Fortran Programming Exercise

Crystal Lattice Energy Calculator

Materials Science Department

Exercise Information

Topic: Computational Materials Science
Estimated Time: 1 hour
Difficulty: Intermediate
Language: Fortran 90/95

1 Problem Statement

Write a Fortran program to calculate the cohesive energy of a 2D crystal lattice using the Lennard-Jones potential. This is a simplified model for understanding atomic interactions in materials.

2 Background

The Lennard-Jones potential describes the interaction energy between two atoms. It captures both the repulsive force at short distances and the attractive van der Waals force at longer distances.

$$V(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{1}$$

Where:

- r is the distance between atoms
- ε (epsilon) is the depth of the potential well (energy parameter)
- σ (sigma) is the distance at which the potential is zero

3 Task Requirements

3.1 Input Specification

Your program should read from a file named `lattice.dat` with the following format:

- Line 1: Number of atoms (N)
- Line 2: Lennard-Jones parameters: ε (eV) and σ (Ångströms)
- Lines 3 to $N + 2$: x, y coordinates of each atom (Ångströms)

3.2 Calculations Required

1. Calculate pairwise distances between all atoms
2. Compute the Lennard-Jones potential for each pair
3. Sum all pairwise interactions to get total potential energy
4. Calculate the cohesive energy per atom:

$$E_{\text{cohesive}} = \frac{E_{\text{total}}}{N} \tag{2}$$

3.3 Output Requirements

Print to console:

- Total potential energy (eV)
- Cohesive energy per atom (eV)
- Nearest neighbor distance (Ångströms)
- Number of pairs calculated

Also write results to `results.dat`

4 Sample Input File

The file `lattice.dat` should look like this:

```
9
0.0104 3.40
0.0 0.0
3.5 0.0
7.0 0.0
0.0 3.5
3.5 3.5
7.0 3.5
0.0 7.0
3.5 7.0
7.0 7.0
```

This represents a 3×3 square lattice with 9 atoms.

5 Expected Behavior

Important Notes

- Handle the case where atoms might be at the same position ($r = 0$)
- Use double precision for all calculations
- The potential should only be calculated once per pair (not double-counted)
- Distance between points (x_1, y_1) and (x_2, y_2) is:

$$d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$$

6 Implementation Hints

- You'll need to use nested loops to iterate over all pairs
- Consider using `SQRT()` for distance calculations
- Each pair should only be counted once (i.e., if you calculate $V(\text{atom}_i, \text{atom}_j)$, don't also calculate $V(\text{atom}_j, \text{atom}_i)$)
- Use a conditional like `DO i = 1, N-1` and `DO j = i+1, N` to avoid double counting
- Remember to declare variables with `REAL(8)` or `DOUBLE PRECISION`

Bonus Challenges (Optional)

If you finish early, try implementing these extensions:

1. Implement a cutoff distance (e.g., 10 Ångströms) beyond which interactions are ignored
2. Calculate and report the average coordination number (number of nearest neighbors per atom)
3. Create a simple visualization by writing coordinates colored by local energy to a file
4. Extend the program to 3D lattices

7 Program Structure Suggestion

Consider organizing your program with the following structure:

```fortran
PROGRAM lattice_energy
  IMPLICIT NONE

  ! Variable declarations
  INTEGER :: N, i, j, num_pairs
  REAL(8) :: epsilon, sigma
  REAL(8), ALLOCATABLE :: x(:), y(:)
  REAL(8) :: total_energy, cohesive_energy
  REAL(8) :: min_distance

  ! Read input file
  ! ...

  ! Calculate pairwise energies
  ! ...

  ! Write output
  ! ...

END PROGRAM lattice_energy
```

8 Grading Criteria

Your program will be evaluated on:

- **Correctness (50%):** Accurate implementation of the Lennard-Jones potential
- **Code Quality (25%):** Clear variable names, proper formatting, comments
- **I/O Handling (15%):** Correct file reading and output formatting
- **Error Handling (10%):** Managing edge cases (e.g., $r = 0$)

Good luck and enjoy exploring computational materials science!