Rigid Dynamics in LAMMPS

David Keffer
Department of Materials Science & Engineering
University of Tennessee, Knoxville
date begun: March 8, 2016
date last updated: March 22, 2016

Table of Contents

I. Purpose of Document

The purpose of this document is to provide a practical introduction to the simulation of rigid molecules in LAMMPS. This is useful, for example, with molecules like carbon dioxide, which have high vibrational frequencies for the C=O bonds. To simulate the flexible system requires a very small time step. Often the approximation of the molecule as a rigid body is sufficient to capture the physics of interest and offers a significant computational savings.

II. Review of Rigid Body Dynamics

We consider a molecule with N_{apm} atoms per molecule. Each atom has a position, $\mathbf{r}_i$, and velocity, $\mathbf{v}_i$, in the "laboratory frame of reference".

The dynamics of a rigid body are divided into translation of the center of mass and rotation about the center of mass. Each molecule has a center of mass position, defined as

$$\mathbf{R}_{\text{com}} \equiv \frac{\sum_{i=1}^{N_{apm}} m_i \mathbf{r}_i}{\sum_{i=1}^{N_{apm}} m_i} \tag{1}$$

The velocity of the center of mass of a molecule

$$\mathbf{v}_{\text{com}} \equiv \frac{d\mathbf{R}_{\text{com}}}{dt} = \frac{\sum_{i=1}^{N_{apm}} m_i \frac{d\mathbf{r}_i}{dt}}{\sum_{i=1}^{N_{apm}} m_i} = \frac{\sum_{i=1}^{N_{apm}} m_i \mathbf{v}_i}{\sum_{i=1}^{N_{apm}} m_i} \tag{2}$$

The acceleration of the center of mass of a molecule

$$\mathbf{a}_{\text{com}} \equiv \frac{d\mathbf{v}_{\text{com}}}{dt} = \frac{\sum_{i=1}^{N_{apm}} m_i \frac{d\mathbf{v}_i}{dt}}{\sum_{i=1}^{N_{apm}} m_i} = \frac{\sum_{i=1}^{N_{apm}} m_i \mathbf{a}_i}{\sum_{i=1}^{N_{apm}} m_i} = \frac{\sum_{i=1}^{N_{apm}} \mathbf{f}_i}{\sum_{i=1}^{N_{apm}} m_i} = \frac{1}{\sum_{i=1}^{N_{apm}} m_i}\mathbf{f}_{\text{com}} = \frac{1}{m_{\text{com}}}\mathbf{f}_{\text{com}} \tag{3}$$

where we have invoked Newton's equation of motion, $\mathbf{f}_i = m_i \mathbf{a}_i$, on a particle basis. This motion of the center of mass constitutes the translational degrees of freedom of the molecule.

We observe that the trajectory of the center of mass can be obtained based upon the forces evaluated at each atomic position, something that LAMMPS is well suited to evaluate.

To describe the rotational degrees of freedom, we must define the torque on the rigid body,

$$\mathbf{T}_{\text{com}} \equiv \sum_{i=1}^{N_{apm}} \left(\mathbf{r}_i - \mathbf{R}_{\text{com}}\right) \times \mathbf{f}_i \tag{4}$$

Again we note that the torque about the center of mass is entirely defined by the point positions and forces. The moment of inertia of a set of points about their center of mass is defined as

$$I_{\text{com}} \equiv \sum_{i=1}^{N_{apm}} m_i \left|\mathbf{r}_i - \mathbf{R}_{\text{com}}\right|^2 \tag{5}$$

Newton's second law for rotational dynamics relates the torque to the angular acceleration, α, and the angular velocity, ω.

$$\mathbf{T}_{\text{com}} = I_{\text{com}}\alpha + \omega \times I_{\text{com}}\omega \tag{6}$$

The angular velocity of a rigid object is the same for all points and can thus be evaluated from any single point be evaluated

$$\omega = \frac{\left(\mathbf{r}_i - \mathbf{R}_{\text{com}}\right) \times \mathbf{v}_i}{\left|\mathbf{r}_i - \mathbf{R}_{\text{com}}\right|^2} \tag{7}$$

These equations thus provide the angular acceleration and angular velocity based on knowledge of the point positions, velocities and forces. The acceleration of any point on the rigid object is given by

$$a_i = \alpha \times \left(\mathbf{r}_i - \mathbf{R}_{\text{com}}\right) + \omega \times \left(\omega \times \left(\mathbf{r}_i - \mathbf{R}_{\text{com}}\right)\right) + \mathbf{a}_{\text{com}} \tag{8}$$

The kinetic energy of the rigid body has translation and rotational components

$$KE = KE_{tran} + KE_{rot} \tag{9}$$

where

$$KE_{tran} = \frac{1}{2} m_{com} \left| \mathbf{v}_{com} \right|^2 \tag{10}$$

$$KE_{rot} = \frac{1}{2} I_{com} \omega^2 \tag{11}$$

For a nonlinear molecule translating and rotating in three-dimensional space, each of these motions contains three degrees of freedom. The molecule can translate in the x, y and z dimensions. The molecule can rotate about the x, y and z axes. Therefore according to the equipartition theorem,

$$KE_{tran} = KE_{rot} = \frac{3}{2} kT \tag{12}$$

Note that the kinetic energy of the system if all atoms were treated independently is

$$KE_{ind} = \frac{1}{2} \sum_{i=1}^{N_{apm}} m_i \left| \mathbf{v}_i \right|^2 = \frac{3}{2} N_{apm} kT \tag{13}$$

This is a totally different quantity. One consequence of this is that the LAMMPS command for creating initial velocities for particles sets them to a specific temperature based on the assumption of indpendence (equation (13)). Therefore, if the system is actually composed of rigid bodies, the initial temperature based on this approach will be wrong for both the translation and rotational degrees of freedom. To my knowledge, LAMMPS does not have a way to create correct initial velocities corresponding to a set point temperature for rigid bodies.

III. Simulation of Rigid Molecules

In this section we first simulate a single molecule of carbon dioxide, then we simulate a system of carbon dioxide molecules.

III.A. Simulation of a Single Carbon Dioxide Molecule

An initial configuration for a single carbon dioxide, CO2, molecule is given in Appendix A `config_co2_1.txt`. The input configuration has 3 atoms of 2 types (C & O), 2 bonds of one type (C=O), and 1 angle of 1 type (O=C=O). Importantly, the distance between atoms corresponds to the equilibrium bond distance, which will not vary during the simulation since the molecule is rigid. In other words, you should make sure that your input configuration is consistent with the rigid potential.

A LAMMPS input file is given in Appendix B, `input_co2_1.txt`. This input file must provide a fake (unused) bond force constant for the bond and angle modes. Here, we input a value of 999.9 to emphasize the artificiality of these numbers. This code runs.

III.B. Simulation of a System of Carbon Dioxide Molecules

We next simulate a system of 125 carbon dioxide molecules. T LAMMPS input file is given in Appendix C, `input_co2_sys.txt`. An initial configuration for a single carbon dioxide, CO2, molecule is given in Appendix D, `config_co2_sys.txt`.

Six different fix commands are given invoking the rigid and rigid/small functionality. Of these only four function when compute commands are present to calculate the translation kinetic energy (ke/rigid) and rotational kinetic energy (erotate). The other two (rigid/nve/small and rigid/nvt/small) cause segmentation faults.

