Fortran implementation of grey atmosphere

August 30, 2017

```
In [1]: cd fortran-src/

/Users/will/Dropbox/Teaching/Estelar/Tarea-03-GreyAtmos/fortran-src


In [2]: from fg4py import fm_p, fm_planck, fm_e2, fm_flux

In [3]: print(fm_planck.__doc__)

rslt = fm_planck(alpha,tau)

Wrapper for ``fm_planck``.

Parameters
----------
alpha : input rank-1 array('f') with bounds (f2py_alpha_d0)
tau : input rank-1 array('f') with bounds (f2py_tau_d0)

Returns
-------
rslt : rank-2 array('f') with bounds (size(alpha),size(tau))
```

Check that the $p(\tau)$ function works

```
In [4]: fm_p([0, 1, 2, 4])

Out[4]: array([ 1.18920708,  0.94574159,  0.84089643,  0.73111045], dtype=float32)
```

Check that $B_\alpha(\tau)$ works for vector of α and a single τ:

```
In [5]: fm_planck([0.001, 1, 3, 9], 1)

Out[5]: array([[  1.62751633e-07],
               [  9.77885053e-02],
               [  2.58752614e-01],
               [  2.25805026e-02]], dtype=float32)
```

Check that $B_\alpha(\tau)$ works for a vector of τ and a single α:

```
In [6]: fm_planck(9.0, [0, 1, 2, 4, 8])
```

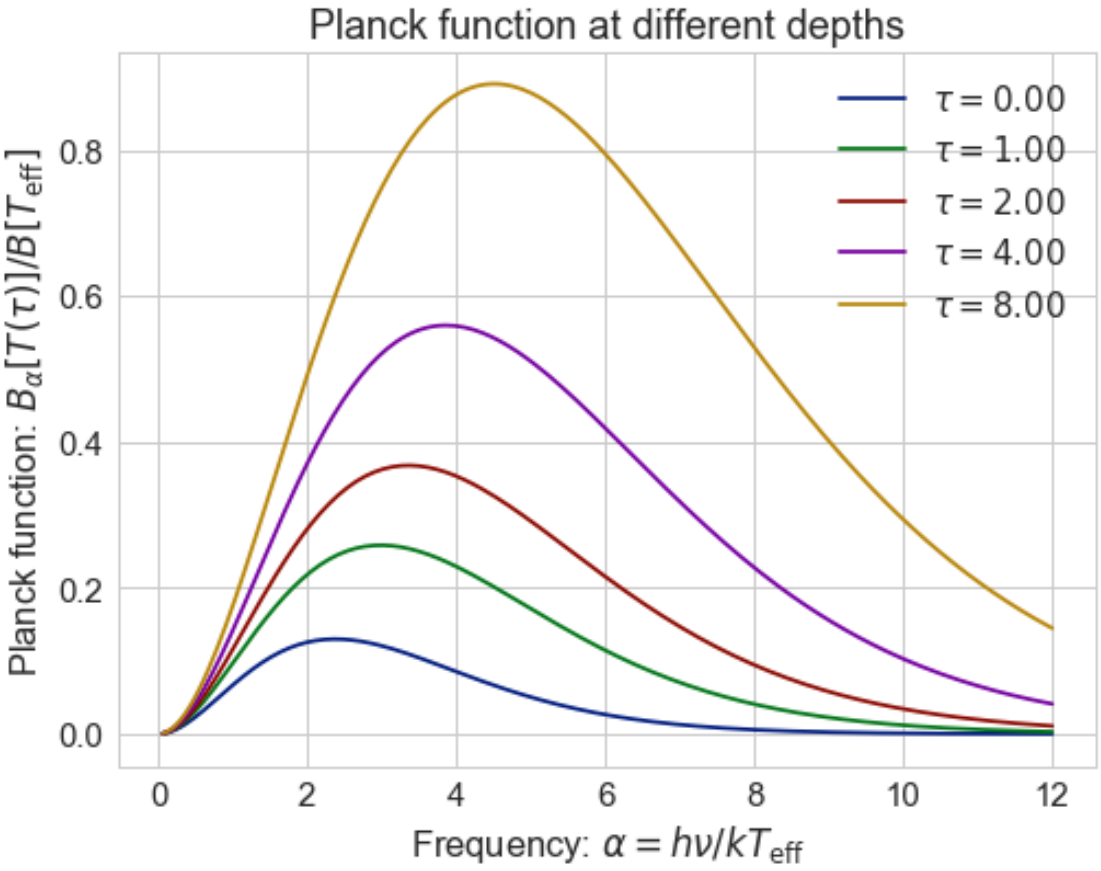
```
Out[6]: array([[ 0.00252368,  0.0225805 ,  0.0580328 ,  0.15601532,  0.40164581]], dtype=float3
```

