

Writing fast Fortran routines for Python

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Overview

Python, unfortunately, does not always come pre-equipped with the speed necessary to perform intense numerical computations in user-defined routines. Ultimately, this is due to Python's flexibility as a programming language. Very efficient programs are often inflexible: every variable is typed as a specific numeric format and all arrays have exactly specified dimensions. Such inflexibility enables programs to assign spots in memory to each variable that can be accessed efficiently, and it eliminates the need to check the type of each variable before performing an operation on it.

Fortunately, it is very easy to maintain the vast majority of Python flexibility and still write very efficient code. We can do this because typically our simulations are dominated by a few bottleneck steps, while the remainder of the code we write is insignificant in terms of computational demands. Things like outputting text to a display, writing data to files, setting up the simulation, keeping track of energy and other averages, and even modifying the simulation while its running (e.g., changing the box size or adding/deleting a particle) are actually not that computationally intensive. On the other hand, computing the total energies and forces on each atom in a *pairwise loop* is quite expensive. This is an order N^2 operation, where the number of atoms N typically varies from 100 to 10000.

The solution is to write the expensive steps in a fast language like Fortran and to keep everything else in Python. Fortunately, this is a very easy task. There are a large number of automated tools for compiling fast code in C, C++, or Fortran into *modules* that can be imported into Python just like any other module. Functions in that module can be called as if they were written in Python, but with the performance of compiled code. There are even now tools for converting Python code into compiled C++ libraries so that one never has to know another programming language other than Python (although these very often have a steep learning curve).

For the purposes of this class, we will use a specific tool called **f2py** that completely automates the compilation of Fortran code into Python modules. The reason we will use this instead of other approaches is that: (1) f2py is relatively stable, very simple to use, and comes built-in with NumPy; (2) Fortran, albeit a somewhat archaic and inflexible language, is simple and actually one of the fastest compiled languages; and (3) a large amount of existing code in the scientific community is written in Fortran and thus you would benefit from being able to both understand and incorporate this code into your own.

Installation

Everything you will need is open source or freely licensed. Moreover, all of the utilities discussed below are cross-platform. If you have installed the Anaconda Distribution, then you should have

most of the necessary files available. You will need to add a Fortran compiler, and on Windows machines, some accessory files. See the course syllabus for details.

Basic Fortran programming

Before we begin compiling routines, we need some background on programming in Fortran. Fortunately, we only need to know the basics of the Fortran language since we will only be writing numerical functions and not coding entire Fortran projects.

We will be using the Fortran 90 standard. There are older versions of Fortran, notably Fortran 77, that are much more difficult to read and use. Fortran 90 files all end in the extension `.f90` and we can put multiple functions in a single `.f90` file—these functions will eventually each appear as separate member functions of the Python module we make from this Fortran file.

Fortran 90 code is actually fairly straightforward to develop, but it is important to keep in mind some main differences from Python:

- Fortran is *not* case-sensitive. That is, the names `atom`, `Atom`, and `ATOM` all designate the same variable.
- The comment character is an exclamation point, `!`, instead of the pound sign in Python.
- Spacing is *unimportant* in Fortran. Instead of using spacing to show the commands included with a subroutine or loop, Fortran uses beginning and closing statements. For example, subroutines begin with `subroutine MyFunction(...)` and end with `end subroutine`.
- Fortran *does* make a distinction between *functions* that return single variable values and *subroutines* that do not return anything but that can modify the contents of variables sent to it. However, in writing code to be compiled for Python, we will always write subroutines and therefore will not need to worry about functions. We will often use the nomenclature "function" interchangeably with subroutine.
- Fortran does not have name binding. Instead, if you change the value of a variable passed to a subroutine via the assignment operation (`=`), the value of that variable is changed for good. Fortunately, Fortran lets us declare whether or not variables can be modified in functions, and a compile error will be thrown if we violate our own rules.
- Every variable should be *typed*. That means that, at the beginning of a function, we should specify the type and size of every variable passed to it, passed from it, and created during it. This is very important to the speed of routines. More on this later.

- Fortran has no list, dictionary, or tuple capabilities. It only has arrays. When we iterate over an array using a loop, we must always create an integer variable that is the loop index. Moreover, Fortran loops are *inclusive* of the upper bound.
- Fortran uses parenthesis () rather than brackets [] to access array elements.
- Fortran array indices start at 1 by default, rather than at 0 as in Python. This can be very confusing, and we will always explicitly override this behavior so that arrays start at 0.

Let's start with a specific example to get us going. We will write a function that takes in a (N,3) array of N atom positions, computes the centroid (the average position), and makes this point the origin by centering the original array. In Python / NumPy, we could accomplish this task using a single line:

```
Pos = Pos - Pos.mean(axis=0)
```

An equivalent Fortran subroutine would look the following:

```
subroutine CenterPos(Pos, Dim, NAtom)
  implicit none
  integer, intent(in) :: Dim, NAtom
  real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Pos
  real(8), dimension(0:Dim-1) :: PosAvg
  integer :: i, j
  PosAvg = sum(Pos, 1) / dble(NAtom)
  do i = 0, NAtom - 1
    do j = 0, Dim - 1
      Pos(i,j) = Pos(i,j) - PosAvg(j)
    end do
  end do
end subroutine
```

In the above example, we defined a subroutine called `CenterPos` that takes three arguments: the array `Pos`, the dimensionality `Dim`, and the number of atoms `NAtom`. The subroutine is entirely contained within the initial `subroutine` and `end subroutine` statements.

Immediately after the declaration statement, we use the phrase `implicit none`. It is a good habit *always* to include this statement immediately after the declaration. It tells the Fortran compiler to raise an error if we do not define a variable that we use. Defining variables is critical to the speed of our code.