For any of these fixes, there appear to be two serious problems. First, the temperature is not the set point temperature. Of course, the initial velocity command can generate the correct initial temperature for a fully flexible system, not a set of rigid objects. *There are several suggestions on the LAMMPS website for manipulating the input file to get the correct temperature, but we found that none of these suggestions delivered the correct set point temperature at the initial configuration.*

Second, for none of the cases is the equipartition theorem satisfied. The sum of the translational and rotational kinetic energies do not sum to 5/2NkT, as they should.

$$KE_{tran} + KE_{rot} = \frac{5}{2} N_{molec} kT \tag{14}$$

We have 5 degrees of freedom here, corresponding to three degrees of translational freedom and 2 degrees of rotational freedom for a linear molecule, like CO_2.

Thus, there remains serious reservations in using the rigid command in LAMMPS. For those that believe that errors, which are not visible in other properties, are okay, proceed with caution.

Appendix A. Carbon Dioxide: `config_co2_1.txt`

```
LAMMPS INPUT FILE FOR co2_1
       3 atoms
       2 bonds
       1 angles
       0 dihedrals
       0 impropers
       2 atom types
       1 bond types
       1 angle types
       0 dihedral types
       0 improper types
  -0.50000000E+02   0.50000000E+02 xlo xhi
  -0.50000000E+02   0.50000000E+02 ylo yhi
  -0.50000000E+02   0.50000000E+02 zlo zhi

 Masses

       1   0.12010700E+02
       2   0.15999000E+02

 Atoms

       1        1        2  -0.35000000E+00  -0.11600000E+01   0.00000000E+00   0.00000000E+00  # O
       2        1        1   0.70000000E+00   0.00000000E+00   0.00000000E+00   0.00000000E+00  # C
       3        1        2  -0.35000000E+00   0.11600000E+01   0.00000000E+00   0.00000000E+00  # O

 Bonds

       1        1        1        2
       2        1        2        3

 Angles

       1        1        1        2        3
```

Appendix B. Carbon Dioxide: `input_co2_1.txt`

```
#
units real
boundary p p p
atom_style full

read_data config_co2_1.txt

# interaction styles
pair_style lj/cut/coul/cut 12.0
bond_style harmonic
angle_style harmonic
pair_modify mix geometric tail yes

# force field parameters
# missing nonbonded parameters are inferred from mixing.
pair_coeff   1 1  0.0537 2.80      # C of CO2 ( 27 K = 0.0537 kcal/mol)
pair_coeff   2 2  0.1570 3.05      # O of CO2 (79 K = 0.1570 kcal/mol)
bond_coeff   1  999.9 1.16    # C=O (999.9 = fake number since not used)
angle_coeff  1  999.9 180.0    # O=C=O (999.9 = fake number since not used)

group all_co2 id <> 1 3

fix 1 all_co2 rigid/nve molecule # my_ketran = finite number

compute my_ketran all_co2 ke/rigid 1
compute my_kerot all_co2 erotate/rigid 1
compute my_temp all_co2 temp

timestep 1.0
reset_timestep 0
neigh_modify every 10 delay 20 check yes
thermo 500
thermo_style custom step c_my_ketran c_my_kerot temp c_my_temp pe ebond eangle

dump 1 all atom 100 dump.lammpstrj

run 0
```

Appendix C. Carbon Dioxide: `input_co2_sys.txt`

```
#
units real
boundary p p p
atom_style full

read_data config_co2_sys.txt

# interaction styles
pair_style lj/cut/coul/cut 12.0
bond_style harmonic
angle_style harmonic
pair_modify mix geometric tail yes

# force field parameters
# missing nonbonded parameters are inferred from mixing.
pair_coeff   1 1  0.0537 2.80      # C of CO2 ( 27 K = 0.0537 kcal/mol)
pair_coeff   2 2  0.1570 3.05      # O of CO2 (79 K = 0.1570 kcal/mol)
bond_coeff   1  999.9 1.16    # C=O (999.9 = fake number since not used)
angle_coeff  1  999.9 180.0    # O=C=O (999.9 = fake number since not used)

velocity all create 100.0 53244 dist gaussian mom no rot no

group clump id <> 1 375

#fix 1 clump rigid/small molecule # my_ketran = finite number
#fix 1 clump rigid/nve/small molecule # doesn't work with computing ke for rigid objects - Segmentation fault
#fix 1 clump rigid/nvt/small molecule temp 100.0 100.0 100.0 # doesn't work with computing ke for rigid objects -
Segmentation fault
#fix 1 clump rigid molecule # my_ketran = finite number
fix 1 clump rigid/nve molecule # my_ketran = finite number
#fix 1 clump rigid/nvt molecule temp 100.0 100.0 100.0 # my_ketran = finite number

compute my_ketran clump ke/rigid 1
compute my_kerot clump erotate/rigid 1
compute my_temp clump temp

##minimize 1.0e-4 1.0e-6 100 1000

timestep 1.0
reset_timestep 0
neigh_modify every 10 delay 20 check yes
thermo 500
```

```
#thermo_style multi
thermo_style custom step c_my_ketran c_my_kerot temp c_my_temp pe ebond eangle

dump 1 all atom 100 dump.lammpstrj

run 0
```

Appendix D. Carbon Dioxide: `config_co2_sys.txt`

```
LAMMPS INPUT FILE FOR co2_system
         375  atoms
         250  bonds
         125  angles
           0  dihedrals
           0  impropers
           2  atom types
       1 bond types
       1 angle types
       0 dihedral types
       0 improper types
  0.0000000E+00   100.000000000000       xlo xhi
  0.0000000E+00   100.000000000000       ylo yhi
  0.0000000E+00   100.000000000000       zlo zhi

 Masses

           1   12.0107000000000
           2   15.9990000000000

 Atoms

         1          1          2  -0.3500000E+00   0.8355413E+00  -0.8046557E+00  -0.2285103E-05
         2          1          1   0.7000000E+00   0.0000000E+00   0.0000000E+00   0.0000000E+00
         3          1          2  -0.3500000E+00  -0.8355413E+00   0.8046557E+00   0.2285103E-05
         4          2          2  -0.3500000E+00  -0.7077159E+00  -0.3379484E+00   0.1914529E+02
         5          2          1   0.7000000E+00   0.0000000E+00   0.0000000E+00   0.2000000E+02
         6          2          2  -0.3500000E+00   0.7077159E+00   0.3379484E+00   0.2085471E+02
         7          3          2  -0.3500000E+00  -0.5723737E+00  -0.3224989E+00   0.4095602E+02
         8          3          1   0.7000000E+00   0.0000000E+00   0.0000000E+00   0.4000000E+02
         9          3          2  -0.3500000E+00   0.5723737E+00   0.3224989E+00   0.3904398E+02
        10          4          2  -0.3500000E+00   0.1052832E+00  -0.8962571E+00   0.5927114E+02
        11          4          1   0.7000000E+00   0.0000000E+00   0.0000000E+00   0.6000000E+02
        12          4          2  -0.3500000E+00  -0.1052832E+00   0.8962571E+00   0.6072886E+02
        13          5          2  -0.3500000E+00   0.8713731E+00   0.4858468E+00   0.8059183E+02
        14          5          1   0.7000000E+00   0.0000000E+00   0.0000000E+00   0.8000000E+02
        15          5          2  -0.3500000E+00  -0.8713731E+00  -0.4858468E+00   0.7940817E+02
        16          6          2  -0.3500000E+00   0.3094261E+00   0.1893983E+02   0.3548246E+00
        17          6          1   0.7000000E+00   0.0000000E+00   0.2000000E+02   0.0000000E+00
        18          6          2  -0.3500000E+00  -0.3094261E+00   0.2106017E+02  -0.3548246E+00
        19          7          2  -0.3500000E+00  -0.7778275E+00   0.1915416E+02   0.2015854E+02
        20          7          1   0.7000000E+00   0.0000000E+00   0.2000000E+02   0.2000000E+02
```