Set up python for plotting the results:

```
In [7]: import numpy as np
        import matplotlib.pyplot as plt
        import seaborn as sns
        %matplotlib inline
        sns.set(context='notebook',
                style='whitegrid',
                palette='dark',
                font_scale=1.5,
                color_codes=True,
                rc={'figure.figsize': (8,6)},
               )
```

```
In [8]: alpha_pts = np.linspace(0.0, 12.0, 200)
        taus = [0.0, 1.0, 2.0, 4.0, 8.0]
        alphas = [1.0, 3.0, 9.0]
        tau_pts = np.linspace(0.0, 20.0, 200)
        tau_label = r'Optical depth: $\tau$'
        alpha_label = r'Frequency: $\alpha = h \nu / k T_\mathrm{eff}$'
        planck_label = r'Planck function: $B_\alpha[T(\tau)] / B[T_\mathrm{eff}]$'
```

```
In [9]: fig, ax = plt.subplots(1, 1)
        for tau in taus:
            B = fm_planck(alpha_pts, tau)
            ax.plot(alpha_pts, B, label=r'$\tau = {:.2f}$'.format(tau))
        ax.legend()
        ax.set_xlabel(alpha_label)
        ax.set_ylabel(planck_label)
        ax.set_title('Planck function at different depths')
        None
```



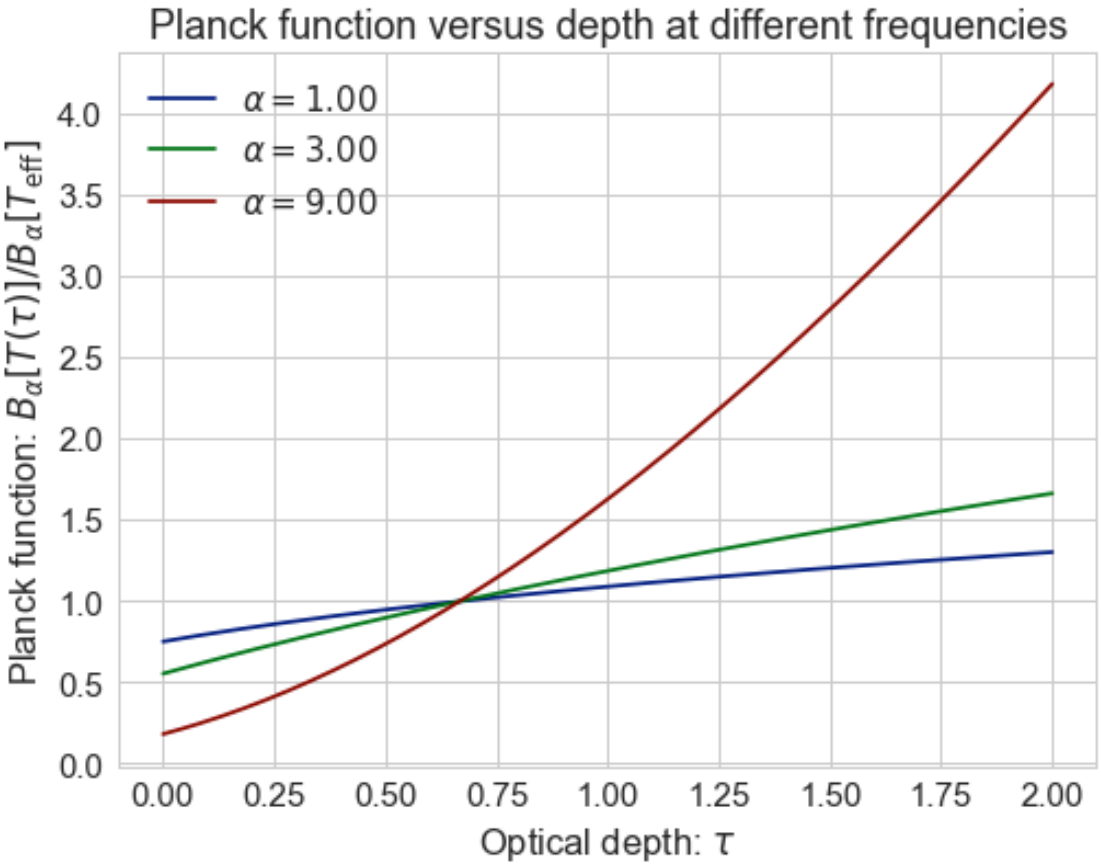
Note that `fm_planck` always returns a rank-2 array, so it doesn't behave quite like the numpy implementation.

```
In [10]: fm_planck(3.0, 0.5)
```