Next we have a series of statements that define all variables, including those that are sent to the function. These statements have the following forms. For arguments to our function that are single values, we use:

```
type TYPE, intent(INTENT) :: NAME
```

For array arguments, we use:

```
type TYPE, intent(INTENT), dimension(DIMENSIONS) :: NAME
```

Finally, for other variables that we use within the function, but that are not arguments/inputs or outputs, we use:

```
type TYPE :: NAME
```

or, for arrays,

```
type TYPE, dimension(DIMENSIONS) :: NAME
```

Here, *TYPE* is a specifier that tells the function the numeric format of a variable. The Fortran equivalents of Python types are:

Python / NumPy	Fortran
float	real(8) (also called <i>double</i>)
int	integer
bool	logical

For arguments, we use the *INTENT* option to tell Python what we are going to do with a variable. There are three such options,

intent	meaning
in	The variable is an input to the subroutine only. Its value must not be changed during the course of the subroutine.
out	The variable is an output from the subroutine only. Its input value is irrelevant. We must assign this variable a value before exiting the subroutine.
inout	The subroutine both uses and modifies the data in the variable. Thus, the initial value is sent and we ultimately make modifications base on it.

For array arguments, we also specify the *DIMENSIONS* of the arrays. For multiple dimensions, we use comma-separated lists. The colon ":" character indicates the range of the dimension. Unlike Python, however, the upper bound is *inclusive*. The statement

```
real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Pos
```

says that the first axis of *Pos* varies from 0 to and including *NAtom-1*, and the second axis from 0 to and including *Dim-1*. We could have also written this statement as

```
real(8), intent(inout), dimension(NAtom, Dim) :: Pos
```

In which case the lower bound of each dimension would have been 1 rather than 0. Instead, we explicitly override this behavior to keep Fortran array indexing the same as that in Python, for clarity in our programming.

Notice that the dimensions are variables that we must declare in and pass to the subroutine when it is called. This, again, is a step that helps achieve faster code. Eventually `f2py` will *automatically* pass these dimensions when the Fortran code is called as a Python module, so that these dimensional arguments are *hidden*. **For that reason, one should always put any arguments that specify dimensions at the end of the argument list.** Notice that all of the dimension variables are at the end of our subroutine declaration:

```
subroutine CenterPos(Pos, Dim, NAtom)
```

Notice that we can list multiple variable names that have the same type, dimensions (if array), and intent (if arguments) on the same line in place of *NAME*.

In addition to the subroutine arguments, we define three additional variables that are used only within our function, created upon entry and destroyed upon exit:

```
real(8), dimension(0:Dim-1) :: PosAvg  
integer :: i, j
```

`PosAvg` is a length-three array that we will use to hold the centroid position we compute. The integers `i` and `j` are the indices we will use when writing loops.

The first line of our program computes the centroid (average position) of our array:

```
PosAvg = sum(Pos, 1) / dble(NAtom)
```

The Fortran function `sum` takes an array argument and sums it, optionally over a specified dimension. Here, we indicate a summation over the *first* axis, that corresponding to the particle number. In other words, Fortran sums all of the `x`, `y`, and `z` values separately and returns a length-three array. It is very important to notice here that the first axis of an array is indicated with 1 rather than 0, as would be the case in Python. This is because Fortran ordering naturally begins at 1.

The `dble` function above takes the integer `NAtom` and converts it to a double-precision number, e.g., of type `real(8)`. It is a good idea to explicitly convert types using such functions in Fortran. Not doing so will force the compiler to insert conversions that many not be what we desired, and could result in extra unanticipated steps that might slow performance. In addition to `dble`, `int(X)` will convert any argument `X` to an integer type.

The lines that follow modify the `Pos` array to subtract the centroid positions from it:

```
do i = 0, NAtom - 1
  do j = 0, Dim - 1
    Pos(i,j) = Pos(i,j) - PosAvg(j)
  end do
end do
```

Notice that we have two loops that iterate over the array indices. Each loop has the following form:

```
do VAR = START, STOP
  COMMANDS
end do
```

In Fortran, such `do` loops involve integers and are inclusive of both the starting and stopping values. Indentation here is optional and just for ease of reading, because it is the `end do` command that signals the end of a loop.

Like Python, Fortran allows array operations. What this means internally is that Fortran will write out the *implied* `do` loop over array elements if we perform array calculations. We could therefore simplify the above code by removing the inner loop:

```
subroutine CenterPos(Pos, Dim, NAtom)
  implicit none
  integer, intent(in) :: Dim, NAtom
  real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Pos
  real(8), dimension(0:Dim-1) :: PosAvg
  integer :: i
  PosAvg = sum(Pos, 1) / dble(NAtom)
  do i = 0, NAtom - 1
    Pos(i,:) = Pos(i,:) - PosAvg(:)
  end do
end subroutine
```

Here, we use Fortran slicing notation to indicate that we want to apply the mathematical operation to each array element.

Slicing of Fortran arrays is very similar to that of NumPy, and uses the `start:stop:step` notation, where each of these can be optional. One small difference is that the upper bounds of arrays are inclusive in Fortran, whereas they are exclusive in Python. In other words, `PosAvg[:2]` takes elements 0 through 1 in Python and `PosAvg(:2)` takes elements 0 through 2 in Fortran.

There is one other, major difference between slicing arrays in Fortran and NumPy: the former does not permit broadcasting. That means that every array in a mathematical operation designed to operate elementwise *must* be the exact same dimensions and size. In NumPy, on the other

hand, broadcasting can be used to automatically up-convert arrays to higher dimensionalities when performing such operations.