21	7	2	-0.3500000E+00	0.7778275E+00	0.2084584E+02	0.1984146E+02
22	8	2	-0.3500000E+00	0.1129006E+01	0.1996001E+02	0.4026334E+02
23	8	1	0.7000000E+00	0.0000000E+00	0.2000000E+02	0.4000000E+02
24	8	2	-0.3500000E+00	-0.1129006E+01	0.2003999E+02	0.3973666E+02
25	9	2	-0.3500000E+00	-0.1122795E+01	0.2003330E+02	0.5971048E+02
26	9	1	0.7000000E+00	0.0000000E+00	0.2000000E+02	0.6000000E+02
27	9	2	-0.3500000E+00	0.1122795E+01	0.1996670E+02	0.6028952E+02
28	10	2	-0.3500000E+00	-0.8863783E-01	0.2098327E+02	0.8060903E+02
29	10	1	0.7000000E+00	0.0000000E+00	0.2000000E+02	0.8000000E+02
30	10	2	-0.3500000E+00	0.8863783E-01	0.1901673E+02	0.7939097E+02
31	11	2	-0.3500000E+00	-0.3438975E+00	0.4110784E+02	0.4872613E-02
32	11	1	0.7000000E+00	0.0000000E+00	0.4000000E+02	0.0000000E+00
33	11	2	-0.3500000E+00	0.3438975E+00	0.3889216E+02	-0.4872613E-02
34	12	2	-0.3500000E+00	-0.8417580E-02	0.4056014E+02	0.2101576E+02
35	12	1	0.7000000E+00	0.0000000E+00	0.4000000E+02	0.2000000E+02
36	12	2	-0.3500000E+00	0.8417580E-02	0.3943986E+02	0.1898424E+02
37	13	2	-0.3500000E+00	-0.5598126E+00	0.3902219E+02	0.4027586E+02
38	13	1	0.7000000E+00	0.0000000E+00	0.4000000E+02	0.4000000E+02
39	13	2	-0.3500000E+00	0.5598126E+00	0.4097781E+02	0.3972414E+02
40	14	2	-0.3500000E+00	-0.4539178E+00	0.4106725E+02	0.5997695E+02
41	14	1	0.7000000E+00	0.0000000E+00	0.4000000E+02	0.6000000E+02
42	14	2	-0.3500000E+00	0.4539178E+00	0.3893275E+02	0.6002305E+02
43	15	2	-0.3500000E+00	0.6971430E+00	0.3907605E+02	0.7992312E+02
44	15	1	0.7000000E+00	0.0000000E+00	0.4000000E+02	0.8000000E+02
45	15	2	-0.3500000E+00	-0.6971430E+00	0.4092395E+02	0.8007688E+02
46	16	2	-0.3500000E+00	-0.9341715E+00	0.6057392E+02	0.3788656E+00
47	16	1	0.7000000E+00	0.0000000E+00	0.6000000E+02	0.0000000E+00
48	16	2	-0.3500000E+00	0.9341715E+00	0.5942608E+02	-0.3788656E+00
49	17	2	-0.3500000E+00	0.1067008E+01	0.5985920E+02	0.2043275E+02
50	17	1	0.7000000E+00	0.0000000E+00	0.6000000E+02	0.2000000E+02
51	17	2	-0.3500000E+00	-0.1067008E+01	0.6014080E+02	0.1956725E+02
52	18	2	-0.3500000E+00	0.6086209E+00	0.6017452E+02	0.4097197E+02
53	18	1	0.7000000E+00	0.0000000E+00	0.6000000E+02	0.4000000E+02
54	18	2	-0.3500000E+00	-0.6086209E+00	0.5982548E+02	0.3902803E+02
55	19	2	-0.3500000E+00	0.4150895E+00	0.6001716E+02	0.6108305E+02
56	19	1	0.7000000E+00	0.0000000E+00	0.6000000E+02	0.6000000E+02
57	19	2	-0.3500000E+00	-0.4150895E+00	0.5998284E+02	0.5891695E+02
58	20	2	-0.3500000E+00	-0.1127984E+01	0.5993139E+02	0.7973819E+02
59	20	1	0.7000000E+00	0.0000000E+00	0.6000000E+02	0.8000000E+02
60	20	2	-0.3500000E+00	0.1127984E+01	0.6006861E+02	0.8026181E+02
61	21	2	-0.3500000E+00	0.6711348E+00	0.7905423E+02	-0.2645362E-01
62	21	1	0.7000000E+00	0.0000000E+00	0.8000000E+02	0.0000000E+00
63	21	2	-0.3500000E+00	-0.6711348E+00	0.8094577E+02	0.2645362E-01
64	22	2	-0.3500000E+00	-0.1776712E+00	0.7885480E+02	0.1994946E+02
65	22	1	0.7000000E+00	0.0000000E+00	0.8000000E+02	0.2000000E+02

66	22	2	-0.3500000E+00	0.1776712E+00	0.8114520E+02	0.2005054E+02
67	23	2	-0.3500000E+00	0.3536869E+00	0.8094811E+02	0.4056709E+02
68	23	1	0.7000000E+00	0.0000000E+00	0.8000000E+02	0.4000000E+02
69	23	2	-0.3500000E+00	-0.3536869E+00	0.7905189E+02	0.3943291E+02
70	24	2	-0.3500000E+00	0.6191410E+00	0.8098012E+02	0.6004037E+02
71	24	1	0.7000000E+00	0.0000000E+00	0.8000000E+02	0.6000000E+02
72	24	2	-0.3500000E+00	-0.6191410E+00	0.7901988E+02	0.5995963E+02
73	25	2	-0.3500000E+00	0.6112207E+00	0.7994683E+02	0.8098447E+02
74	25	1	0.7000000E+00	0.0000000E+00	0.8000000E+02	0.8000000E+02
75	25	2	-0.3500000E+00	-0.6112207E+00	0.8005317E+02	0.7901553E+02
76	26	2	-0.3500000E+00	0.2076414E+02	0.8103951E+00	-0.3239712E+00
77	26	1	0.7000000E+00	0.2000000E+02	0.0000000E+00	0.0000000E+00
78	26	2	-0.3500000E+00	0.1923586E+02	-0.8103951E+00	0.3239712E+00
79	27	2	-0.3500000E+00	0.2113885E+02	-0.1644978E+00	0.2014687E+02
80	27	1	0.7000000E+00	0.2000000E+02	0.0000000E+00	0.2000000E+02
81	27	2	-0.3500000E+00	0.1886115E+02	0.1644978E+00	0.1985313E+02
82	28	2	-0.3500000E+00	0.2085459E+02	-0.2912865E+00	0.3927170E+02
83	28	1	0.7000000E+00	0.2000000E+02	0.0000000E+00	0.4000000E+02
84	28	2	-0.3500000E+00	0.1914541E+02	0.2912865E+00	0.4072830E+02
85	29	2	-0.3500000E+00	0.1964239E+02	-0.5481121E+00	0.6095775E+02
86	29	1	0.7000000E+00	0.2000000E+02	0.0000000E+00	0.6000000E+02
87	29	2	-0.3500000E+00	0.2035761E+02	0.5481121E+00	0.5904225E+02
88	30	2	-0.3500000E+00	0.2114226E+02	-0.2020738E+00	0.7999726E+02
89	30	1	0.7000000E+00	0.2000000E+02	0.0000000E+00	0.8000000E+02
90	30	2	-0.3500000E+00	0.1885774E+02	0.2020738E+00	0.8000274E+02
91	31	2	-0.3500000E+00	0.2020277E+02	0.2110196E+02	0.3002772E+00
92	31	1	0.7000000E+00	0.2000000E+02	0.2000000E+02	0.0000000E+00
93	31	2	-0.3500000E+00	0.1979723E+02	0.1889804E+02	-0.3002772E+00
94	32	2	-0.3500000E+00	0.2106855E+02	0.1960819E+02	0.2022426E+02
95	32	1	0.7000000E+00	0.2000000E+02	0.2000000E+02	0.2000000E+02
96	32	2	-0.3500000E+00	0.1893145E+02	0.2039181E+02	0.1977574E+02
97	33	2	-0.3500000E+00	0.1959870E+02	0.1893002E+02	0.4019924E+02
98	33	1	0.7000000E+00	0.2000000E+02	0.2000000E+02	0.4000000E+02
99	33	2	-0.3500000E+00	0.2040130E+02	0.2106998E+02	0.3980076E+02
100	34	2	-0.3500000E+00	0.2097821E+02	0.2062127E+02	0.6005219E+02
101	34	1	0.7000000E+00	0.2000000E+02	0.2000000E+02	0.6000000E+02
102	34	2	-0.3500000E+00	0.1902179E+02	0.1937873E+02	0.5994781E+02
103	35	2	-0.3500000E+00	0.2007904E+02	0.2074070E+02	0.7911078E+02
104	35	1	0.7000000E+00	0.2000000E+02	0.2000000E+02	0.8000000E+02
105	35	2	-0.3500000E+00	0.1992096E+02	0.1925930E+02	0.8088922E+02
106	36	2	-0.3500000E+00	0.1905858E+02	0.3974971E+02	-0.6298214E+00
107	36	1	0.7000000E+00	0.2000000E+02	0.4000000E+02	0.0000000E+00
108	36	2	-0.3500000E+00	0.2094142E+02	0.4025029E+02	0.6298214E+00
109	37	2	-0.3500000E+00	0.2073633E+02	0.4009123E+02	0.1910832E+02
110	37	1	0.7000000E+00	0.2000000E+02	0.4000000E+02	0.2000000E+02