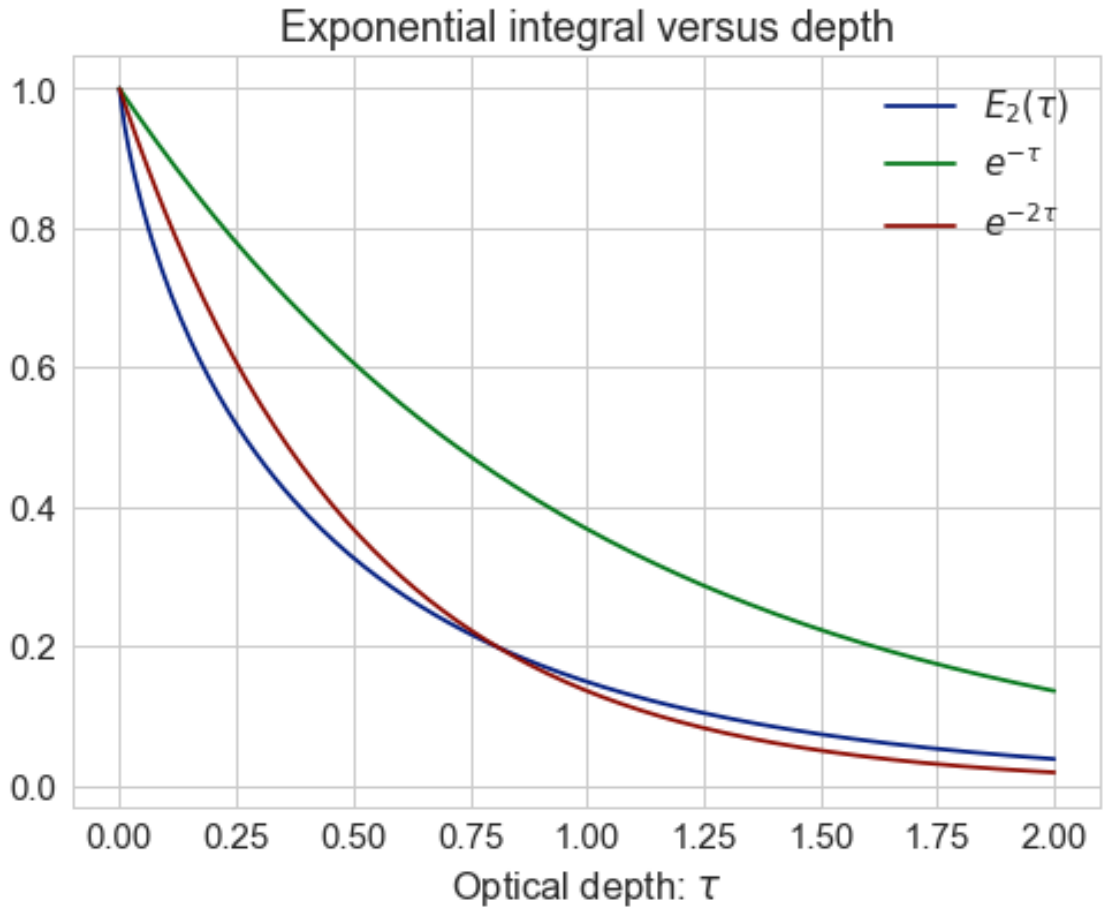
```
Out[10]: array([[ 0.19576064]], dtype=float32)
```