A Fortran case study

To illustrate the Fortran language, we will consider the following subroutine that computes the total potential energy and force on each atom for a system of Lennard-Jones particles. Here, total potential energy is given by a sum of pairwise interactions:

$$U = \sum_{i < j} u(r_{ij})$$

$$u(r_{ij}) = 4\epsilon \left[\left(\frac{r_{ij}}{\sigma} \right)^{-12} - \left(\frac{r_{ij}}{\sigma} \right)^{-6} \right]$$

The force in the x-direction on a particular atom is given by:

$$\begin{aligned} F_{i,x} &= -\frac{\partial U}{\partial x_i} \\ &= -\frac{\partial}{\partial x_i} \sum_{j \neq i} u(r_{ij}) \\ &= -\sum_{j \neq i} \frac{\partial r_{ij}}{\partial x_i} \frac{\partial}{\partial r_{ij}} u_{12}(r_{ij}) \end{aligned}$$

But since $r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$,

$$F_{i,x} = -\sum_{j \neq i} \left(\frac{x_i - x_j}{r_{ij}} \right) \frac{\partial}{\partial r_{ij}} u(r_{ij})$$

Thus, generalizing to all three coordinates and using vector notation for $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$:

$$\begin{aligned} \mathbf{F}_i &= \sum_{j \neq i} \left(\frac{\mathbf{r}_{ij}}{r_{ij}} \right) \frac{\partial}{\partial r_{ij}} u(r_{ij}) \\ &= \sum_{j \neq i} \left(\frac{\mathbf{r}_{ij}}{r_{ij}} \right) \left(\frac{4\epsilon}{\sigma} \right) \left[-12 \left(\frac{r_{ij}}{\sigma} \right)^{-13} + 6 \left(\frac{r_{ij}}{\sigma} \right)^{-7} \right] \\ &= \sum_{j \neq i} \mathbf{r}_{ij} \left(\frac{\epsilon}{\sigma} \right) \left[-48 \left(\frac{r_{ij}}{\sigma} \right)^{-14} + 24 \left(\frac{r_{ij}}{\sigma} \right)^{-8} \right] \end{aligned}$$

These equations form the basis of our pairwise interaction loop. We notice that we will need to compute vectors, like \mathbf{r}_{ij} , as well as distances, like r_{ij} . In addition, a large portion of our computational overhead will involve raising quantities to powers.

We must also consider the effects of periodic boundary conditions when computing \mathbf{r}_{ij} and r_{ij} . Each particle should see only those images of other particles that are closest to it. We can accomplish this task by finding the minimum image distance between each pair of particles \mathbf{r}_{ij}^0 . For each component, we use the rounding function `nint`, which returns the nearest integer value:

$$\mathbf{r}_{ij}^0 = \mathbf{r}_{ij} - L \text{ nint}(\mathbf{r}_{ij}/L)$$

Here L is the length of the simulation box, and may be a vector for non-cubic boxes. Notice that this equation implies a separate operation for each component x , y , and z .

Finally, we have to treat the truncation of our potential. We will introduce a cutoff at a pairwise distance r_c , beyond which the value of the potential will be zero; typically $r_c = 2.5\sigma$ or greater. We will also shift our entire potential up in energy by the value at r_c so that the potential energy between any pair of particles continuously approaches zero at r_c . Thus we have:

$$u(r_{ij}) = \begin{cases} 4\epsilon \left[\left(\frac{r_{ij}}{\sigma}\right)^{-12} - \left(\frac{r_{ij}}{\sigma}\right)^{-6} \right] - 4\epsilon \left[\left(\frac{r_c}{\sigma}\right)^{-12} - \left(\frac{r_c}{\sigma}\right)^{-6} \right] & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c \end{cases}$$

In our simulation, we will work with dimensionless units such that values for positions/distances and energies are given in units of σ and ϵ respectively. Thus, our pairwise potential function actually looks like:

$$u(r_{ij}) = \begin{cases} 4[r_{ij}^{-12} - r_{ij}^{-6}] - 4[r_c^{-12} - r_c^{-6}] & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c \end{cases}$$

We are now ready to write our subroutine. A naïve implementation unoptimized for speed might look like:

```

ljlib1.f90
subroutine EnergyForces(Pos, L, rc, PEnergy, Forces, Dim, NAtom)
  implicit none
  integer, intent(in) :: Dim, NAtom
  real(8), intent(in), dimension(0:NAtom-1, 0:Dim-1) :: Pos
  real(8), intent(in) :: L, rc
  real(8), intent(out) :: PEnergy
  real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Forces
  real(8), dimension(Dim) :: rij, Fij
  real(8) :: d, Shift

```

```

integer :: i, j
PEnergy = 0.
Forces = 0.
Shift = -4. * (rc**(-12) - rc**(-6))
do i = 0, NAtom - 1
  do j = i + 1, NAtom - 1
    rij = Pos(j,:) - Pos(i,:)
    rij = rij - L * dnint(rij / L)
    d = sqrt(sum(rij * rij))
    if (d > rc) then
      cycle
    end if
    PEnergy = PEnergy + 4. * (d**(-12) - d**(-6)) + Shift
    Fij = rij * (-48. * d**(-14) + 24. * d**(-12))
    Forces(i,:) = Forces(i,:) + Fij
    Forces(j,:) = Forces(j,:) - Fij
  enddo
enddo
end subroutine

```

Let's consider the features of this subroutine. The arguments `Pos`, `L`, and `rc` are all sent to the function using the `intent(in)` attribute and are not modified. The float `PEnergy` is `intent(out)`, meaning that it will be returned from our function. The array `Forces` is `intent(inout)`. The reason that we did not use `intent(out)` for `Forces` is that this will ultimately imply creation of a new array each time the function is called, after we compile with `f2py`. By declaring the array as `intent(inout)`, we will be able to re-use an existing array for storing the forces, thus avoiding any performance hit that would accompany new array creation. Finally, the arguments `Dim` and `NAtom` give the sizes of various array dimensions.