111	37	2	-0.3500000E+00	0.1926367E+02	0.3990877E+02	0.2089168E+02
112	38	2	-0.3500000E+00	0.1961909E+02	0.4027247E+02	0.3893874E+02
113	38	1	0.7000000E+00	0.2000000E+02	0.4000000E+02	0.4000000E+02
114	38	2	-0.3500000E+00	0.2038091E+02	0.3972753E+02	0.4106126E+02
115	39	2	-0.3500000E+00	0.1915000E+02	0.4068863E+02	0.5961414E+02
116	39	1	0.7000000E+00	0.2000000E+02	0.4000000E+02	0.6000000E+02
117	39	2	-0.3500000E+00	0.2085000E+02	0.3931137E+02	0.6038586E+02
118	40	2	-0.3500000E+00	0.1904555E+02	0.3941541E+02	0.8030476E+02
119	40	1	0.7000000E+00	0.2000000E+02	0.4000000E+02	0.8000000E+02
120	40	2	-0.3500000E+00	0.2095445E+02	0.4058459E+02	0.7969524E+02
121	41	2	-0.3500000E+00	0.2061676E+02	0.5905346E+02	0.2631995E+00
122	41	1	0.7000000E+00	0.2000000E+02	0.6000000E+02	0.0000000E+00
123	41	2	-0.3500000E+00	0.1938324E+02	0.6094654E+02	-0.2631995E+00
124	42	2	-0.3500000E+00	0.2090459E+02	0.5973587E+02	0.2067642E+02
125	42	1	0.7000000E+00	0.2000000E+02	0.6000000E+02	0.2000000E+02
126	42	2	-0.3500000E+00	0.1909541E+02	0.6026413E+02	0.1932358E+02
127	43	2	-0.3500000E+00	0.1904642E+02	0.6021538E+02	0.3937559E+02
128	43	1	0.7000000E+00	0.2000000E+02	0.6000000E+02	0.4000000E+02
129	43	2	-0.3500000E+00	0.2095358E+02	0.5978462E+02	0.4062441E+02
130	44	2	-0.3500000E+00	0.2028985E+02	0.5935720E+02	0.5907892E+02
131	44	1	0.7000000E+00	0.2000000E+02	0.6000000E+02	0.6000000E+02
132	44	2	-0.3500000E+00	0.1971015E+02	0.6064280E+02	0.6092108E+02
133	45	2	-0.3500000E+00	0.1940818E+02	0.5939294E+02	0.8079173E+02
134	45	1	0.7000000E+00	0.2000000E+02	0.6000000E+02	0.8000000E+02
135	45	2	-0.3500000E+00	0.2059182E+02	0.6060706E+02	0.7920827E+02
136	46	2	-0.3500000E+00	0.1979142E+02	0.7888740E+02	-0.2534143E+00
137	46	1	0.7000000E+00	0.2000000E+02	0.8000000E+02	0.0000000E+00
138	46	2	-0.3500000E+00	0.2020858E+02	0.8111260E+02	0.2534143E+00
139	47	2	-0.3500000E+00	0.1965620E+02	0.8106056E+02	0.1967968E+02
140	47	1	0.7000000E+00	0.2000000E+02	0.8000000E+02	0.2000000E+02
141	47	2	-0.3500000E+00	0.2034380E+02	0.7893944E+02	0.2032032E+02
142	48	2	-0.3500000E+00	0.1973549E+02	0.7933783E+02	0.4091497E+02
143	48	1	0.7000000E+00	0.2000000E+02	0.8000000E+02	0.4000000E+02
144	48	2	-0.3500000E+00	0.2026451E+02	0.8066217E+02	0.3908503E+02
145	49	2	-0.3500000E+00	0.2103178E+02	0.8038721E+02	0.5963792E+02
146	49	1	0.7000000E+00	0.2000000E+02	0.8000000E+02	0.6000000E+02
147	49	2	-0.3500000E+00	0.1896822E+02	0.7961279E+02	0.6036208E+02
148	50	2	-0.3500000E+00	0.2032827E+02	0.8091767E+02	0.7937094E+02
149	50	1	0.7000000E+00	0.2000000E+02	0.8000000E+02	0.8000000E+02
150	50	2	-0.3500000E+00	0.1967173E+02	0.7908233E+02	0.8062906E+02
151	51	2	-0.3500000E+00	0.4074241E+02	0.7714055E-01	-0.8879620E+00
152	51	1	0.7000000E+00	0.4000000E+02	0.0000000E+00	0.0000000E+00
153	51	2	-0.3500000E+00	0.3925759E+02	-0.7714055E-01	0.8879620E+00
154	52	2	-0.3500000E+00	0.3890641E+02	-0.3610078E+00	0.1986091E+02
155	52	1	0.7000000E+00	0.4000000E+02	0.0000000E+00	0.2000000E+02

