2D Surface Creation Using Intel MKL

R. Steven Turley
Brigham Young University, turley@byu.edu

Follow this and additional works at: https://scholarsarchive.byu.edu/facpub

Part of the Physics Commons

BYU ScholarsArchive Citation
Turley, R. Steven, "2D Surface Creation Using Intel MKL" (2017). All Faculty Publications. 1965.
https://scholarsarchive.byu.edu/facpub/1965

This Report is brought to you for free and open access by BYU ScholarsArchive. It has been accepted for inclusion in All Faculty Publications by an authorized administrator of BYU ScholarsArchive. For more information, please contact scholarsarchive@byu.edu, ellen_amatangelo@byu.edu.
2D Surface Creation Using Intel MKL

Steve Turley

July 18, 2017

Contents

1. Introduction ................................................................. 1
   1.1. Creating Random Frequency Amplitudes ......................... 2
   1.2. Fourier Transform ............................................... 4
   1.3. Low Pass Filter .................................................. 5
   1.4. Setting RMS Height ............................................. 7

2. Setting Frequency Filter .................................................. 7

3. Setting RMS Height ...................................................... 8

4. FFT Routines .................................................................. 9

5. Plot Routines .................................................................. 10

6. Interpolation .................................................................... 11

7. CMake File ...................................................................... 12
   A. CMakeLists.txt ......................................................... 13
   B. simple_plot.f90 ......................................................... 15
   C. fft_surface.f95 .......................................................... 18
   D. fft_example.f95 ........................................................ 21

1. Introduction

This document illustrates how to use the Intel Math Kernel Library (which is installed on nystrom and marylou) to create surfaces with a given cut-off spatial frequency and rms height. I've included example Fortran-95 code which is included in its entirety in the Appendix.
In this introduction, I'll go through the theory of what the program accomplishes. Implementation details are found in later sections. Section 2 discusses how to set up the frequency filter. Section 3 discusses how to force the desired RMS surface height. Section 4 has implementation details about the inverse Fourier Transform. The plot routines are described in Section 5. Section 6 discusses how to interpolate to arbitrary points on the FFT surface and find the partial derivatives of the surface there. Finally, Section A discusses how to use cmake to compile and link the example programs.

Constructing the surface involves the following steps:

1. Create random surface height.
2. Transform the surface from the to k-space using a Fourier Transform (FFT).
3. Pass the amplitudes through a low pass filter.
4. Use an inverse FFT to reconstruct the filtered surface from the frequency amplitudes.
5. Adjust the height of the surface to have the desired RMS height.
6. Interpolate from the Fourier points to the desired surface points.

1.1. Creating Random Frequency Amplitudes

In order to compute the effects of roughness from a variety of arbitrary surfaces, it is important to be able to generate different surfaces each time. Doing so requires generating random values for the frequency amplitudes. Random number generators in FORTRAN aren't truly random. Rather, they produce a sequence of uncorrelated numbers based on an initial starting point or seed. In the examples below, I'll use the same default seed each time. To get a random seed, you could set the seed using the system clock. Here is an example code snippet to do that.

```fortran
  integer :: seed_size, clock
  integer, allocatable :: seed(:)

  call random_seed(size=seed_size)
  allocate(seed(seed_size))
  call system_clock(clock)
  seed = clock/1000 + 37 * (/ (i=0,n-1) /)
  call random_seed(put=seed)
  deallocate(seed)
```

the system random number generator in FORTRAN generates a number which is equally likely to have any value between 0 and 1. It's physically more realistic to expect the surface heights to have a gaussian probability distribution.

\[ P_x \propto \exp \left( -\frac{x^2}{2\sigma^2} \right) \]  

(1)
where $\sigma$ is the rms surface height. The following module uses the Box-Muller transform to create pseudorandom numbers centered about 0 with unit variance. These numbers are generated from the standard Fortran random number generator, so they can be seeded the same way outlined above.

module normal

! "use Box–Muller transform to create pseudorandom numbers centered about zero with a unit variance"

use iso_fortran_env, only: real64
implicit none

private

real(real64):: second
logical:: first = .TRUE.

public nrand

contains

function nrand()

  real(real64):: n(2), sr, nrand
  real(real64), parameter:: pi = 4.0d0*atan(1.0d0)

  if(first) then
    call random_number(n)
    sr = sqrt(-2.0d0*log(n(1)))
    nrand = sr*cos(2*pi*n(2))
    second = sr*sin(2*pi*n(2))
    first = .FALSE.
  else
    nrand = second
    first = .TRUE.
  end if

end function nrand

end module normal

This module is utilized in the random_surface subroutine to generate the initial surface heights.

subroutine filter(z, sigma)

use iso_fortran_env
implicit none

real(real64), intent(inout) :: z(:,:)
real(real64), intent(in) :: sigma
integer :: i, j
real(real64):: x
Figure 1: Original random surface before filtering.

\[
\text{do } i = 1, \text{size}(y, 1) \\
x = i - 1 \\
y(i) = y(i) \ast \exp(-x^2/(2*\text{sigma}^2)) \\
\text{end do} \\
\text{end subroutine filter}
\]

Figure 1 is a graph of the random surface generated by this routine before filtering.