Upon entering the subroutine, we zero the values of the potential energy and forces since we will add to these variables during the pairwise loop. We also precalculate the values of any constants that will be used during the loop, such as the energy shift due to the pairwise potential truncation.

In the pairwise loop, we compute the minimum image distance using the code

```

rij = Pos(j,:) - Pos(i,:)
rij = rij - L * dnint(rij / L)

```

Notice that `rij` is a length-three array and thus these lines are actually implied loops over each element. Here, `dnint` is the Fortran function returning the nearest integer of its argument as a type `double` or `real(8)` (the same as a Python float).

The absolute distance is computed and we then determine whether or not a pair of atoms is beyond the distance cutoff:

```

d = sqrt(sum(rij * rij))
if (d > rc) then

```

```
cycle
end if
```

The `cycle` statement in Fortran is equivalent to `continue` in Python, and it immediately causes the innermost loop to advance and return to the next iteration. Here, we use it to skip ahead to the next atom pair if two atoms are beyond the cutoff.

Notice the formatting of the `if` statement. In general, Fortran conditional statements have the form:

```
if (CONDITION) then
  COMMANDS
else if (CONDITION) then
  COMMANDS
else
  COMMANDS
end if
```

The test condition can be any conditional expression built from comparison operators, parenthesis, and compound statements. In Fortran, conditional comparisons are given by `=`, `<`, `>`, `<=`, `>=` and `/=`. Only the last of these, which signifies “not equals to”, is different from Python. Moreover, in Fortran compound expressions can be written using `.and.`, `.or.`, and `.not.` which differ from Python only by the presence of a preceding and trailing period. Similarly, the Boolean constants in Fortran are written as `.true.` and `.false.`

After calculating the force, we add this vector to the force array for particle `i` and the negative vector for particle `j` in the loop:

```
Fij = rij * (-48. * d**(-14) + 24. * d**(-12))
Forces(i,:) = Forces(i,:) + Fij
Forces(j,:) = Forces(j,:) - Fij
```

Notice that, like Python, the power operator is written as `**`.

In addition to the `sqrt` function used in this example, Fortran provides a large number of mathematical operations, almost all of which can be used to operate on entire arrays at a time. These functions include:

```
mod, sin, cos, tan, cotan, asin, acos, atan, sinh, cosh,
tanh, asinh, acosh, atanh, exp, log, log10, sqrt,
ceiling, floor, nint, erf, erfc, huge, tiny, epsilon
```

For many of these, the default versions of the functions return single-precision numbers. To obtain double-precision return values, the equivalent of Python floats, there are versions of the functions that start with “d”, such as `dnint` from `nint`.

In addition there are a number of functions that return information about arrays or perform array-specific mathematical operations:

```
count, sum, product, minval, maxval, minloc, maxloc,  
matmul, transpose
```

Many of these functions accept an optional argument `axis=X` that will perform the indicated operation over the specified axis only, returning an array of one smaller dimension. Keep in mind that in Fortran the first axis is `axis=1`, as opposed to Python's `axis=0`.

Maximizing computational efficiency in Fortran code

While the above code appears simple and straightforward, there are a number of ways in which it might be rewritten to require much fewer floating point calculations.

First, we never need to find the absolute distance between two particles; rather, all computations can be rewritten in terms of the squared distance. Thus we can remove the square root operation, which will result in significant time savings.

Second, we can take much greater control over the exponentiation performed to specify exactly the number of multiplications. In particular, the force calculation relies on terms that have overlap with the potential calculation.

Third, we can copy the position of particle *i* into a temporary array to be used in the loop over *j*. This will save the effort of having to locate *i*'s position in memory each time we loop through *j*, as large multidimensional array access can be slow.

With these considerations, our optimized computation looks like:

```
lplib2.f90
```

```
subroutine EnergyForces(Pos, L, rc, PEnergy, Forces, Dim, NAtom)  
  implicit none  
  integer, intent(in) :: Dim, NAtom  
  real(8), intent(in), dimension(0:NAtom-1, 0:Dim-1) :: Pos  
  real(8), intent(in) :: L, rc  
  real(8), intent(out) :: PEnergy  
  real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Forces  
  real(8), dimension(Dim) :: rij, Fij, Posi  
  real(8) :: d2, id2, id6, id12  
  real(8) :: rc2, Shift  
  integer :: i, j  
  PEnergy = 0.  
  Forces = 0.  
  Shift = -4. * (rc**(-12) - rc**(-6))  
  rc2 = rc * rc  
  do i = 0, NAtom - 1  
    !store Pos(i,:) in a temporary array for faster access in j loop
```

```

Posi = Pos(i,:)
do j = i + 1, NAtom - 1
  rij = Pos(j,:) - Posi
  rij = rij - L * dnint(rij / L)
  !compute only the squared distance and compare to squared cut
  d2 = sum(rij * rij)
  if (d2 > rc2) then
    cycle
  end if
  id2 = 1. / d2           !inverse squared distance
  id6 = id2 * id2 * id2   !inverse sixth distance
  id12 = id6 * id6       !inverse twelvth distance
  PEnergy = PEnergy + 4. * (id12 - id6) + Shift
  Fij = rij * ((-48. * id12 + 24. * id6) * id2)
  Forces(i,:) = Forces(i,:) + Fij
  Forces(j,:) = Forces(j,:) - Fij
enddo
enddo
end subroutine

```

Some general considerations for writing fast routines are:

