Packed In A Glassy Structure (ver.3 on 3/20)
2009 Skadron Prize In Computational Physics

When we cool down a liquid consisting of two kinds of atoms (*e.g.*, Au/Si), these atoms sometimes do not form a crystalline solid where they are orderly arranged on a regular lattice structure. Instead, they are almost randomly arranged in a so-called glassy or amorphous structure, which corresponds to a local minimum in the total potential energy function that depends on the positions of the atoms. For such a system that cools down to a glassy structure, its total potential energy function is known to have many local minima each corresponding to a different glassy structure.

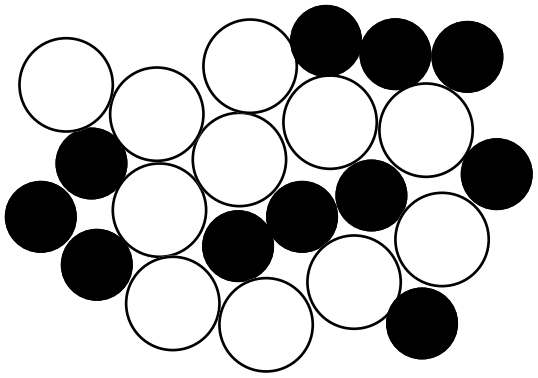
For this year's Skadron prize, we ask you to create a subroutine that finds an atomic structure for a "two-dimensional" system of atoms that are confined in a square with side L. The goal is to find an atomic structure with the lowest value for the following total potential energy function V:

$$V = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\phi\left(\left|\vec{r}_i^{(A)} - \vec{r}_j^{(A)}\right|\right) + 1.4^{12}\sum_{k=1}^{N-1}\sum_{l=k+1}^{N}\phi\left(\left|\vec{r}_k^{(B)} - \vec{r}_l^{(B)}\right|\right) + 1.2^{12}\sum_{i=1}^{N}\sum_{k=1}^{N}\phi\left(\left|\vec{r}_i^{(A)} - \vec{r}_k^{(B)}\right|\right),$$

where $\vec{r}_i^{(A)}$ and $\vec{r}_k^{(B)}$ are the two-dimensional position vectors for the i-th atom of type A and the k-th atom of type B, respectively: $\vec{r}_i^{(A)} = \left(x_i^{(A)}, y_i^{(A)}\right)$ and $\vec{r}_k^{(B)} = \left(x_k^{(B)}, y_k^{(B)}\right)$, where $0 \le x_i^{(A)} \le L$, $0 \le y_i^{(A)} \le L$, $0 \le x_k^{(B)} \le L$, and $0 \le y_k^{(B)} \le L$. $\left|\vec{r} - \vec{r}\,'\right|$ is the distance between two atoms at positions $\vec{r} = (x, y)$ and $\vec{r}\,' = (x', y')$: $\left|\vec{r} - \vec{r}\,'\right| = \sqrt{(x - x')^2 + (y - y')^2}$ N is the total number of each type of atoms. For the contest, we will choose $N = 5000$ and $L = 111.8$. The function $\phi(r)$ in the definition of V is defined by

$$\phi(r) = \begin{cases} \dfrac{1}{r^{12}} & (0 \le r \le 4.5) \\ 0 & (4.5 < r) \end{cases}$$

Finding an atomic structure that minimize V is analogous to finding an arrangement of soft rubber disks of two different sizes all packed in a square box of side L. The diameter of a type-A disk is 1 while the diameter of a type-B disk is 1.4 when they are not squeezed into smaller sizes and a type-A disk can "touch" a type-B disk when their centers are separated by a distance of 1.2 as $1/2 + 1.4/2 = 2.4/2 = 1.2$. With our choice of $N = 5000$ and $L = 111.8$, some of the disks must be squeezed into smaller sizes. CAUTION: it is known that for this system, a simple regular crystalline structure such as a triangular structure does not correspond to the lowest value of the total potential energy function.



Challenge

Write a FORTRAN subroutine "pack.f" that must start with the following 2 lines:

```
subroutine pack (xa, ya, xb, yb, n, al)
dimension xa(n), ya(n), xb(n), yb(n)
```

where

n is the total number *N* of each type of atoms. xa and ya are real array variables of size n. xa(i) and ya(i) represent the *x* and *y* coordinates of the *i*-th atom of type A. xb and yb are real array variables of size n. xb(k) and yb(k) represent the *x* and *y* coordinates of the *k*-th atom of type B. al is the length *L* of each side of the square in which all the atoms must be placed. For the contest, we will use the following values for n and al: n = 5000 and al = 111.8 However, your subroutine should be able to run for any arbitrary values of n and al.

The Skadron Prize committee will run your subroutine "pack.f" with the main program "skmain09.f" (to be provided by the committee) that checks if the position of each atom selected by your subroutine is inside the square of side *L* and calculates the value of the total potential energy function *V* for the atomic structure created by your subroutine. The main program also creates a data file "pack.dat" that contains the data for all the atomic coordinates for the structure generated by your subroutine so that you can look at the structure using "Kaleidagraph." The first prize goes to the contestant whose subroutine creates the atomic structure with the lowest value of *V*. Your subroutine must also complete its computation within 5 minutes.

To test your subroutine "pack.f" on our computer "meitner":

1. Copy the main program "skmain09.f" on "meitner" to your account on "meitner":

   ```
   copy ~hmb/hmb/skmain09.f skmain09.f
   ```

2. Compile and run your subroutine with the main program:

   ```
   g95 skmain09.f pack.f
   a.out
   ```

To visualize the atomic structure generated by your subroutine "pack.f":

1. Copy the data file "pack.dat" generated by the main program to an iMac you are using.
2. Launch "Kaleidagraph."
3. Use the "Open" command in the "File" pull-down menu in "Kaleidagraph" to open "pack.dat." Before locating "pack.dat," enable "All Documents" in the dialog box.
4. In the "Text File Input Format" dialog box, select "Space" for "Delimiter:" and ">=1" for "Number:". Type in "1" in the box below "Lines Skipped" and deselect "Read Titles" under "Options:".
5. You find four columns filled with numbers: the column 1 lists the number given to each atom ranging from 1 to 5000; the column 2 lists the *x*-coordinate of the type-A atom with the number in the column 1; the column 3 lists the *y*-coordinate of that type-A atom; the column 4 lists the *x*-coordinate of the type-B atom with the number in the column 1; the column 5 lists the *y*-coordinate of that type-B atom. You can plot the atomic positions using a linear scatter plot.

Prizes: $ 200 for the first place, $100 for the second place.

Who can participate: Physics majors at ISU. **Deadline:** 4 p.m. on Friday, April 17, 2009.