# 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.

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 actually a bit faster and simpler than C and other 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 Python(x,y) on a Windows machine
with NumPy, SciPy, and the Mingw compilers, then you should be ready to go. If you have NOT installed Python(x,y), the following is a brief outline of the steps that you should follow.

**Step 1.** Install Python, NumPy, and SciPy. You probably have already done this, as we discussed in an earlier tutorial.

**Step 2.** Install a Fortran compiler. A reasonable open-source option is GNU Fortran, or gfortran. This compiler will be used by f2py to generate compiled Fortran modules. Installation binaries and source files can be found here:

http://gcc.gnu.org/fortran

**Step 3.** Configure environment variables. The compilation steps depend on the presence of *environment variables*, which are operating system variables that, among other things, typically give the path locations of needed files for compilation.

In a Windows system, you can access environment variables by right-clicking on My Computer > Properties > Advanced > Environment Variables. When the “Environment Variables” window comes up, you will need to edit two variables under the “System Variables” section.
First, click on the variable Path and hit Edit. Then you want to add two items to the end of the list in “variable value”. Add the text “;c:\python27;c:\python27\scripts”. Make sure there is a semicolon but no spaces in between this text and whatever preceded it. (Note: whatever currently exists in “Path” for your machine may differ from the image below. Be sure to keep the existing text.)

![Edit System Variable](image)

Click ok and then go back to the “Environment Variables” window. Click on New in the “System Variables” section. You will add a new variable “C\_INCLUDE\_PATH” with value “c:\gfortran\include”:

![Edit System Variable](image)

**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 explanation 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:

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

An equivalent Fortran subroutine would look the following:

```fortran
subroutine CenterPos(Pos, Dim, NAtom)
    implicit none
    integer, intent(in) :: Dim, NAtom
```

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(INENT) :: NAME
```

For array arguments, we use:

```
type TYPE, intent(INENT), 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:

<table>
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<th>Python / NumPy</th>
<th>Fortran</th>
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<td>float</td>
<td>real(8) (also called double)</td>
</tr>
<tr>
<td>int</td>
<td>integer</td>
</tr>
<tr>
<td>bool</td>
<td>logical</td>
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For arguments, we use the *INTENT* option to tell Python what we are going to do with a variable. There are three such options,

<table>
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<th>intent</th>
<th>meaning</th>
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<tr>
<td>in</td>
<td>The variable is an input to the subroutine only. Its value must not be changed during the course of the subroutine.</td>
</tr>
<tr>
<td>out</td>
<td>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.</td>
</tr>
<tr>
<td>inout</td>
<td>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.</td>
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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

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

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

```fortran
real(8), intent(inout), dimension(NAAtom, 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:

```fortran
subroutine CenterPos(Pos, Dim, NAAtom)
```

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:

```fortran
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:

\[
\text{PosAvg} = \frac{\text{sum}(\text{Pos}, 1)}{\text{dble}(\text{NAtom})}
\]

The Fortran function \texttt{sum} takes an array argument and sums it, optionally over a specified dimension. Here, we indicate a summation over the \textit{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 \texttt{dble} function above takes the integer \texttt{NAtom} and converts it to a double-precision number, e.g., of type \texttt{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 \texttt{dble}, \texttt{int(X)} will convert any argument \texttt{X} to an integer type.

The lines that follow modify the \texttt{Pos} array to subtract the centroid positions from it:

\[
\text{do } i = 0, \text{NAtom} - 1 \\
\quad \text{do } j = 0, \text{Dim} - 1 \\
\quad\quad \text{Pos}(i,j) = \text{Pos}(i,j) - \text{PosAvg}(j) \\
\quad \text{end do} \\
\text{end do}
\]

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

\[
\text{do } \text{VAR} = \text{START}, \text{STOP} \\
\quad \text{COMMANDS} \\
\text{end do}
\]

In Fortran, such \texttt{do} loops involve integers and are inclusive of both the starting and stopping values. Indentation here is optional and just for ease of reading, as it is the \texttt{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 \textit{implied} \texttt{do} loop over array elements if we perform array calculations. We could therefore simplify the above code by removing the inner loop:
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:

\[
F_{i,x} = -\frac{\partial U}{\partial x_i} = -\frac{\partial}{\partial x_i} \sum_{j \neq i} u(r_{ij})
\]
But since $r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2$, 

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

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

$$\mathbf{F}_i = \sum_{j \neq i} \left( \frac{\mathbf{r}_{ij}}{r_{ij}} \right) \frac{\partial}{\partial r_{ij}} u(r_{ij})$$

$$= \sum_{j \neq i} \left( \frac{\mathbf{r}_{ij}}{r_{ij}} \right) \left[ 4\varepsilon \left( \frac{r_{ij}}{\sigma} \right)^{-13} - 12 \left( \frac{r_{ij}}{\sigma} \right)^{-14} + 6 \left( \frac{r_{ij}}{\sigma} \right)^{-7} \right]$$

$$= \sum_{j \neq i} \mathbf{r}_{ij} \left( \frac{\varepsilon}{\sigma} \right) \left[ -48 \left( \frac{r_{ij}}{\sigma} \right)^{-14} + 24 \left( \frac{r_{ij}}{\sigma} \right)^{-8} \right]$$

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:

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

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

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

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

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

```fortran
 subroutine EnergyForces(Pos, L, rc, PEnergy, Forces, Dim, NAAtom)
   implicit none
   integer, intent(in) :: Dim, NAAtom
   real(8), intent(in), dimension(0:NAAtom-1, 0:Dim-1) :: Pos
   real(8), intent(in) :: L, rc
   real(8), intent(out) :: PEnergy
   real(8), intent(inout), dimension(0:NAAtom-1, 0:Dim-1) :: Forces
   real(8) :: d, Shift
   integer :: i, j
   PEnergy = 0.
   Forces = 0.
   Shift = -4. * (rc**(-12) - rc**(-6))
   do i = 0, NAAtom - 1
     do j = i + 1, NAAtom - 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 \( \text{Pos}, \text{L}, \text{and} \text{rc} \) are all sent to the function using the \texttt{intent(in)} attribute and are not modified. The float \( \text{PEnergy} \) is \texttt{intent(out)}, meaning that it will be returned from our function. The array \( \text{Forces} \) is \texttt{intent(inout)}. The reason that we did not use \texttt{intent(out)} for \( \text{Forces} \) 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

```fortran
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:

```fortran
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:

```fortran
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
Forces(j,:) = Forces(j,:) – Fij

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

In addition to the \texttt{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:

\begin{itemize}
  \item mod, \sin, \cos, \tan, \cotan, \asin, \acos, \atan, \sinh,
  \item \cosh, \tanh, \asinh, \acosh, \atanh, \exp, \log, \log10,
  \item \sqrt, \text{ceiling}, \text{floor}, \text{nint}, \text{erf}, \text{erfc}, \text{huge}, \text{tiny},
  \item \text{epsilon}
\end{itemize}

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 \texttt{dnint} from \texttt{nint}.

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

\begin{itemize}
  \item \text{count}, \text{sum}, \text{product}, \text{minval}, \text{maxval}, \text{minloc}, \text{maxloc},
  \item \text{matmul}, \text{transpose}
\end{itemize}

Many of these functions accept an optional argument \texttt{axis} 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 \texttt{axis=1}, as opposed to Python's \texttt{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:

```fortran
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) :: 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 * dmin(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
        end do
    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 \( \text{id6} \).

• 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, \( x\times(x\times(x+1)+1)+1 \) 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 \( \sqrt{\cdot} \) 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 \( \text{Pos}(i,j) \) is the fastest if \( i \) is the inner loop and \( j \) the outer. Similarly, expressions like \( \text{Pos}(::,j) \) are faster than \( \text{Pos}(j,:) \). 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 \( \text{Pos} \) 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:
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) :: rc2, Shift
    integer :: i, j
    PEnergy = 0.
    Forces = 0.
    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(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, KEnergy, PEnergy, Dim, NAtom)
    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. Professional commercial packages (e.g., not free) include the Intel Visual Fortran programming suite:
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(inout) :: 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. Running f2py without any arguments prints out a long help file:
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 -c <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 `--fcompiler=gnu95` and `--compiler=mingw32` 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:

```
f2py -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 Fortran Compiler
--fcompiler=g95 G95 Fortran Compiler
--fcompiler=gnu GNU Fortran 77 compiler
--fcompiler=intele 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=hpx 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
```
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 --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 fcompiler/compaq.py)

running build

running config_cc

unifying config_cc, config, build_clib, build_ext, build commands --compiler options

running config_f90

unifying config_f90, 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\tmp14tj-f\src.win32-2.5\ljlibmodule.c

creating c:\docume-1\shell\locals-1\temp\tmp14tj-f

creating c:\docume-1\shell\locals-1\temp\tmp14tj-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"...

energyforces = energyforces(pos,1,rc,forces,[dim,natom])

Constructing wrapper function "vvintegrate"...

vvintegrate(pos,vel,accel,kinenergy,penergy = vvintegrate(pos,vel,accel,1,cutsq,dt,[dim,natom])

Wrote C/API module "ljlib" to file "c:\docume-1\shell\locals-1\temp\tmp14tj-f\src.win32-2.5\ljlibmodule.c"

adding 'c:\docume-1\shell\locals-1\temp\tmp14tj-f\src.win32-2.5\fortranobject.c' to sources.

adding 'c:\docume-1\shell\locals-1\temp\tmp14tj-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\tmp14tj-f\src.win32-2.5

copying C:\Python25\lib\site-packages\numpy\f2py\src\fortranobject.h -> c:\docume-1\shell\locals-1\temp\tmp14tj-f\src.win32-2.5

running build_ext

customize Mingw32CCompiler

customize Mingw32CCompiler using build_ext

customize Gnu95FCCompiler

Found executable C:\gfortran\bin\gfortran.exe

Building 'ljlib' extension

compiling C sources
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 \textit{MODULENAME} option.

The \texttt{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 ljlib
```

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:

```python
>>> 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: \( \text{pos}, \text{l}, \text{rc}, \text{and forces} \). 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 \( \text{dim} \) and \( \text{natom} \), as these will be taken automatically from the shape of the argument \( \text{pos} \).

The docstring also tells us that the function will return two arguments, \( \text{penergy} \) and \( \text{forces} \). 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:

```python
>>> 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:

```python
>>> print ljlib.vvintegrate.__doc__
vintegrate - Function signature:
    penergy, forces = vintegrate(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
```

© 2012 M. Scott Shell
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:

```python
>>> 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://wwwwasdoc.web.cern.ch/wwwwasdoc/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