- Store values that are used multiple times in temporary variables to avoid repeating calculations. In the above example, r_{ij}^{-6} was used a number of times for each pair and stored as its own variable `id6`.
- Break down large polynomial expressions so that fewer multiplications are needed. For example, $x^3 + x^2 + x + 1$ requires four multiplication and three addition operations. Alternatively, $x * (x * (x + 1) + 1) + 1$ requires only two multiplication and three addition operations, but gives the same result. In a similar manner, x^8 can be evaluated fastest by $((x^2)^2)^2$.
- If expensive mathematical operations like `log`, `exp`, or `sqrt` can be avoided, rewrite your code to do so.
- If the same elements of a large array are to be accessed many times in succession during a loop, copy these values into a temporary variable first. Fortran will be able to read and write values in variables or smaller, single-dimensional arrays much faster than in large arrays because memory access can be slow and small variables can be optimized to sit in faster parts of memory.
- In Fortran, arrays are traversed most efficiently in memory if the leftmost array index varies the fastest. For example, a double loop over `Pos(i, j)` is the fastest if `i` is the inner loop and `j` the outer. Similarly, expressions like `Pos(:, j)` are faster than `Pos(j, :)`. Unfortunately, writing code in this way is not always possible given the way in which it is natural to define arrays in Python and how Python passes variables to

Fortran. In the above example, we were not able to make the inner index vary fastest because `Pos` was passed with the (x,y,z) coordinates in the second index, which we need to access all at one time. However, if given the option, choose loops that vary the fastest over the leftmost array indices.

Multiple functions in each Fortran file

We can put multiple subroutines inside the same Fortran file. Generally it is a good idea to group functions together in files by their purpose and level of generality. In other words, keep functions specific to the potential energy function in a separate Fortran file from those which perform generic geometric manipulations (e.g., rotation of a rigid body). When compiled for Python, all of the subroutines in a given Fortran file will appear as functions in the same imported module.

Here is the example from above extended with a subroutine that advances the positions and velocities of each atom using the velocity Verlet algorithm:

```
lplib3.f90
```

```
subroutine EnergyForces(Pos, L, rc, PEnergy, Forces, Dim, NAtom)
  implicit none
  integer, intent(in) :: Dim, NAtom
  real(8), intent(in), dimension(0:NAtom-1, 0:Dim-1) :: Pos
  real(8), intent(in) :: L, rc
  real(8), intent(out) :: PEnergy
  real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Forces
  real(8), dimension(Dim) :: rij, Fij, Posi
  real(8) :: d2, id2, id6, id12
  real(8) :: rc2, Shift
  integer :: i, j
  PEnergy = 0.
  Forces = 0.
  Shift = -4. * (rc**(-12) - rc**(-6))
  rc2 = rc * rc
  do i = 0, NAtom - 1
    !store Pos(i,:) in a temporary array for faster access in j loop
    Posi = Pos(i,:)
    do j = i + 1, NAtom - 1
      rij = Pos(j,:) - Posi
      rij = rij - L * dnint(rij / L)
      !compute only the squared distance and compare to squared cut
      d2 = sum(rij * rij)
      if (d2 > rc2) then
        cycle
      end if
      id2 = 1. / d2           !inverse squared distance
      id6 = id2 * id2 * id2   !inverse sixth distance
      id12 = id6 * id6       !inverse twelvth distance
      PEnergy = PEnergy + 4. * (id12 - id6) + Shift
      Fij = rij * ((-48. * id12 + 24. * id6) * id2)
      Forces(i,:) = Forces(i,:) + Fij
      Forces(j,:) = Forces(j,:) - Fij
    enddo
  enddo
end subroutine
```

```

subroutine VVIntegrate(Pos, Vel, Accel, L, CutSq, dt, KEnergy, PEnergy, Dim, NAtom)
  implicit none
  integer, intent(in) :: Dim, NAtom
  real(8), intent(in) :: L, CutSq, dt
  real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Pos, Vel, Accel
  real(8), intent(out) :: KEnergy, PEnergy
  external :: EnergyForces
  Pos = Pos + dt * Vel + 0.5 * dt*dt * Accel
  Vel = Vel + 0.5 * dt * Accel
  call EnergyForces(Pos, L, CutSq, PEnergy, Accel, Dim, NAtom)
  Vel = Vel + 0.5 * dt * Accel
  KEnergy = 0.5 * sum(Vel*Vel)
end subroutine

```

Notice that the `VVIntegrate` function calls the `EnergyForces` function within it. When a Fortran function calls another function, we must also declare the latter using the `external` keyword as we wrote above. This tells the compiler that the function we are calling lies somewhere else in the code we wrote. In addition, called subroutines must be preceded with the keyword `call`.

Compiling and debugging

Once we have written our Fortran source code, we must compile it. Ultimately this will be done automatically by `f2py` in the creation of a Python module from the `.f90` file. However, to debug our code, it is often useful to first try to compile the Fortran source directly. To compile our code above, we write at the command line:

```
c:\> gfortran -c ljlib3.f90
```

If there were no errors in our program, `gfortran` will return quietly with no output and a file `ljlib3.o` will have been created, an object file that can be subsequently linked into an executable file. We will have no use for the `.o` file here, since we are only concerned with identifying errors in our code at this point, and thus it is safe to delete it.

If `gfortran` finds a problem with our code, it will return an error message. For example, if we used the assignment `k=1` in our code, but forgot to explicitly define the type of `k`, `gfortran` would return:

```

ljlib3.f90:50.5:
      k = 1
      1
Error: Symbol 'k' at (1) has no IMPLICIT type

```

In the first line, we are given the line (50) and column (5) numbers where it found the error, as well as the specific error message. The number 1 is used underneath the offending line to show where the error occurred.

