value_of_xi 2 0.0000000000E+00
desired_temperature 2 -1.00000000E+00
temp_step 2 0.00000000E+00
pin_const 2 1.1.1.1

value_of_xi 3 0.0000000000E+00
desired_temperature 3 -1.00000000E+00
temp_step 3 0.00000000E+00
pin_const 3 1.1.1.1

value_of_xi 4 0.0000000000E+00
desired_temperature 4 -1.00000000E+00
temp_step 4 0.00000000E+00
pin_const 4 1.1.1.1

pin_pt_filename

stat_time_const_tau 1.000000E-14
B3. PINNING POINT FILE

Exhibit B5. Pinning File

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1.375325E-08</td>
<td>-6.978250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>2</td>
<td>-1.375325E-08</td>
<td>-6.436250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>3</td>
<td>-1.375325E-08</td>
<td>-5.894250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>4</td>
<td>-1.375325E-08</td>
<td>-5.352250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>5</td>
<td>-1.375325E-08</td>
<td>-4.810250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>6</td>
<td>-1.375325E-08</td>
<td>-4.268250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>7</td>
<td>-1.375325E-08</td>
<td>-3.726250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>8</td>
<td>-1.375325E-08</td>
<td>-3.184250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>9</td>
<td>-1.375325E-08</td>
<td>-2.642250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>10</td>
<td>-1.375325E-08</td>
<td>-2.100250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>11</td>
<td>-1.375325E-08</td>
<td>-1.558250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>12</td>
<td>-1.375325E-08</td>
<td>-1.016250E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>13</td>
<td>-1.375325E-08</td>
<td>-4.742500E-10</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>14</td>
<td>-1.375325E-08</td>
<td>6.774978E-11</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>15</td>
<td>-1.375325E-08</td>
<td>6.097496E-10</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>16</td>
<td>-1.375325E-08</td>
<td>1.151750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>17</td>
<td>-1.375325E-08</td>
<td>1.693750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>18</td>
<td>-1.375325E-08</td>
<td>2.235750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>19</td>
<td>-1.375325E-08</td>
<td>2.777750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>20</td>
<td>-1.375325E-08</td>
<td>3.319750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>21</td>
<td>-1.375325E-08</td>
<td>3.861750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>22</td>
<td>-1.375325E-08</td>
<td>4.403750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>23</td>
<td>-1.375325E-08</td>
<td>4.945750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>24</td>
<td>-1.375325E-08</td>
<td>5.487750E-09</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>25</td>
<td>-1.375325E-08</td>
<td>6.029750E-09</td>
<td>0.0000000E+00</td>
</tr>
</tbody>
</table>

B4. OUTPUT FILE

The following output file was created from the sample input file of 13 atoms.

Exhibit B6. 13-Atom Output File

```
points = 13
format = ascii
header = marker "Start data\n"
field = locations, velocities, species
structure = 3-vector, 3-vector, scalar
type = float, float, int
dependency = positions, positions, positions
interleaving = field
end
```

- Status Data -

B-5
date_time 970615165724
t_this_filename 06151657.24
last_filename 13RICA.atm
first_filename 13rica.atm
t=0__filename 13RIC.atm

#_of_atoms 13
evolution_time 1.0000000000E-014
cut_off 9.0000000E-010

kin_engy 5.739603E-033
current_temperature 2.131865E-011
t_stat_work 1 0.0000000E+000
t_stat_work 2 0.0000000E+000
t_stat_work 3 0.0000000E+000
t_stat_work 4 0.0000000E+000

- Control Data -

integration_steps_this_run 10
write_data_every 2000000

time_step 1.00000E-015

value_of_xi 1 0.0000000000E+000
desired_temperature 1 -5.0000000E-008
temp_step 1 0.0000000E+000
pin_const 1 1.0000000E-001 1.0000000E-001 1.0000000E-001

value_of_xi 2 0.0000000000E+000
desired_temperature 2 -1.0000000E+000
temp_step 2 0.0000000E+000
pin_const 2 1.0000000E-001 1.0000000E-001 1.0000000E-001