This means that we have to use the transpose when we plot against τ

```
In [11]: fig, ax = plt.subplots(1, 1)
         for alpha in alphas:
             B = fm_planck(alpha, tau_pts/10)/fm_planck(alpha, 2./3.)
             ax.plot(tau_pts/10, B.T, label=r'$\alpha = {:.2f}$'.format(alpha))
         ax.legend(loc='upper left')
         ax.set_xlabel(tau_label)
         ax.set_ylabel(planck_label.replace('B[', r'B_\alpha['))
         ax.set_title('Planck function versus depth at different frequencies')
         None
```



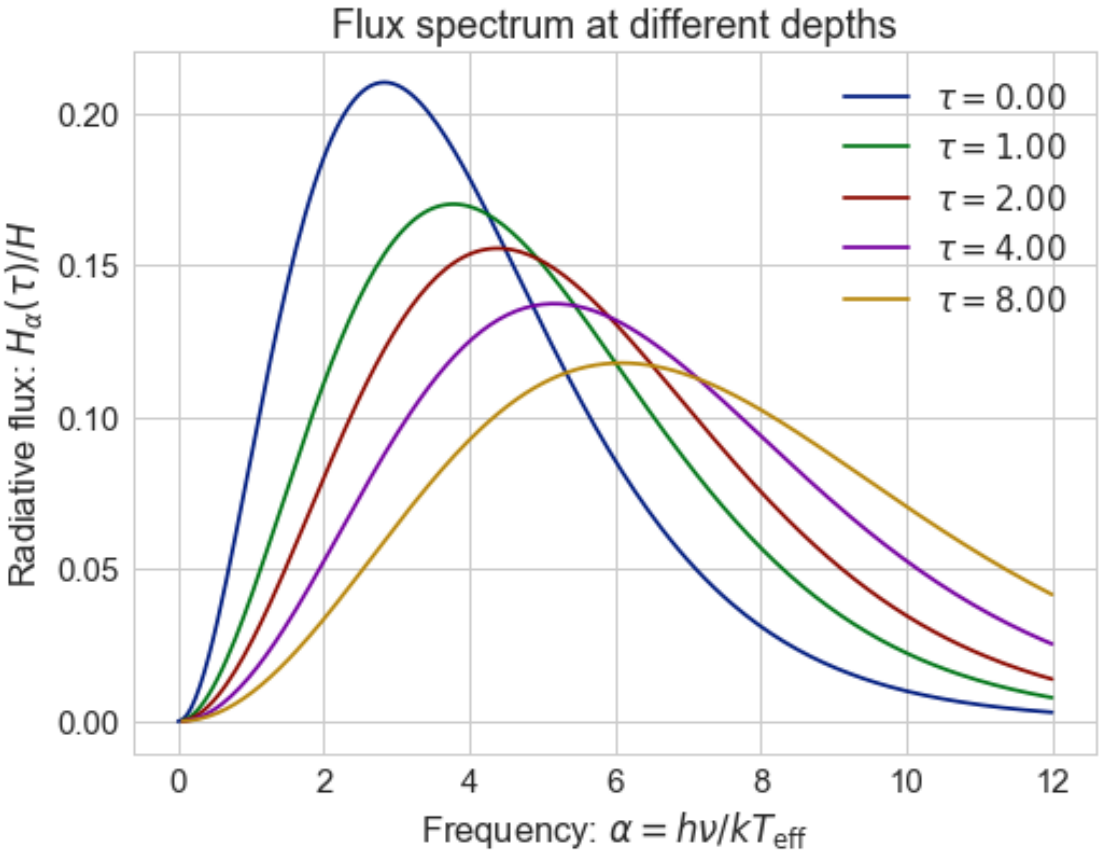
In [12]:
```
fig, ax = plt.subplots(1, 1)
t = 0.00001 + tau_pts/10
e = fm_e2(t)
ax.plot(t, e, label=r'$E_2(\tau)$')
ax.plot(t, np.exp(-t), label=r'$e^{-\tau}$')
ax.plot(t, np.exp(-t/0.5), label=r'$e^{-2\tau}$')
ax.legend(loc='upper right')
ax.set_xlabel(tau_label)
ax.set_ylabel('')
ax.set_title('Exponential integral versus depth')
None
```