156	52	2	-0.3500000E+00	0.4109359E+02	0.3610078E+00	0.2013909E+02
157	53	2	-0.3500000E+00	0.3981034E+02	-0.5133891E+00	0.4102277E+02
158	53	1	0.7000000E+00	0.4000000E+02	0.0000000E+00	0.4000000E+02
159	53	2	-0.3500000E+00	0.4018966E+02	0.5133891E+00	0.3897723E+02
160	54	2	-0.3500000E+00	0.3911390E+02	0.1660410E+00	0.6072997E+02
161	54	1	0.7000000E+00	0.4000000E+02	0.0000000E+00	0.6000000E+02
162	54	2	-0.3500000E+00	0.4088610E+02	-0.1660410E+00	0.5927003E+02
163	55	2	-0.3500000E+00	0.3892428E+02	0.4128036E+00	0.8013422E+02
164	55	1	0.7000000E+00	0.4000000E+02	0.0000000E+00	0.8000000E+02
165	55	2	-0.3500000E+00	0.4107572E+02	-0.4128036E+00	0.7986578E+02
166	56	2	-0.3500000E+00	0.3948189E+02	0.2092986E+02	0.4609907E+00
167	56	1	0.7000000E+00	0.4000000E+02	0.2000000E+02	0.0000000E+00
168	56	2	-0.3500000E+00	0.4051811E+02	0.1907014E+02	-0.4609907E+00
169	57	2	-0.3500000E+00	0.3980882E+02	0.1889398E+02	0.1970712E+02
170	57	1	0.7000000E+00	0.4000000E+02	0.2000000E+02	0.2000000E+02
171	57	2	-0.3500000E+00	0.4019118E+02	0.2110602E+02	0.2029288E+02
172	58	2	-0.3500000E+00	0.4012099E+02	0.2115103E+02	0.4007803E+02
173	58	1	0.7000000E+00	0.4000000E+02	0.2000000E+02	0.4000000E+02
174	58	2	-0.3500000E+00	0.3987901E+02	0.1884897E+02	0.3992197E+02
175	59	2	-0.3500000E+00	0.3946110E+02	0.1951442E+02	0.5909479E+02
176	59	1	0.7000000E+00	0.4000000E+02	0.2000000E+02	0.6000000E+02
177	59	2	-0.3500000E+00	0.4053890E+02	0.2048558E+02	0.6090521E+02
178	60	2	-0.3500000E+00	0.3961356E+02	0.2001118E+02	0.7890632E+02
179	60	1	0.7000000E+00	0.4000000E+02	0.2000000E+02	0.8000000E+02
180	60	2	-0.3500000E+00	0.4038644E+02	0.1998882E+02	0.8109368E+02
181	61	2	-0.3500000E+00	0.4104864E+02	0.4039352E+02	-0.3018209E+00
182	61	1	0.7000000E+00	0.4000000E+02	0.4000000E+02	0.0000000E+00
183	61	2	-0.3500000E+00	0.3895136E+02	0.3960648E+02	0.3018209E+00
184	62	2	-0.3500000E+00	0.4066502E+02	0.3930109E+02	0.2064411E+02
185	62	1	0.7000000E+00	0.4000000E+02	0.4000000E+02	0.2000000E+02
186	62	2	-0.3500000E+00	0.3933498E+02	0.4069891E+02	0.1935589E+02
187	63	2	-0.3500000E+00	0.3959651E+02	0.4080243E+02	0.4073410E+02
188	63	1	0.7000000E+00	0.4000000E+02	0.4000000E+02	0.4000000E+02
189	63	2	-0.3500000E+00	0.4040349E+02	0.3919757E+02	0.3926590E+02
190	64	2	-0.3500000E+00	0.4100364E+02	0.3980229E+02	0.6054701E+02
191	64	1	0.7000000E+00	0.4000000E+02	0.4000000E+02	0.6000000E+02
192	64	2	-0.3500000E+00	0.3899636E+02	0.4019771E+02	0.5945299E+02
193	65	2	-0.3500000E+00	0.4060019E+02	0.3981915E+02	0.7902395E+02
194	65	1	0.7000000E+00	0.4000000E+02	0.4000000E+02	0.8000000E+02
195	65	2	-0.3500000E+00	0.3939981E+02	0.4018085E+02	0.8097605E+02
196	66	2	-0.3500000E+00	0.4059209E+02	0.5902646E+02	0.2173894E+00
197	66	1	0.7000000E+00	0.4000000E+02	0.6000000E+02	0.0000000E+00
198	66	2	-0.3500000E+00	0.3940791E+02	0.6097354E+02	-0.2173894E+00
199	67	2	-0.3500000E+00	0.3909385E+02	0.5931855E+02	0.1975482E+02
200	67	1	0.7000000E+00	0.4000000E+02	0.6000000E+02	0.2000000E+02

201	67	2	-0.3500000E+00	0.4090615E+02	0.6068145E+02	0.2024518E+02
202	68	2	-0.3500000E+00	0.4111451E+02	0.5969635E+02	0.4010618E+02
203	68	1	0.7000000E+00	0.4000000E+02	0.6000000E+02	0.4000000E+02
204	68	2	-0.3500000E+00	0.3888549E+02	0.6030365E+02	0.3989382E+02
205	69	2	-0.3500000E+00	0.3912348E+02	0.6045222E+02	0.5938943E+02
206	69	1	0.7000000E+00	0.4000000E+02	0.6000000E+02	0.6000000E+02
207	69	2	-0.3500000E+00	0.4087652E+02	0.5954778E+02	0.6061057E+02
208	70	2	-0.3500000E+00	0.4103661E+02	0.5958111E+02	0.7969085E+02
209	70	1	0.7000000E+00	0.4000000E+02	0.6000000E+02	0.8000000E+02
210	70	2	-0.3500000E+00	0.3896339E+02	0.6041889E+02	0.8030915E+02
211	71	2	-0.3500000E+00	0.4026068E+02	0.7985413E+02	-0.1120879E+01
212	71	1	0.7000000E+00	0.4000000E+02	0.8000000E+02	0.0000000E+00
213	71	2	-0.3500000E+00	0.3973932E+02	0.8014587E+02	0.1120879E+01
214	72	2	-0.3500000E+00	0.4032325E+02	0.7930461E+02	0.1912963E+02
215	72	1	0.7000000E+00	0.4000000E+02	0.8000000E+02	0.2000000E+02
216	72	2	-0.3500000E+00	0.3967675E+02	0.8069539E+02	0.2087037E+02
217	73	2	-0.3500000E+00	0.4000564E+02	0.8079578E+02	0.4084398E+02
218	73	1	0.7000000E+00	0.4000000E+02	0.8000000E+02	0.4000000E+02
219	73	2	-0.3500000E+00	0.3999436E+02	0.7920422E+02	0.3915602E+02
220	74	2	-0.3500000E+00	0.4070046E+02	0.8056484E+02	0.5926794E+02
221	74	1	0.7000000E+00	0.4000000E+02	0.8000000E+02	0.6000000E+02
222	74	2	-0.3500000E+00	0.3929954E+02	0.7943516E+02	0.6073206E+02
223	75	2	-0.3500000E+00	0.3960669E+02	0.7906517E+02	0.7943697E+02
224	75	1	0.7000000E+00	0.4000000E+02	0.8000000E+02	0.8000000E+02
225	75	2	-0.3500000E+00	0.4039331E+02	0.8093483E+02	0.8056303E+02
226	76	2	-0.3500000E+00	0.5985168E+02	-0.4140728E-01	-0.1149734E+01
227	76	1	0.7000000E+00	0.6000000E+02	0.0000000E+00	0.0000000E+00
228	76	2	-0.3500000E+00	0.6014832E+02	0.4140728E-01	0.1149734E+01
229	77	2	-0.3500000E+00	0.6004604E+02	-0.1133278E+01	0.2024323E+02
230	77	1	0.7000000E+00	0.6000000E+02	0.0000000E+00	0.2000000E+02
231	77	2	-0.3500000E+00	0.5995396E+02	0.1133278E+01	0.1975677E+02
232	78	2	-0.3500000E+00	0.6010826E+02	-0.3246343E+00	0.4110837E+02
233	78	1	0.7000000E+00	0.6000000E+02	0.0000000E+00	0.4000000E+02
234	78	2	-0.3500000E+00	0.5989174E+02	0.3246343E+00	0.3889163E+02
235	79	2	-0.3500000E+00	0.6072579E+02	0.2755542E+00	0.5913808E+02
236	79	1	0.7000000E+00	0.6000000E+02	0.0000000E+00	0.6000000E+02
237	79	2	-0.3500000E+00	0.5927421E+02	-0.2755542E+00	0.6086192E+02
238	80	2	-0.3500000E+00	0.6084127E+02	-0.6454398E+00	0.8047039E+02
239	80	1	0.7000000E+00	0.6000000E+02	0.0000000E+00	0.8000000E+02
240	80	2	-0.3500000E+00	0.5915873E+02	0.6454398E+00	0.7952961E+02
241	81	2	-0.3500000E+00	0.5887404E+02	0.2021437E+02	0.1784829E+00
242	81	1	0.7000000E+00	0.6000000E+02	0.2000000E+02	0.0000000E+00
243	81	2	-0.3500000E+00	0.6112596E+02	0.1978563E+02	-0.1784829E+00
244	82	2	-0.3500000E+00	0.6076577E+02	0.1947117E+02	0.2069249E+02
245	82	1	0.7000000E+00	0.6000000E+02	0.2000000E+02	0.2000000E+02