Sometimes our program compiles just fine, but we still experience numerical problems in running our code. At this point, it often becomes useful to track values of variables throughout the program execution. In Python, we could place `print` statements throughout the code to periodically report on variable values. If we also need to see the values of variables during called Fortran routines, we can similarly place `print` statements within our Fortran code during test production. In Fortran a `print` statement has the form:

```
print *, var1, var2, var3
```

Here, one must always include the “*,” indicator after the Fortran `print` statement to tell it that you want to send the values to the terminal (screen), and not to a file or attached device.

There are also many Fortran source code editors with a graphical user interface that color-code statements and functions for ease of viewing, and that will often check for simple errors. The Spyder editor included with the Anaconda Distribution is one such editor.

Preparing code for f2py

Generally, if we write Fortran code that strongly types and specifies intents for all variables, then there is very little that we need to do before using `f2py` to convert it into a Python-importable module. However, for *array variables* with the `intent(inout)` attribute, we typically need to add a small *directive* that tells `f2py` how we want to deal with this particular kind of variable. `f2py` directives are small comments at the beginning of lines (no preceding spaces) that start as “!f2py”. For `intent(inout)` variables, we simply add

```
!f2py intent(in,out) :: VAR
```

to the line after an argument declaration statement.

Consider the `EnergyForces` function. Here, we need to place an `f2py` directive immediately after the type declaration for the `Forces` variable:

```
...  
    real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Forces  
    !f2py intent(in,out) :: Forces  
...
```

Since our directive begins with the Fortran comment character “!”, it will not affect compilation by Fortran during debugging. However, the addition of `intent(in,out) :: Forces` will tell `f2py` that we want the Python version of our Fortran function to treat the array `Forces` as an argument and also as a return value as a part of the return tuple.

We need to similarly modify the code for `VVIntegrate`:


```
...
    real(8), intent(inout), dimension(0:NAtom-1, 0:Dim-1) :: Pos, Vel, Accel
!f2py intent(in,out) :: Pos, Vel, Accel
...
```

Running f2py

Once we have written and debugged our Fortran source code, we are ready to compile it into a Python module using the f2py utility. If your environment variables are set up correctly, you should be able to run f2py directly from the command line or terminal. On a Windows system, start an Anaconda Prompt to open a terminal.

Running f2py without any arguments prints out a long help file:

```
c:\> f2py.py
Usage:

1) To construct extension module sources:

    f2py [<options>] <fortran files> [[[only:]]|[[skip:]] \
        <fortran functions> ] \
        [: <fortran files> ...]

2) To compile fortran files and build extension modules:

    f2py -c [<options>, <build_flib options>, <extra options>] <fortran files>

3) To generate signature files:

    f2py -h <filename.pyf> ...< same options as in (1) >

Description: This program generates a Python C/API file (<modulename>module.c)
that contains wrappers for given fortran functions so that they
can be called from Python. With the -c option the corresponding
extension modules are built.

...
```

If this did not work on your system, you may need to explicitly run with Python as well as give the full path to f2py:

```
c:\> python c:\python26\scripts\f2py.py
```

f2py is a powerful utility that enables a lot of control over how modules are compiled. Here we will only describe a specific subset of its abilities. To compile our code into a module on a Windows platform we use a command of the following form:

```
f2py.py -c -m MODULENAME SOURCE.f90 --fcompiler=gnu95 --compiler=mingw32
```

Here, *MODULENAME* is the name we want for our module after it is compiled. *SOURCE.f90* is the name of the file containing the Fortran source code. The `-c` and `-m` flags indicate compilation and the name specification, respectively. The option `--fcompiler=gnu95` tells f2py to use

the GFortran compiler that we downloaded and installed earlier. There are other Fortran compilers that will work with f2py that could be specified here. To see what compilers are present and recognized on your system, use the following command:

```
c:\> f2py.py -c --help-fcompiler
Fortran compilers found:
  --fcompiler=compaqv  DIGITAL or Compaq Visual Fortran Compiler (6.6)
  --fcompiler=gnu95    GNU Fortran 95 compiler (4.4.0)
Compilers available for this platform, but not found:
  --fcompiler=absoft  Absoft Corp Fortran Compiler
  --fcompiler=g95     G95 Fortran Compiler
  --fcompiler=gnu     GNU Fortran 77 compiler
  --fcompiler=intelev Intel Visual Fortran Compiler for Itanium apps
  --fcompiler=intelv  Intel Visual Fortran Compiler for 32-bit apps
Compilers not available on this platform:
  --fcompiler=compaq  Compaq Fortran Compiler
  --fcompiler=hpux    HP Fortran 90 Compiler
  --fcompiler=ibm     IBM XL Fortran Compiler
  --fcompiler=intel   Intel Fortran Compiler for 32-bit apps
  --fcompiler=intele  Intel Fortran Compiler for Itanium apps
  --fcompiler=intelem Intel Fortran Compiler for EM64T-based apps
  --fcompiler=lahey   Lahey/Fujitsu Fortran 95 Compiler
  --fcompiler=mips    MIPSpro Fortran Compiler
  --fcompiler=nag     NAGWare Fortran 95 Compiler
  --fcompiler=none    Fake Fortran compiler
  --fcompiler=pg      Portland Group Fortran Compiler
  --fcompiler=sun     Sun or Forte Fortran 95 Compiler
  --fcompiler=vast    Pacific-Sierra Research Fortran 90 Compiler
For compiler details, run 'config_fc --verbose' setup command.
```

Part of the f2py process involves the automated writing and compilation of C wrapper code around the Fortran routines. The option `--compiler=mingw32` tells f2py to use the MinGW C compiler that comes with gfortran. This compiler is specific to the Windows system. On other systems, this option might be omitted to use the default C compiler, or another C compiler could be specified directly (e.g., `--compiler=gcc`).