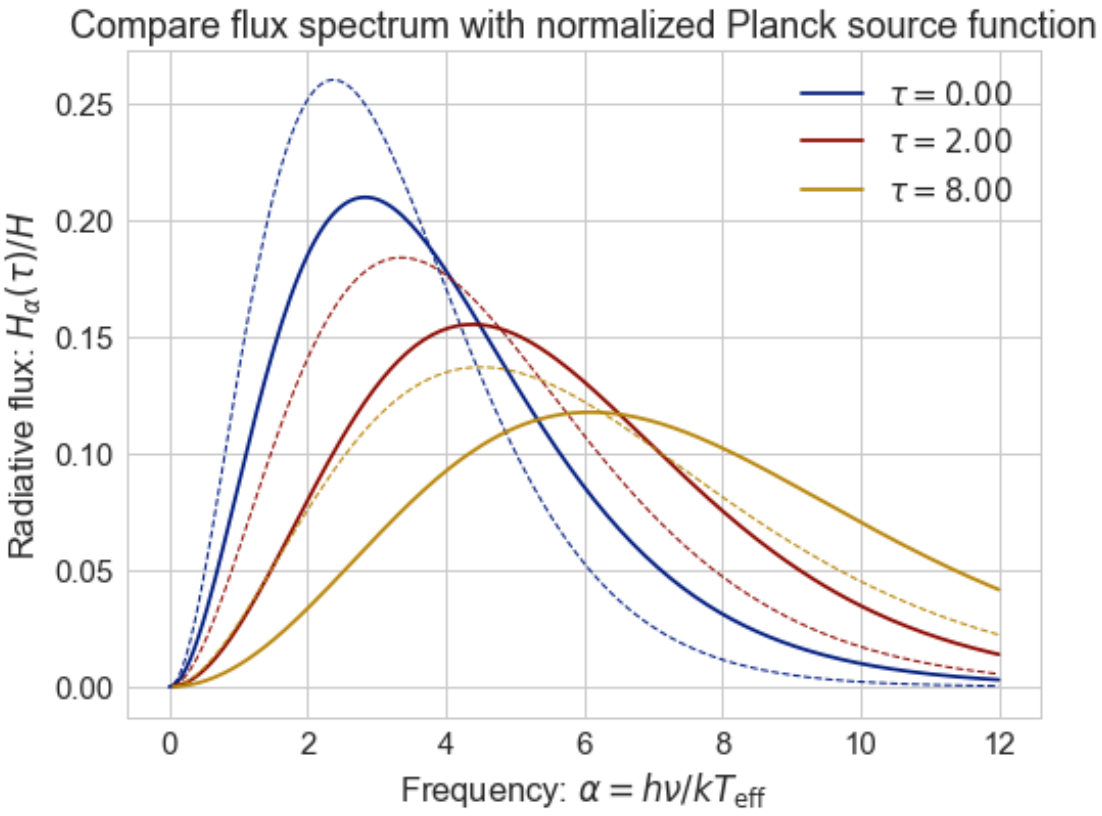
Now, try out the flux integral. This is just repeating all the plots in the python version, but with the `fm_*` fortran routines, instead of the python ones.

```
In [13]: flux_label = r'Radiative flux: $H_\alpha(\tau) / H$'
```

```
In [14]: fig, ax = plt.subplots(1, 1)
         Hlist = []
         for tau in taus:
             H = fm_flux(alpha_pts, tau)
             ax.plot(alpha_pts, H, label=r'$\tau = {:.2f}$'.format(tau))
             Hlist.append(H)
         ax.legend()
         ax.set_xlabel(alpha_label)
         ax.set_ylabel(flux_label)
         ax.set_title('Flux spectrum at different depths')
         None
```




```
In [16]: fig, ax = plt.subplots(1, 1)
         colors = 'bry'
         for tau, H, color in zip(taus[::2], Hlist[::2], colors):
             ax.plot(alpha_pts, H, c=color,
                     label=r'$\tau = {:.2f}$'.format(tau))
             B = fm_p(tau)**4 * fm_planck(alpha_pts, tau)
             ax.plot(alpha_pts, B, lw=1, ls='--', c=color, label=None)
         ax.legend()
         ax.set_xlabel(alpha_label)
         ax.set_ylabel(flux_label)
         ax.set_title('Compare flux spectrum with normalized Planck source function')
         None
```



As far as I can see, these curves are identical to the pure-python ones. The only thing remaining to do is the schwarschild integral for the mean intensity.