246	82	2	-0.3500000E+00	0.5923423E+02	0.2052883E+02	0.1930751E+02
247	83	2	-0.3500000E+00	0.5894306E+02	0.2038161E+02	0.4028784E+02
248	83	1	0.7000000E+00	0.6000000E+02	0.2000000E+02	0.4000000E+02
249	83	2	-0.3500000E+00	0.6105694E+02	0.1961839E+02	0.3971216E+02
250	84	2	-0.3500000E+00	0.5967422E+02	0.2020961E+02	0.5890660E+02
251	84	1	0.7000000E+00	0.6000000E+02	0.2000000E+02	0.6000000E+02
252	84	2	-0.3500000E+00	0.6032578E+02	0.1979039E+02	0.6109340E+02
253	85	2	-0.3500000E+00	0.6048184E+02	0.2096769E+02	0.8042073E+02
254	85	1	0.7000000E+00	0.6000000E+02	0.2000000E+02	0.8000000E+02
255	85	2	-0.3500000E+00	0.5951816E+02	0.1903231E+02	0.7957927E+02
256	86	2	-0.3500000E+00	0.5909509E+02	0.3993188E+02	0.7225586E+00
257	86	1	0.7000000E+00	0.6000000E+02	0.4000000E+02	0.0000000E+00
258	86	2	-0.3500000E+00	0.6090491E+02	0.4006812E+02	-0.7225586E+00
259	87	2	-0.3500000E+00	0.5908672E+02	0.3928523E+02	0.2002519E+02
260	87	1	0.7000000E+00	0.6000000E+02	0.4000000E+02	0.2000000E+02
261	87	2	-0.3500000E+00	0.6091328E+02	0.4071477E+02	0.1997481E+02
262	88	2	-0.3500000E+00	0.5907155E+02	0.4013073E+02	0.3931700E+02
263	88	1	0.7000000E+00	0.6000000E+02	0.4000000E+02	0.4000000E+02
264	88	2	-0.3500000E+00	0.6092845E+02	0.3986927E+02	0.4068300E+02
265	89	2	-0.3500000E+00	0.5988173E+02	0.4067959E+02	0.6093261E+02
266	89	1	0.7000000E+00	0.6000000E+02	0.4000000E+02	0.6000000E+02
267	89	2	-0.3500000E+00	0.6011827E+02	0.3932041E+02	0.5906739E+02
268	90	2	-0.3500000E+00	0.6103419E+02	0.4028690E+02	0.8044015E+02
269	90	1	0.7000000E+00	0.6000000E+02	0.4000000E+02	0.8000000E+02
270	90	2	-0.3500000E+00	0.5896581E+02	0.3971310E+02	0.7955985E+02
271	91	2	-0.3500000E+00	0.5963214E+02	0.6107389E+02	-0.2388226E+00
272	91	1	0.7000000E+00	0.6000000E+02	0.6000000E+02	0.0000000E+00
273	91	2	-0.3500000E+00	0.6036786E+02	0.5892611E+02	0.2388226E+00
274	92	2	-0.3500000E+00	0.5971231E+02	0.5928712E+02	0.2086869E+02
275	92	1	0.7000000E+00	0.6000000E+02	0.6000000E+02	0.2000000E+02
276	92	2	-0.3500000E+00	0.6028769E+02	0.6071288E+02	0.1913131E+02
277	93	2	-0.3500000E+00	0.5929571E+02	0.5914337E+02	0.4034022E+02
278	93	1	0.7000000E+00	0.6000000E+02	0.6000000E+02	0.4000000E+02
279	93	2	-0.3500000E+00	0.6070429E+02	0.6085663E+02	0.3965978E+02
280	94	2	-0.3500000E+00	0.6053997E+02	0.6080253E+02	0.5935970E+02
281	94	1	0.7000000E+00	0.6000000E+02	0.6000000E+02	0.6000000E+02
282	94	2	-0.3500000E+00	0.5946003E+02	0.5919747E+02	0.6064030E+02
283	95	2	-0.3500000E+00	0.5886004E+02	0.5998340E+02	0.7978594E+02
284	95	1	0.7000000E+00	0.6000000E+02	0.6000000E+02	0.8000000E+02
285	95	2	-0.3500000E+00	0.6113996E+02	0.6001660E+02	0.8021406E+02
286	96	2	-0.3500000E+00	0.5986267E+02	0.8010015E+02	0.1147480E+01
287	96	1	0.7000000E+00	0.6000000E+02	0.8000000E+02	0.0000000E+00
288	96	2	-0.3500000E+00	0.6013733E+02	0.7989985E+02	-0.1147480E+01
289	97	2	-0.3500000E+00	0.6055878E+02	0.7900192E+02	0.2019289E+02
290	97	1	0.7000000E+00	0.6000000E+02	0.8000000E+02	0.2000000E+02