Running f2py for our Lennard-Jones example looks something like the following:

```
c:\>f2py.py -c -m ljlib ljlib3.f90 --fcompiler=gnu95 --compiler=mingw32
Ignoring "Python was built with Visual Studio version 7.1, and extensions need to be built
with the same version of the compiler, but it isn't installed." (one should fix me in fco
mpiler/compaq.py)
running build
running config_cc
unifing config_cc, config, build_clib, build_ext, build commands --compiler options
running config_fc
unifing config_fc, config, build_clib, build_ext, build commands --fcompiler options
running build_src
building extension "ljlib" sources
f2py options: []
f2py:> c:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5\ljlibmodule.c
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5
Reading fortran codes...
  Reading file 'ljlib3.f90' (format:free)
Post-processing...
  Block: ljlib
                                Block: energyforces
                                Block: vvintegrate
```

```

Post-processing (stage 2)...
Building modules...
  Building module "ljlib"...
    Constructing wrapper function "energyforces"...
      penergy,forces = energyforces(pos,l,rc,forces,[dim,natom])
    Constructing wrapper function "vvintegrate"...
      pos,vel,accel,kenergy,penergy = vvintegrate(pos,vel,accel,l,cutsq,dt,[di
m,natom])
    Wrote C/API module "ljlib" to file "c:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win
32-2.5\ljlibmodule.c"
    adding 'c:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5\fortranobject.c' to sour
ces.
    adding 'c:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5' to include_dirs.
    copying C:\Python25\lib\site-packages\numpy\f2py\src\fortranobject.c -> c:\docume~1\shell\
locals~1\temp\tmpl4tj-f\src.win32-2.5
    copying C:\Python25\lib\site-packages\numpy\f2py\src\fortranobject.h -> c:\docume~1\shell\
locals~1\temp\tmpl4tj-f\src.win32-2.5
    running build_ext
    customize Mingw32CCompiler
    customize Mingw32CCompiler using build_ext
    customize Gnu95FCompiler
    Found executable C:\gfortran\bin\gfortran.exe
    Found executable C:\gfortran\bin\gfortran.exe
    customize Gnu95FCompiler using build_ext
    building 'ljlib' extension
    compiling C sources
    C compiler: gcc -mno-cygwin -O2 -Wall -Wstrict-prototypes

creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1\temp
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1\temp\tm
pl4tj-f
creating c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1\temp\tm
pl4tj-f\src.win32-2.5
compile options: '-Ic:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5 -IC:\Python25\
lib\site-packages\numpy\core\include -IC:\Python25\include -IC:\Python25\PC -c'
gcc -mno-cygwin -O2 -Wall -Wstrict-prototypes -Ic:\docume~1\shell\locals~1\temp\tmpl4tj-f\
src.win32-2.5 -IC:\Python25\lib\site-packages\numpy\core\include -IC:\Python25\include -IC
:\Python25\PC -c c:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5\fortranobject.c -
o c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1\temp\tmpl4tj-f
\src.win32-2.5\fortranobject.o
Found executable C:\gfortran\bin\gcc.exe
gcc -mno-cygwin -O2 -Wall -Wstrict-prototypes -Ic:\docume~1\shell\locals~1\temp\tmpl4tj-f\
src.win32-2.5 -IC:\Python25\lib\site-packages\numpy\core\include -IC:\Python25\include -IC
:\Python25\PC -c c:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5\ljlibmodule.c -o c:\
docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1\temp\tmpl4tj-f\src.
win32-2.5\ljlibmodule.o
compiling Fortran sources
Fortran f77 compiler: C:\gfortran\bin\gfortran.exe -Wall -ffixed-form -fno-second-undersco
re -mno-cygwin -O3 -funroll-loops -march=nocona -m386 -msse2 -fomit-frame-pointer -malign-
double
Fortran f90 compiler: C:\gfortran\bin\gfortran.exe -Wall -fno-second-underscore -mno-cygni
n -O3 -funroll-loops -march=nocona -m386 -msse2 -fomit-frame-pointer -malign-double
Fortran fix compiler: C:\gfortran\bin\gfortran.exe -Wall -ffixed-form -fno-second-undersco
re -mno-cygwin -Wall -fno-second-underscore -mno-cygwin -O3 -funroll-loops -march=nocona -
m386 -msse2 -fomit-frame-pointer -malign-double
compile options: '-Ic:\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5 -IC:\Python25\
lib\site-packages\numpy\core\include -IC:\Python25\include -IC:\Python25\PC -c'
gfortran.exe:f90: ljlib3.f90
C:\gfortran\bin\gfortran.exe -Wall -mno-cygwin -Wall -mno-cygwin -shared c:\docume~1\shell
\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1\temp\tmpl4tj-f\src.win32-2.5\ljlibmo
dule.o c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\docume~1\shell\locals~1\temp\tmpl
4tj-f\src.win32-2.5\fortranobject.o c:\docume~1\shell\locals~1\temp\tmpl4tj-f\Release\mdli
b.o -Lc:\gfortran\lib\gcc\i586-pc-mingw32\4.4.0 -LC:\Python25\libs -LC:\Python25\PCbuild -
lpython25 -lgfortran -o .\ljlib.pyd
running scones
Removing build directory c:\docume~1\shell\locals~1\temp\tmpl4tj-f

```

A fair amount of text is outputted when running f2py. You will know that your code has compiled successfully when (1) the final lines of the f2py output contain “Removing build directory...” and there are no signs of errors, and (2) a compiled module file now exists. On Windows, your module file will end in .pyd, while on Linux it will typically end in .so. The name of your file is that which you specified in the *MODULENAME* option.