In [ ]:

0.0.1 How to use fortran cells in a jupyter notebook

Test of fortran-magic, see this blog post

```
In [18]: %load_ext fortranmagic
```

```
The fortranmagic extension is already loaded. To reload it, use:
  %reload_ext fortranmagic
```

We test with a simple function, implemented as a subroutine with an `intent(out)` argument. We also use a module for furher communication with the function.

```
In [2]: %%fortran --opt='-O3'
        module myparams
            real :: constant = 1.0
        end module
```

```
        subroutine add_constant(x, rslt)
            use myparams
            real, intent(in) :: x(:)
            real, intent(out) :: rslt(size(x))
            rslt = x + constant
        end subroutine
```

When we evaluate the above cell, it compiles the fortran and exports `add_constant` as a function that can be called from python.

```
In [5]: import numpy as np

In [6]: add_constant([1.0, 2.0, 3.0])

Out[6]: array([ 2.,  3.,  4.], dtype=float32)
```

We can also access the variables in the `myparams` module.

```
In [7]: myparams.constant = -2.0
        add_constant([1.0, 2.0, 3.0])

Out[7]: array([ 2.,  3.,  4.], dtype=float32)
```

Unfortunately, there does not seem to be an easy way, within a `%%fortran` cell, to `use` a module that was defined in another cell. So we need to put everything inside one cell. (We can access the modules within python cells however).

```
In [ ]: %%fortran --opt='-O3'
        module myparams
            real :: constant = 1.0
        end module

        subroutine raise_to_power(x, rslt)
            use myparams
            real, intent(in) :: x(:)
            real, intent(out) :: rslt(size(x))
            rslt = x**constant
        end subroutine

In [8]: myparams.constant = -1.0
        raise_to_power([1.0, 2.0, 3.0])

Out[8]: array([ 1.        ,  0.5       ,  0.33333334], dtype=float32)
```

Trying out `elemental` functions, which can simplify the whole-array operations on the fortran side, since you just write one function of scalar arguments, which can then be applied to arrays of any shape. But with the proviso that all the arguments *plus* the result must all be the same shape.

```
In [42]: %%fortran --opt='-O3' -v
         module myparams
           real :: constant = 1.0
         contains
           elemental function raise_product_to_power(x, y) result(rslt)
             real, intent(in) :: x, y
             real :: rslt
             rslt = (x*y)**constant
           end function
         end module myparams

         subroutine fm_raise(x, y, rslt)
           use myparams, only: raise_product_to_power
           real, intent(in) :: x(:), y(:)
           real, intent(out) :: rslt(size(x), size(y))
           real :: xx(size(x), size(y)), yy(size(x), size(y))
           xx = spread(x, dim=2, ncopies=size(y))
           yy = spread(y, dim=1, ncopies=size(x))
           rslt = raise_product_to_power(xx, yy)
         end subroutine fm_raise


Ok. The following fortran objects are ready to use: fm_raise, myparams
```

We want to apply this to a function of two vector arguments, where the vectors are over incommensurate dimensions (e.g., frequency and depth), so it is a kind of outer product: like $x \times y^{\mathrm{T}}$. Fortran doesn't do any sort of broadcasting of degenerate array dimensions, so we do this explicitly with the fortran intrinsic `spread` function.

```
In [54]: fm_raise([1, 2, 3], [10, 100])

Out[54]: array([[  10.,  100.],
                [  20.,  200.],
                [  30.,  300.]], dtype=float32)
```

So, if we send in two vectors, we get out a 2d array.

```
In [55]: fm_raise([1, 2, 3], 99)

Out[55]: array([[  99.],
                [ 198.],
                [ 297.]], dtype=float32)
```

And we can also make the second argument a scalar, in which case we get a column vector result.

```
In [56]: fm_raise(2, [10, 100])

Out[56]: array([[  20.,  200.]], dtype=float32)
```

Or make the first argument a scalar, to give a row vector result. But in both cases, they are really still 2D results, but with one dim of size 1.

```
In [53]: np.array([[1, 2]]) * np.array([[2, 3, 4]]).T
```

```
Out[53]: array([[2, 4],
                [3, 6],
                [4, 8]])
```

0.0.2 Earlier version of grey atmosphere routines using fortan magic

I had a *lot* of trouble with paths to shared libraries (they were found at compile time, but then couldn't be found at run time). So, I eventually decided to just use the normal f2py machinery instead. But I leave this here for historical reference.

```
In [1]: %load_ext fortranmagic
```

```
/Users/will/anaconda/lib/python3.6/site-packages/fortranmagic.py:147: UserWarning: get_ipython_
  self._lib_dir = os.path.join(get_ipython_cache_dir(), 'fortran')
```