291	97	2	-0.3500000E+00	0.5944122E+02	0.8099808E+02	0.1980711E+02
292	98	2	-0.3500000E+00	0.5965345E+02	0.7890844E+02	0.3981560E+02
293	98	1	0.7000000E+00	0.6000000E+02	0.8000000E+02	0.4000000E+02
294	98	2	-0.3500000E+00	0.6034655E+02	0.8109156E+02	0.4018440E+02
295	99	2	-0.3500000E+00	0.5911329E+02	0.8046163E+02	0.5941158E+02
296	99	1	0.7000000E+00	0.6000000E+02	0.8000000E+02	0.6000000E+02
297	99	2	-0.3500000E+00	0.6088671E+02	0.7953837E+02	0.6058842E+02
298	100	2	-0.3500000E+00	0.5949999E+02	0.7981899E+02	0.7896907E+02
299	100	1	0.7000000E+00	0.6000000E+02	0.8000000E+02	0.8000000E+02
300	100	2	-0.3500000E+00	0.6050001E+02	0.8018101E+02	0.8103093E+02
301	101	2	-0.3500000E+00	0.7951823E+02	0.1046670E+01	-0.1340859E+00
302	101	1	0.7000000E+00	0.8000000E+02	0.0000000E+00	0.0000000E+00
303	101	2	-0.3500000E+00	0.8048177E+02	-0.1046670E+01	0.1340859E+00
304	102	2	-0.3500000E+00	0.8062666E+02	0.9579918E+00	0.2018747E+02
305	102	1	0.7000000E+00	0.8000000E+02	0.0000000E+00	0.2000000E+02
306	102	2	-0.3500000E+00	0.7937334E+02	-0.9579918E+00	0.1981253E+02
307	103	2	-0.3500000E+00	0.8110623E+02	-0.3191631E+00	0.4014140E+02
308	103	1	0.7000000E+00	0.8000000E+02	0.0000000E+00	0.4000000E+02
309	103	2	-0.3500000E+00	0.7889377E+02	0.3191631E+00	0.3985860E+02
310	104	2	-0.3500000E+00	0.7921918E+02	-0.6231624E+00	0.6058956E+02
311	104	1	0.7000000E+00	0.8000000E+02	0.0000000E+00	0.6000000E+02
312	104	2	-0.3500000E+00	0.8078082E+02	0.6231624E+00	0.5941044E+02
313	105	2	-0.3500000E+00	0.7961317E+02	-0.8928735E+00	0.7936854E+02
314	105	1	0.7000000E+00	0.8000000E+02	0.0000000E+00	0.8000000E+02
315	105	2	-0.3500000E+00	0.8038683E+02	0.8928735E+00	0.8063146E+02
316	106	2	-0.3500000E+00	0.8011418E+02	0.2001731E+02	0.1154237E+01
317	106	1	0.7000000E+00	0.8000000E+02	0.2000000E+02	0.0000000E+00
318	106	2	-0.3500000E+00	0.7988582E+02	0.1998269E+02	-0.1154237E+01
319	107	2	-0.3500000E+00	0.7940403E+02	0.2070460E+02	0.1929717E+02
320	107	1	0.7000000E+00	0.8000000E+02	0.2000000E+02	0.2000000E+02
321	107	2	-0.3500000E+00	0.8059597E+02	0.1929540E+02	0.2070283E+02
322	108	2	-0.3500000E+00	0.7943943E+02	0.2098991E+02	0.3977318E+02
323	108	1	0.7000000E+00	0.8000000E+02	0.2000000E+02	0.4000000E+02
324	108	2	-0.3500000E+00	0.8056057E+02	0.1901009E+02	0.4022682E+02
325	109	2	-0.3500000E+00	0.8088798E+02	0.2011742E+02	0.6073709E+02
326	109	1	0.7000000E+00	0.8000000E+02	0.2000000E+02	0.6000000E+02
327	109	2	-0.3500000E+00	0.7911202E+02	0.1988258E+02	0.5926291E+02
328	110	2	-0.3500000E+00	0.8070646E+02	0.2086631E+02	0.8030987E+02
329	110	1	0.7000000E+00	0.8000000E+02	0.2000000E+02	0.8000000E+02
330	110	2	-0.3500000E+00	0.7929354E+02	0.1913369E+02	0.7969013E+02
331	111	2	-0.3500000E+00	0.7922648E+02	0.4082407E+02	0.2611022E+00
332	111	1	0.7000000E+00	0.8000000E+02	0.4000000E+02	0.0000000E+00
333	111	2	-0.3500000E+00	0.8077352E+02	0.3917593E+02	-0.2611022E+00
334	112	2	-0.3500000E+00	0.8066749E+02	0.4088854E+02	0.1966751E+02
335	112	1	0.7000000E+00	0.8000000E+02	0.4000000E+02	0.2000000E+02

```
       336         112          2  -0.3500000E+00   0.7933251E+02   0.3911146E+02   0.2033249E+02
       337         113          2  -0.3500000E+00   0.8069549E+02   0.3954844E+02   0.3918884E+02
       338         113          1   0.7000000E+00   0.8000000E+02   0.4000000E+02   0.4000000E+02
       339         113          2  -0.3500000E+00   0.7930451E+02   0.4045156E+02   0.4081116E+02
       340         114          2  -0.3500000E+00   0.8007865E+02   0.4112683E+02   0.5973607E+02
       341         114          1   0.7000000E+00   0.8000000E+02   0.4000000E+02   0.6000000E+02
       342         114          2  -0.3500000E+00   0.7992135E+02   0.3887317E+02   0.6026393E+02
       343         115          2  -0.3500000E+00   0.8096299E+02   0.4019568E+02   0.7938358E+02
       344         115          1   0.7000000E+00   0.8000000E+02   0.4000000E+02   0.8000000E+02
       345         115          2  -0.3500000E+00   0.7903701E+02   0.3980432E+02   0.8061642E+02
       346         116          2  -0.3500000E+00   0.7903127E+02   0.5945997E+02   0.3398998E+00
       347         116          1   0.7000000E+00   0.8000000E+02   0.6000000E+02   0.0000000E+00
       348         116          2  -0.3500000E+00   0.8096873E+02   0.6054003E+02  -0.3398998E+00
       349         117          2  -0.3500000E+00   0.8112387E+02   0.5972470E+02   0.2008208E+02
       350         117          1   0.7000000E+00   0.8000000E+02   0.6000000E+02   0.2000000E+02
       351         117          2  -0.3500000E+00   0.7887613E+02   0.6027530E+02   0.1991792E+02
       352         118          2  -0.3500000E+00   0.8015299E+02   0.5889828E+02   0.4032923E+02
       353         118          1   0.7000000E+00   0.8000000E+02   0.6000000E+02   0.4000000E+02
       354         118          2  -0.3500000E+00   0.7984701E+02   0.6110172E+02   0.3967077E+02
       355         119          2  -0.3500000E+00   0.7890693E+02   0.6006545E+02   0.6038278E+02
       356         119          1   0.7000000E+00   0.8000000E+02   0.6000000E+02   0.6000000E+02
       357         119          2  -0.3500000E+00   0.8109307E+02   0.5993455E+02   0.5961722E+02
       358         120          2  -0.3500000E+00   0.7909845E+02   0.5930084E+02   0.7979030E+02
       359         120          1   0.7000000E+00   0.8000000E+02   0.6000000E+02   0.8000000E+02
       360         120          2  -0.3500000E+00   0.8090155E+02   0.6069916E+02   0.8020970E+02
       361         121          2  -0.3500000E+00   0.7905708E+02   0.8067231E+02  -0.6699613E-01
       362         121          1   0.7000000E+00   0.8000000E+02   0.8000000E+02   0.0000000E+00
       363         121          2  -0.3500000E+00   0.8094292E+02   0.7932769E+02   0.6699613E-01
       364         122          2  -0.3500000E+00   0.8072867E+02   0.8034531E+02   0.1916609E+02
       365         122          1   0.7000000E+00   0.8000000E+02   0.8000000E+02   0.2000000E+02
       366         122          2  -0.3500000E+00   0.7927133E+02   0.7965469E+02   0.2083391E+02
       367         123          2  -0.3500000E+00   0.7996616E+02   0.7890097E+02   0.3963043E+02
       368         123          1   0.7000000E+00   0.8000000E+02   0.8000000E+02   0.4000000E+02
       369         123          2  -0.3500000E+00   0.8003384E+02   0.8109903E+02   0.4036957E+02
       370         124          2  -0.3500000E+00   0.7916423E+02   0.8041742E+02   0.6068763E+02
       371         124          1   0.7000000E+00   0.8000000E+02   0.8000000E+02   0.6000000E+02
       372         124          2  -0.3500000E+00   0.8083577E+02   0.7958258E+02   0.5931237E+02
       373         125          2  -0.3500000E+00   0.7897990E+02   0.7955697E+02   0.7967028E+02
       374         125          1   0.7000000E+00   0.8000000E+02   0.8000000E+02   0.8000000E+02
       375         125          2  -0.3500000E+00   0.8102010E+02   0.8044303E+02   0.8032972E+02

Bonds

         1           1           1           2
         2           1           2           3
```

3	1	4	5
4	1	5	6
5	1	7	8
6	1	8	9
7	1	10	11
8	1	11	12
9	1	13	14
10	1	14	15
11	1	16	17
12	1	17	18
13	1	19	20
14	1	20	21
15	1	22	23
16	1	23	24
17	1	25	26
18	1	26	27
19	1	28	29
20	1	29	30
21	1	31	32
22	1	32	33
23	1	34	35
24	1	35	36
25	1	37	38
26	1	38	39
27	1	40	41
28	1	41	42
29	1	43	44
30	1	44	45
31	1	46	47
32	1	47	48
33	1	49	50
34	1	50	51
35	1	52	53
36	1	53	54
37	1	55	56
38	1	56	57
39	1	58	59
40	1	59	60
41	1	61	62
42	1	62	63
43	1	64	65
44	1	65	66
45	1	67	68
46	1	68	69
47	1	70	71