1.2. Fourier Transform

In order to get a surface dominated by low spatial frequencies, the surface first has to be transformed to the spatial frequency domain. We do this using the Intel Math Kernel Library (MKL).

The symbols needed to control the FFT are included with the statement

use MKL_DFTI

The initialization then requires the following steps:

1. Setting the x and y dimensions of the FFT
2. Creating a descriptor

3. Committing the descriptor

Here is a code fragment the accomplishes these steps.

```fortran
integer, intent(out) :: status
integer :: l(2)
type(DFTI_DESCRIPTOR), POINTER :: handle

! Initialize data descriptors
l(1)=nx
l(2)=ny
status = DftiCreateDescriptor(handle, DFTI_DOUBLE,&
                          DFTI_COMPLEX, 2, 1)
status = DftiCommitDescriptor(handle)
```

The array l of dimension 2 hold the length of the x and y data for the transform. The call to DftiCreateDescriptor specifies that we are doing a double precision transform of an array of complex numbers. The third argument is the number of dimensions in the transform. If changes to the default parameters were needed, it would be done between the call to DftiCreateDescriptor and DftiCommitDescriptor. After the required space is computer and defaults are set for various parameters, the call to DftiCommitDescriptor allocates this space and precomputes some needed constants.

After initialization, the forward transform is accomplished in a single call. All of the DFTI routines return a status integer which is 0 on success and has a non-zero error code otherwise.

```fortran
status = DftiComputeForward(handle, z)
```

### 1.3. Low Pass Filter

Once in the spatial frequency domain, random frequency amplitudes need to be passed through a low pass filter. At first, a simple cut-off frequency might seem appropriate, but that will add ringing to the surface after the Fourier transform (like the side bands that appear from passing through a slit with a sharp cut-off). There are a number of filters that are commonly used in signal processing to provide smooth frequency cut-offs. The Wikipedia page at [https://en.wikipedia.org/wiki/Window_function](https://en.wikipedia.org/wiki/Window_function) discusses some of the possibilities. I chose a half-gaussian filter for our case.

\[
f(\nu) = e^{-\frac{\nu^2}{2\sigma^2}}
\]  

(2)

where \( \nu \) is the frequency in Fourier space. Another possibility to try would be an error function (\( \text{erf}(x) \)) joined to a constant function.

In applying the filter, I have assumed the \( \delta k \) is the same in the x and y directions.

Figure 2 is the filtered surface corresponding the the data in Figure 1. Note how the characteristic length scale between bumps on the surface is much large after the filtering.
Figure 2: Random surface after filtering.
1.4. Setting RMS Height

Depending on the width of the filter, the surface in real space will have a varying RMS height. To select a particular RMS height, one needs to calculate the RMS height of the surface and then scale it as desired. Let $\langle h \rangle$ be the mean height and $\langle h^2 \rangle$ be the mean of the square of the height. The RMS height is

$$\Delta h = \sqrt{\langle h^2 \rangle - \langle h \rangle^2}. \quad (3)$$

If the desired height is $\delta$, that can be achieved by multiplying each height $y_i$ by $\delta/\Delta h$.

2. Setting Frequency Filter

Once in the spatial frequency domain, we can filter out the highest frequencies in the surface noise. This is complicated by the fact that the FFT doesn’t store the transformed data completely in order of increasing frequency. For a transform with an even number of points, the transform first stores the positive frequencies

$$k_i = \frac{(i-1)2\pi}{L}, \, i = 1, \frac{n}{2} + 1$$

followed by the negative frequencies in increasing order.

$$k_i = \frac{(i-1)2\pi}{L} - \frac{2n\pi}{L}, \, i = \frac{n}{2} + 2, n$$

(4)

(5)

For ease of computation, I scale the $k_i$ values by the frequency increment

$$dk = \frac{2\pi}{L} \quad (6)$$

so that the actual values of $k_i$ are integers.

$$k_i = \begin{cases} 
  i - 1 & \text{for } i \leq \frac{n}{2} + 1 \\
  i - n - 1 & \text{for } i > \frac{n}{2} + 1 
\end{cases} \quad (7)$$