First, we do a direct translation of some functions from the python version.
General strategy:

1. Define wrapper functions `fm_*` (where fm stands for fortran magic) that conform to the odd way that f2py likes to have things defined. That is, subroutines with `intent(out)` argument for the return value, instead of a function.
2. These subroutines include the module `fgrey`, in which we are free to write more idiomatic fortran (although when I tried to use `public` and `private` it didn't work - not sure why).

```
In [10]: %fortran_config --defaults
```

```
Deleted custom config. Back to default arguments for %%fortran
```

```
In [74]: %%fortran -vvv --opt='-O3' --extra './libfgrey.so'  --f90flags='-Wl,-rpath,.' --f77fla
```

```
          subroutine fm_e2(t, rslt)
            use fspecial, only: e2
            real, intent(in) :: t(:)
            real, intent(out) :: rslt(size(t))
            integer :: i
            rslt = (/(e2(t(i)), i = 1, size(t))/)
          end subroutine

          subroutine fm_p(tau, rslt)
              use planck_grey, only: p
              real, intent(in) :: tau(:)
              real, intent(out) :: rslt(size(tau))
```

```
            rslt = p(tau)
        end subroutine

        subroutine fm_planck(alpha, tau, rslt)
            use planck_grey, only: planck
            real, intent(in) :: alpha(:), tau(:)
            real, intent(out) :: rslt(size(alpha), size(tau))
            real :: aalpha(size(alpha), size(tau)), ttau(size(alpha), size(tau))
            aalpha = spread(alpha, dim=2, ncopies=size(tau))
            ttau = spread(tau, dim=1, ncopies=size(alpha))
            rslt = planck(aalpha, ttau)
        end subroutine

Running...
   /Users/will/anaconda/bin/python -m numpy.f2py --fcompiler=gnu95 --f90flags='-Wl,-rpath,.' --
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
build_src
building extension "_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87" sources
f2py options: []
f2py:> /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3.6/
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3
Reading fortran codes...
        Reading file '/Users/will/.ipython/fortran/_fortran_magic_de8a64c7025eb58b0899ce8f4f1ee
Post-processing...
        Block: _fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87
                        Block: fm_e2
In: :_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87:/Users/will/.ipython/fortran/_fortran_magi
get_useparameters: no module fspecial info used by fm_e2
                        Block: fm_p
In: :_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87:/Users/will/.ipython/fortran/_fortran_magi
get_useparameters: no module planck_grey info used by fm_p
                        Block: fm_planck
In: :_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87:/Users/will/.ipython/fortran/_fortran_magi
get_useparameters: no module planck_grey info used by fm_planck
Post-processing (stage 2)...
Building modules...
        Building module "_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87"...
                Creating wrapper for Fortran subroutine "fm_e2"("fm_e2")...
                Constructing wrapper function "fm_e2"...
                  rslt = fm_e2(t)
                Creating wrapper for Fortran subroutine "fm_p"("fm_p")...
                Constructing wrapper function "fm_p"...
                  rslt = fm_p(tau)
```

```
                Creating wrapper for Fortran subroutine "fm_planck"("fm_planck")...
                Constructing wrapper function "fm_planck"...
                  rslt = fm_planck(alpha,tau)
        Wrote C/API module "_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87" to file "/var/fold
        Fortran 77 wrappers are saved to "/var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpn
  adding '/var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3
  adding '/var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3
copying /Users/will/anaconda/lib/python3.6/site-packages/numpy/f2py/src/fortranobject.c -> /var
copying /Users/will/anaconda/lib/python3.6/site-packages/numpy/f2py/src/fortranobject.h -> /var
  adding '/var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3
build_src: building npy-pkg config files
running build_ext
customize UnixCCompiler
customize UnixCCompiler using build_ext
customize Gnu95FCompiler
Found executable /usr/local/bin/gfortran
customize Gnu95FCompiler using build_ext
building '_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87' extension
compiling C sources
C compiler: gcc -Wno-unused-result -Wsign-compare -Wunreachable-code -DNDEBUG -g -fwrapv -O3 -W

creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/var
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/var/folders
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/var/folders/rm
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/var/folders/rm/hnrktx9s22