The f2py utility will generate automatically all of the code necessary to pass NumPy arrays in between Python and your compiled Fortran routines. In particular, it makes sure that function arguments obey the right types and dimensioning. As a part of this effort to make sure Python arrays are Fortran-friendly, NumPy can sometimes make a copy of an input array to send to the compiled function.

Sometimes it is convenient to know when copies are made of arrays sent to Fortran routines, rather than the original Python arrays themselves, since such copying can create a performance hit. One can compile f2py with the additional option `-DF2PY_REPORT_ON_ARRAY_COPY=1` to have Fortran-compiled routines print out messages in real-time each time such a copying event occurs. This is useful for debugging / optimizing code, but final production code should not use this option.

Help with f2py

There are a number of online resources for reading about additional options with and for troubleshooting the f2py utility. The main website can be found at the SciPy development page:

<http://www.scipy.org/F2py>

More extensive documentation can be found at links therein, and at the following:

<http://cens.ioc.ee/projects/f2py2e/>

For those who are using f2py on Windows,

http://www.scipy.org/F2PY_Windows

Importing and using f2py-compiled modules in Python

Once we have compiled our Fortran source code into a module using f2py, it is as easy to import as any other module:

```
>>> import ljl
```

f2py embeds information about the functions it compiles into docstrings. To see these docstrings, use the `print` statement with the `__doc__` special property:

```

>>> print ljlib.__doc__
This module 'ljlib' is auto-generated with f2py (version:2_5972).
Functions:
  penergy, forces = energyforces(pos, l, rc, forces, dim=shape(pos, 1), natom=
shape(pos, 0))
  pos, vel, accel, kenergy, penergy = vvintegrate(pos, vel, accel, l, cutsq, dt, dim=
shape(pos, 1), natom=shape(pos, 0))

```

Here, the docstring tells us that the module contains two functions, `energyforces` and `vvintegrate`. Notice that `f2py` converts all Fortran variable and function names to lowercase format by default.

In addition to their names, the module docstring tells us the format of a call to each of the functions. We can get more detailed information by examining the docstrings of the individual functions:

```

>>> print ljlib.energyforces.__doc__
energyforces - Function signature:
  penergy, forces = energyforces(pos, l, rc, forces, [dim, natom])
Required arguments:
  pos : input rank-2 array('d') with bounds (natom, dim)
  l : input float
  rc : input float
  forces : rank-2 array('d') with bounds (natom, dim)
Optional arguments:
  dim := shape(pos, 1) input int
  natom := shape(pos, 0) input int
Return objects:
  penergy : float
  forces : rank-2 array('d') with bounds (natom, dim)

```

Here, we are told that there are four arguments we must provide: `pos`, `l`, `rc`, and `forces`. These arguments correspond to any for which we specified the `intent(in)` or `intent(inout)` attributes. However, we do not need to specify the dimension variables `dim` and `natom`, as these will be taken automatically from the shape of the argument `pos`.

The docstring also tells us that the function will return two arguments, `penergy` and `forces`. These correspond to any Fortran arguments for which we specified `intent(out)` or `intent(inout)`. Thus a call from Python to the `energyforces` routine would look like:

```

>>> penergy, forces = ljlib.energyforces(pos, l, rc, forces)

```

where we would have needed to supply the vector of positions, box length, cutoff, and force array. If we had specified `intent(out)` for `forces`, it would not have appeared as an argument and Python instead would have created a new force array with each function call.

Similarly, we can examine the docstring of the `vvintegrate` function:

```

>>> print ljlib.vvintegrate.__doc__
vvintegrate - Function signature:
  pos,vel,accel,kenergy,penergy = vvintegrate(pos,vel,accel,l,cutsq,dt,
[dim,natom])
Required arguments:
  pos : rank-2 array('d') with bounds (natom,dim)
  vel : rank-2 array('d') with bounds (natom,dim)
  accel : rank-2 array('d') with bounds (natom,dim)
  l : input float
  cutsq : input float
  dt : input float
Optional arguments:
  dim := shape(pos,1) input int
  natom := shape(pos,0) input int
Return objects:
  pos : rank-2 array('d') with bounds (natom,dim)
  vel : rank-2 array('d') with bounds (natom,dim)
  accel : rank-2 array('d') with bounds (natom,dim)
  kenergy : float
  penergy : float

```

A call to `vvintegrate` would therefore look like:

```

>>> pos, vel, accel, kenergy, penergy = ljlib.vvintegrate(pos, vel, accel,
...                                                    l, cutsq, dt)

```

Note that `f2py` automatically makes the conversions / equivalencies of Fortran `real(8)` and Python `float` types.

And that's it! You are now ready to use your Fortran routines with Python.

Tutorials and references for Fortran

It is beyond the scope of this document to cover the entire Fortran language. However, a number of excellent tutorials for Fortran programming are available online. Keep in mind that many of these discuss broader programmatic issues, like file input/output and modules, that are irrelevant for the much simpler task of compiling numerical functions for Python.

<http://www.dur.ac.uk/resources/its/info/guides/138fortran90.pdf>

<http://www.pcc.qub.ac.uk/tec/courses/f90/ohp/f90-ohp.html>

<http://www.cisl.ucar.edu/tcg/consweb/Fortran90/F90Tutorial/tutorial.html>

<http://www.cs.mtu.edu/~shene/COURSES/cs201/NOTES/fortran.html>

<http://wwwasdoc.web.cern.ch/wwwasdoc/f90.html>

<http://www.liv.ac.uk/HPC/HTMLF90Course/HTMLF90CourseSlides.html>

A large reference for language constructs and available functions can be found at:

<http://docs.hp.com/en/B3908-90002/>

A convenient “cheat sheet” can also be found at:

http://www.pa.msu.edu/~duxbury/courses/phy480/fortran90_refcard.pdf