48	1	71	72
49	1	73	74
50	1	74	75
51	1	76	77
52	1	77	78
53	1	79	80
54	1	80	81
55	1	82	83
56	1	83	84
57	1	85	86
58	1	86	87
59	1	88	89
60	1	89	90
61	1	91	92
62	1	92	93
63	1	94	95
64	1	95	96
65	1	97	98
66	1	98	99
67	1	100	101
68	1	101	102
69	1	103	104
70	1	104	105
71	1	106	107
72	1	107	108
73	1	109	110
74	1	110	111
75	1	112	113
76	1	113	114
77	1	115	116
78	1	116	117
79	1	118	119
80	1	119	120
81	1	121	122
82	1	122	123
83	1	124	125
84	1	125	126
85	1	127	128
86	1	128	129
87	1	130	131
88	1	131	132
89	1	133	134
90	1	134	135
91	1	136	137
92	1	137	138

93	1	139	140
94	1	140	141
95	1	142	143
96	1	143	144
97	1	145	146
98	1	146	147
99	1	148	149
100	1	149	150
101	1	151	152
102	1	152	153
103	1	154	155
104	1	155	156
105	1	157	158
106	1	158	159
107	1	160	161
108	1	161	162
109	1	163	164
110	1	164	165
111	1	166	167
112	1	167	168
113	1	169	170
114	1	170	171
115	1	172	173
116	1	173	174
117	1	175	176
118	1	176	177
119	1	178	179
120	1	179	180
121	1	181	182
122	1	182	183
123	1	184	185
124	1	185	186
125	1	187	188
126	1	188	189
127	1	190	191
128	1	191	192
129	1	193	194
130	1	194	195
131	1	196	197
132	1	197	198
133	1	199	200
134	1	200	201
135	1	202	203
136	1	203	204
137	1	205	206

138	1	206	207
139	1	208	209
140	1	209	210
141	1	211	212
142	1	212	213
143	1	214	215
144	1	215	216
145	1	217	218
146	1	218	219
147	1	220	221
148	1	221	222
149	1	223	224
150	1	224	225
151	1	226	227
152	1	227	228
153	1	229	230
154	1	230	231
155	1	232	233
156	1	233	234
157	1	235	236
158	1	236	237
159	1	238	239
160	1	239	240
161	1	241	242
162	1	242	243
163	1	244	245
164	1	245	246
165	1	247	248
166	1	248	249
167	1	250	251
168	1	251	252
169	1	253	254
170	1	254	255
171	1	256	257
172	1	257	258
173	1	259	260
174	1	260	261
175	1	262	263
176	1	263	264
177	1	265	266
178	1	266	267
179	1	268	269
180	1	269	270
181	1	271	272
182	1	272	273

183	1	274	275
184	1	275	276
185	1	277	278
186	1	278	279
187	1	280	281
188	1	281	282
189	1	283	284
190	1	284	285
191	1	286	287
192	1	287	288
193	1	289	290
194	1	290	291
195	1	292	293
196	1	293	294
197	1	295	296
198	1	296	297
199	1	298	299
200	1	299	300
201	1	301	302
202	1	302	303
203	1	304	305
204	1	305	306
205	1	307	308
206	1	308	309
207	1	310	311
208	1	311	312
209	1	313	314
210	1	314	315
211	1	316	317
212	1	317	318
213	1	319	320
214	1	320	321
215	1	322	323
216	1	323	324
217	1	325	326
218	1	326	327
219	1	328	329
220	1	329	330
221	1	331	332
222	1	332	333
223	1	334	335
224	1	335	336
225	1	337	338
226	1	338	339
227	1	340	341

```
       228          1        341        342
       229          1        343        344
       230          1        344        345
       231          1        346        347
       232          1        347        348
       233          1        349        350
       234          1        350        351
       235          1        352        353
       236          1        353        354
       237          1        355        356
       238          1        356        357
       239          1        358        359
       240          1        359        360
       241          1        361        362
       242          1        362        363
       243          1        364        365
       244          1        365        366
       245          1        367        368
       246          1        368        369
       247          1        370        371
       248          1        371        372
       249          1        373        374
       250          1        374        375

Angles

         1          1          1          2          3
         2          1          4          5          6
         3          1          7          8          9
         4          1         10         11         12
         5          1         13         14         15
         6          1         16         17         18
         7          1         19         20         21
         8          1         22         23         24
         9          1         25         26         27
        10          1         28         29         30
        11          1         31         32         33
        12          1         34         35         36
        13          1         37         38         39
        14          1         40         41         42
        15          1         43         44         45
        16          1         46         47         48
        17          1         49         50         51
        18          1         52         53         54
        19          1         55         56         57
```

20	1	58	59	60
21	1	61	62	63
22	1	64	65	66
23	1	67	68	69
24	1	70	71	72
25	1	73	74	75
26	1	76	77	78
27	1	79	80	81
28	1	82	83	84
29	1	85	86	87
30	1	88	89	90
31	1	91	92	93
32	1	94	95	96
33	1	97	98	99
34	1	100	101	102
35	1	103	104	105
36	1	106	107	108
37	1	109	110	111
38	1	112	113	114
39	1	115	116	117
40	1	118	119	120
41	1	121	122	123
42	1	124	125	126
43	1	127	128	129
44	1	130	131	132
45	1	133	134	135
46	1	136	137	138
47	1	139	140	141
48	1	142	143	144
49	1	145	146	147
50	1	148	149	150
51	1	151	152	153
52	1	154	155	156
53	1	157	158	159
54	1	160	161	162
55	1	163	164	165
56	1	166	167	168
57	1	169	170	171
58	1	172	173	174
59	1	175	176	177
60	1	178	179	180
61	1	181	182	183
62	1	184	185	186
63	1	187	188	189
64	1	190	191	192

65	1	193	194	195
66	1	196	197	198
67	1	199	200	201
68	1	202	203	204
69	1	205	206	207
70	1	208	209	210
71	1	211	212	213
72	1	214	215	216
73	1	217	218	219
74	1	220	221	222
75	1	223	224	225
76	1	226	227	228
77	1	229	230	231
78	1	232	233	234
79	1	235	236	237
80	1	238	239	240
81	1	241	242	243
82	1	244	245	246
83	1	247	248	249
84	1	250	251	252
85	1	253	254	255
86	1	256	257	258
87	1	259	260	261
88	1	262	263	264
89	1	265	266	267
90	1	268	269	270
91	1	271	272	273
92	1	274	275	276
93	1	277	278	279
94	1	280	281	282
95	1	283	284	285
96	1	286	287	288
97	1	289	290	291
98	1	292	293	294
99	1	295	296	297
100	1	298	299	300
101	1	301	302	303
102	1	304	305	306
103	1	307	308	309
104	1	310	311	312
105	1	313	314	315
106	1	316	317	318
107	1	319	320	321
108	1	322	323	324
109	1	325	326	327

110	1	328	329	330
111	1	331	332	333
112	1	334	335	336
113	1	337	338	339
114	1	340	341	342
115	1	343	344	345
116	1	346	347	348
117	1	349	350	351
118	1	352	353	354
119	1	355	356	357
120	1	358	359	360
121	1	361	362	363
122	1	364	365	366
123	1	367	368	369
124	1	370	371	372
125	1	373	374	375