value_of_xi 3 0.0000000000E+000
desired_temperature 3 -1.0000000E+000
temp_step 3 0.0000000E+000
pin_const 3 1.0000000E-001 1.0000000E-001 1.0000000E-001

value_of_xi 4 0.0000000000E+000
desired_temperature 4 -1.0000000E+000
temp_step 4 0.0000000E+000
pin_const 4 1.0000000E-001 1.0000000E-001 1.0000000E-001

pin_pt_filename
t-stat_time_const_tau 1.00000E-014
Start data
1.4612984E-031 2.4355249E-031 1.1690387E-030 4.8709947E-017 8.6241014E-022 7.3064920E-017 2.066
3.2947775E-010 5.4801143E-032 1.6473937E-010 6.7466970E-005 1.2178349E-017 1.2172221E-004 2.066
1.0181461E-010 3.1335182E-010 1.6473937E-010 5.2646169E-005 6.3185794E-005 1.1828024E-004 2.066
-2.6655297E-010 1.9366227E-010 1.6473937E-010 3.2905193E-005 1.6241691E-006 9.1760050E-005 2.066
-2.6655297E-010 1.9366227E-010 1.6473937E-010 3.2905193E-005 1.6241691E-006 9.1760050E-005 2.066
1.0181461E-010 3.1335182E-010 1.6473937E-010 5.2646169E-005 6.3185794E-005 1.1828024E-004 2.066
1.0181461E-010 3.1335182E-010 1.6473937E-010 5.2646169E-005 6.3185794E-005 1.1828024E-004 2.066
2.6655297E-010 1.9366227E-010 1.6473937E-010 3.2905193E-005 1.6241691E-006 9.1760050E-005 2.066
-1.0181461E-010 3.1335182E-010 1.6473937E-010 5.2646169E-005 6.3185794E-005 1.1828024E-004 2.066
-3.2947775E-010 1.8263888E-032 1.6473937E-010 6.7466970E-005 7.1239549E-022 1.2172221E-004 2.066
-1.0181461E-010 3.1335182E-010 1.6473937E-010 5.2646169E-005 6.3185794E-005 1.1828024E-004 2.066
2.6655297E-010 1.9366227E-010 1.6473937E-010 3.2905193E-005 1.6241691E-006 9.1760050E-005 2.066

B5. COMMAND–LINE SCREEN DISPLAY

Exhibit B7 is the command–line screen output for the thirteen atom input file. The run was piped to file, hence only the messages displayed to the screen by MDEM appear. In this run, the user elected to create the TM file, with a write frequency of one.

Exhibit B7. Command–Line Screen Display

PLEASE REVIEW THE FOLLOWING DATA.

Edit the header of the seed file 13rica.atm if they are incorrect.

There are 13 atoms in the system.
They have evolved for 0.000000E+000 seconds, originally from the file 13RIC.atm

System ke and temperature are 0.000000E+000 J and 0.000000E+000 kelvins

Recall that Tstat<0 implies xi=constant=xi0.

Thermostat 1 is set for -5.000000E-008 kelvins
and will change at temp_step 1 = 0.000000E+000 kelvins per step.
x10 1 = 0.000000E+000 N/s/m
Thermostat 2 is set for -1.000000E+000 kelvins
and will change at temp_step 2 = 0.000000E+000 kelvins per step.
x10 2 = 0.000000E+000 N/s/m
Thermostat 3 is set for -1.000000E+000 kelvins
and will change at temp_step 3 = 0.000000E+000 kelvins per step.
x10 3 = 0.000000E+000 N/s/m
Thermostat 4 is set for -1.000000E+000 kelvins
and will change at temp_step 4 = 0.000000E+000 kelvins per step.
x10 4 = 0.000000E+000 N/s/m

The Tstat time constant is 1.000000E-014 seconds
10 integration time steps are scheduled

B–7
each step of length 1.000000E-015 seconds
A *atm file will be saved every 2000000 steps.

The force cut off length is 9.000000E-010 meters.
To modify these conditions, quit now and change the seed file.

The interatomic force model is called several times in move_atoms()
by a name that should start with "force_". Both move_atoms() and
force_* are in the file mdemutl.c; look there for details.

Do you want to create a separate temperature output file?
Enter either a 'Y' or 'N.'