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/var/folders/rm/hnrktx9s22
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/var/folders/rm/hnrktx9s22
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/var/folders/rm/hnrktx9s22
compile options: '-I/var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10
gcc: /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3.6/_
In file included from /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-1
In file included from /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-1
In file included from /Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy
In file included from /Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy
In file included from /Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy
/Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy/npy_1_7_deprecated_ap
#warning "Using deprecated NumPy API, disable it by " \
 ^
1 warning generated.
gcc: /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3.6/fo
In file included from /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-1
In file included from /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-1
In file included from /Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy
In file included from /Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy
In file included from /Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy
/Users/will/anaconda/lib/python3.6/site-packages/numpy/core/include/numpy/npy_1_7_deprecated_ap
#warning "Using deprecated NumPy API, disable it by " \
 ^
```

```
/var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_64-3.6/fortra
        if (size < sizeof(notalloc)) {
            ~~~~ ^ ~~~~~~~~~~~~~~~~
2 warnings generated.
compiling Fortran sources
Fortran f77 compiler: /usr/local/bin/gfortran -Wl,-rpath,. -m64 -fPIC -O3
Fortran f90 compiler: /usr/local/bin/gfortran -Wl,-rpath,. -m64 -fPIC -O3
Fortran fix compiler: /usr/local/bin/gfortran -Wall -g -ffixed-form -fno-second-underscore -Wl
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/Users
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/Users/will
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/Users/will/.ipython
creating /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/Users/will/.ipython/forti
compile options: '-I/var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10
gfortran:f90: /Users/will/.ipython/fortran/_fortran_magic_de8a64c7025eb58b0899ce8f4f1eee87.f90
gfortran:f77: /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6/src.macosx-10.7-x86_
/usr/local/bin/gfortran -Wall -g -m64 -Wall -g -undefined dynamic_lookup -bundle /var/folders/
Removing build directory /var/folders/rm/hnrktx9s22g8sbms445k0z000000gn/T/tmpnqnhn2p6
```

```
ImportError                               Traceback (most recent call last)

<ipython-input-74-55ae0315cf04> in <module>()
----> 1 get_ipython().run_cell_magic('fortran', "-vvv --opt='-O3' --extra './libfgrey.so'


~/anaconda/lib/python3.6/site-packages/IPython/core/interactiveshell.py in run_cell_mag
   2101             magic_arg_s = self.var_expand(line, stack_depth)
   2102             with self.builtin_trap:
-> 2103                 result = fn(magic_arg_s, cell)
   2104             return result
   2105


<decorator-gen-127> in fortran(self, line, cell)


~/anaconda/lib/python3.6/site-packages/IPython/core/magic.py in <lambda>(f, *a, **k)
    185     # but it's overkill for just that one bit of state.
    186     def magic_deco(arg):
--> 187         call = lambda f, *a, **k: f(*a, **k)
    188
    189         if callable(arg):


~/anaconda/lib/python3.6/site-packages/fortranmagic.py in fortran(self, line, cell)
```

```
    380
    381         self._code_cache[key] = module_name
--> 382         module = imp.load_dynamic(module_name, module_path)
    383         self._import_all(module, verbosity=args.verbosity)
    384
```

```
    ~/anaconda/lib/python3.6/imp.py in load_dynamic(name, path, file)
    340         spec = importlib.machinery.ModuleSpec(
    341             name=name, loader=loader, origin=path)
--> 342         return _load(spec)
    343
    344 else:
```

```
    ~/anaconda/lib/python3.6/importlib/_bootstrap.py in _load(spec)
```

```
    ~/anaconda/lib/python3.6/importlib/_bootstrap.py in _load_unlocked(spec)
```

```
    ~/anaconda/lib/python3.6/importlib/_bootstrap.py in module_from_spec(spec)
```

```
    ~/anaconda/lib/python3.6/importlib/_bootstrap_external.py in create_module(self, spec)
```

```
    ~/anaconda/lib/python3.6/importlib/_bootstrap.py in _call_with_frames_removed(f, *args
```

```
    ImportError: dlopen(/Users/will/.ipython/fortran/_fortran_magic_de8a64c7025eb58b0899ce8
  Referenced from: /Users/will/.ipython/fortran/_fortran_magic_de8a64c7025eb58b0899ce8f4f1
  Reason: image not found
```