Enter the interval to use when writing a *.tm file.
Enter a 1 (one) to update after every step, or
a 5 for every fifth step, etc.

Choose 'continue' if data are correct.
c -continue; q -quit

The atom data have loaded successfully.

There are 13 Ar atoms in this data set.

Choose 'continue' if data are correct.
c -continue; q -quit

00001 +2.134e-013K +5.746e-035J
00002 +8.536e-013K +2.298e-034J
00003 +1.921e-012K +5.171e-034J
00004 +3.414e-012K +9.192e-034J
00005 +5.334e-012K +1.436e-033J
00006 +7.680e-012K +2.068e-033J
00007 +1.045e-011K +2.814e-033J
00008 +1.365e-011K +3.675e-033J
00009 +1.727e-011K +4.650e-033J
00010 +2.132e-011K +5.740e-033J

stop time: 165724
start time: 165724
Execution time = 0.00 seconds
Mean compute time per 1.000e-015 sec of simulation time
for a system of 13 atoms
was 0.000e+000 sec

mdem done
C1. GENERAL INFORMATION

DJGPP is a freeware port of GNU C to the 32-bit development system. It is designed for the Intel 30836 PCs (and higher) running the DOS architecture. Many of the GNU development utilities have been ported to DJGPP.

A fairly extensive list of sites from which to download DJGPP exists. Delorie Software’s Home Page (www.delorie.com) is the best starting point for more information on DJGPP.

C2. INSTALLATION

To get started with DJGPP, download the binary distributions. To build C programs, the following zip files are required.

- README.1ST
- djdev201.zip
- gcc2721b.zip
- bnu27b.zip

The README.1ST file details the procedures for installing DJGPP. An important note is to understand the amount of DMPi memory configured for the target machine as compared to that required by DJGPP. The FAQ archives (www.delorie.com/djgpp/v2faq) contain complete information on the minimal and optimal configurations for developing and running programs using DJGPP.

C3. COMPILcE FLAGS USED

In the development of MDEM, the major goal was to decrease the operation time. One method used to address this objective was the use of the various compiler flags.
compile flag -O1 — reduces code size and execution time of the program

compile flag -O2 — signals all optional optimization, except loop unrolling and function inlining

compile flag -O3 — includes all optimizations from -O2 as well as the "inline-function" option

Binaries for optimization for the Pentium became available at the end of the MDEM development effort.
D1. GENERAL INFORMATION

Microsoft Visual C++ (version 5.0) was the development environment for the GUI version of MDEM. With Visual C++, the developer can choose from the following.

Table D1. Configuration Choices

<table>
<thead>
<tr>
<th>Category</th>
<th>Type</th>
<th>Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>C++ Language</td>
<td>Pointer-to-Member</td>
<td>✪ Best Case Always</td>
</tr>
<tr>
<td></td>
<td>Representation</td>
<td>✪ General Purpose Always</td>
</tr>
<tr>
<td></td>
<td>Enable exception</td>
<td>handling</td>
</tr>
<tr>
<td>Code Generation</td>
<td>Processor</td>
<td>✪ 80386</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ 80486</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ Pentium</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ Pentium Pro</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ Blend</td>
</tr>
<tr>
<td></td>
<td>Run-time Library</td>
<td>✪ Single-threaded</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ Multithreaded</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ Multithreaded DLL</td>
</tr>
<tr>
<td></td>
<td>Calling Convention</td>
<td>✪ _cdecl</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ _fastcall</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ _stdcall</td>
</tr>
<tr>
<td></td>
<td>Struct Member Alignment</td>
<td>✪ 1 byte</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ 2 bytes</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ 4 bytes</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ 8 bytes</td>
</tr>
<tr>
<td></td>
<td></td>
<td>✪ 16 bytes</td>
</tr>
</tbody>
</table>
Visual C++ has a processor code generation options option for the each of the Intel PC processors. However, the flag for the Intel 80386 processor is being phased out. The following describes the processor choices considered during Mdem development: (“/G (Optimize for Processor) Options”, Microsoft Visual C++’s (version 5.0) help page).

- **Blend** — “Optimizes the code created to favor the Pentium. It blends the optimizations for the 80386, 80486, Pentium, and Pentium Pro options. This option forces a value of 500 for the _M_IX86 preprocessor macro.”

- **Pentium** — “Optimizes the code created to favor the Pentium. Use this option for programs meant only for the Pentium. This option forces a value of 500 for the _M_IX86 preprocessor macro.”

- **Pentium Pro** — “Optimizes the code created to favor the Pentium Pro. Use this option for programs meant only for the Pentium Pro. This option forces a value of 600 for the _M_IX86 preprocessor macro.”

No hard and fast statement can be given regarding which combination of processor/optimization options produced the fastest executable. In general though, the processor option “Blend” and the optimization “Global” produced the fastest code for both the Pentium and the Pentium Pro. MDEM.exe and MDEM_GUI.exe were delivered using these options.
RasMol is a molecular-graphics viewer available free from the Internet. The program renders the three-dimensional coordinates for a molecule using the pdb file format. It displays the molecule in various representations and allows the user to rotate the molecule interactively.

Two sites from which RasMol can be obtained are:

- University of Edinburgh (ftp.dcs.ed.ac.uk)
- Sunsite Europe (sunsite.doc.ic.ac.uk)

MDEM output files must be reformatted to the pdb file format, which involves creating a new file from the *.atm file. The pdb file consists of records of 80 characters each. The following table shows the structure of the record.

<table>
<thead>
<tr>
<th>COLUMN</th>
<th>FIELD</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 — 6</td>
<td>keyword: ‘ATOM’ or ‘HETATM’</td>
</tr>
<tr>
<td>7 — 11</td>
<td>atom serial number</td>
</tr>
<tr>
<td>13 — 16</td>
<td>atom name, in the IUPAC format</td>
</tr>
<tr>
<td>17</td>
<td>alternate location indicator indicated by A, B, or C</td>
</tr>
<tr>
<td>18 — 20</td>
<td>residue name, in IUPAC format</td>
</tr>
<tr>
<td>23 — 26</td>
<td>residue sequence number</td>
</tr>
<tr>
<td>27</td>
<td>code for insertions of residues</td>
</tr>
<tr>
<td>31 - 38</td>
<td>X-coordinate</td>
</tr>
<tr>
<td>39 — 46</td>
<td>Y-coordinate</td>
</tr>
<tr>
<td>47 — 54</td>
<td>Z-coordinate</td>
</tr>
<tr>
<td>55 — 60</td>
<td>occupancy</td>
</tr>
<tr>
<td>61 — 66</td>
<td>Temperature Factor</td>
</tr>
<tr>
<td>68 — 70</td>
<td>Footnote Number</td>
</tr>
</tbody>
</table>

More detailed information can be found in RasMol v2.5 User’s Manual. Exhibit E1 is a sample pdb input file.
### Exhibit E1. Sample PDB Input File

<table>
<thead>
<tr>
<th>HETATM</th>
<th>1</th>
<th>Ni</th>
<th>1</th>
<th>-3.096</th>
<th>-26.745</th>
<th>4.008</th>
<th>1.00</th>
<th>-0.26</th>
</tr>
</thead>
<tbody>
<tr>
<td>HETATM</td>
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<td>Ni</td>
<td>1</td>
<td>-5.356</td>
<td>12.247</td>
<td>7.768</td>
<td>1.00</td>
<td>-0.49</td>
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<td>15.101</td>
<td>-3.710</td>
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<td>-0.33</td>
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<td>-0.11</td>
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<td>-3.735</td>
<td>-6.815</td>
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<td>-0.30</td>
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<td>-0.581</td>
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<td>-0.37</td>
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<td>-0.30</td>
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<td>Ni</td>
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<td>-37.974</td>
<td>-9.365</td>
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<td>-0.04</td>
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<tr>
<td>HETATM</td>
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<td>Ni</td>
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<td>-9.719</td>
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<td>0.42</td>
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<td>-14.719</td>
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<td>-0.39</td>
</tr>
<tr>
<td>HETATM</td>
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<td>29.005</td>
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<td>4.216</td>
<td>1.00</td>
<td>-0.47</td>
</tr>
</tbody>
</table>
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