Here is the code snippet to filter the random frequency surface with a cut-off frequency of $\sigma$. To allow for different surface resolutions, I found it easiest to

```fortran
subroutine filter(z, sigma)
  use iso_fortran_env
  implicit none
  complex(real64), intent(inout) :: z(nx,ny)
  real(real64), intent(in) :: sigma
  integer :: i,j
  real(real64):: kx,ky,ksq,zf

  ! Assume even number of points
```
do i=1,nx
   if(i <= nx/2+1) then
      kx=i-1
   else
      kx=i-nx-1
   end if
! if j = 1, do nothing, we are multiplying by 1
do j=1,ny
   if(j <= ny/2+1) then
      ky = j-1
   else
      ky = j-ny-1
   end if
   ksq=kx**2+ky**2
   zf = exp(-ksq/(2*sigma**2))
   z(i,j)=z(i,j)*zf
end do
end do
end subroutine filter

The filtering is followed by an inverse FFT to transform the data back to the spatial domain and convert the transform from complex values (with a zero imaginary part) to a real array.

status = DftiComputeBackward(handle,z)
s = real(z)/(nx*ny)

I have verified that the imaginary parts are close to zero after that transform, which they wouldn’t be if different spatial frequencies had different attenuations.

3. Setting RMS Height

After an inverse fourier transform, we set the RMS of the surface to the desired value $\sigma$ using the following routine.

subroutine setrms(y, sigma)
   use iso_fortran_env
   implicit none
   real(real64), intent(inout) :: y(:)
   real(real64), intent(in) :: sigma
   real(real64) :: sm, smsq, rms
   integer :: n

   n = size(y)
   sm = sum(y)/n
   smsq = sum(y*y)/n
\( \text{rms} = \sqrt{\text{msq} - \text{sm}^{**2}} \)
\( y = y \cdot \text{sigma} / \text{rms} \)
end subroutine setrms

4. FFT Routines

The MKL FFT routines require setup, the FFT call, and then cleanup of the auxiliary storage. The routines return a status in the stat variable which will be zero on success. I haven’t been checking the status to make sure it is zero in the code, but we probably should. There is a POINTER variable ‘handle’ of type DFTI_DESCRIPTOR declared at the top level of the module to provide storage for internal data needed by the FFT.

type (DFTI_DESCRIPTOR), POINTER :: handle

Here is the initialization routine which needs to be called first.

subroutine fft_init (status)
use MKL_DFTI
use iso_fortran_env
integer, intent(out) :: status
integer :: l(2)

! Initialize data descriptors
l(1) = nx
l(2) = ny
status = DftiCreateDescriptor(handle, DFTI_DOUBLE,&
   DFTI_COMPLEX, 2, l)
status = DftiCommitDescriptor(handle)
end subroutine fft_init

Here is the routine for the forward FFT.

subroutine fft_forward (z, status)
use iso_fortran_env
implicit none
integer, intent(out) :: status
complex(real64), intent(inout) :: z(:)

status = DftiComputeForward(handle, z)
end subroutine fft_forward

This is the call to a routine for the inverse FFT.

function fft_backward (z, status) result (s)
use iso_fortran_env
implicit none
integer, intent(out) :: status
5. Plot Routines

I used the plotting routines we use in the Helmholtz program to plot the FFT results. They were based on piping calls to the gplot program. While the gplot program is adequate for 1d plots, it wasn't very good for surface plots. I replaced that package with driver's based on the plplot library which has higher quality graphics routines. The simple_plot module declares a plot class which handles a lot of the details of the library. To use the library, first add the public module symbols with a use statement.

```
use simple_plot
```

Next declare a variable of type plot.

```
type (plot) plt
```

In the executable code, create a plot object of this type. There are two possible constructors. The default constructor draws the plots in a graphics window.

```
plt = plot ()
```

To plot the graphics in a PNG file, specify the output file name in the constructor.

```
plt = plot ("osurf.png")
```

To plot a surface, call the splot method in the class with three arguments, the array of x coordinates, the array of y coordinates, and the surface height.

```
use iso_fortran_env , only: real64
integer , parameter :: NPTS=128
real (real64) :: y(NPTS,NPTS), xp(NPTS) , yp(NPTS)
...%ut %splot (xp,yp,y)
```
You can call splot multiple times before calling the done method. If you are plotting to a window, the window will display the plots in sequence when you right-click on the window. Right-clicking on the window while displaying the final plot will exit the window and return control to the calling program. If you are plotting to a file, the program will create a sequence of graphics files with each plot with trailing numbers to distinguish them. For example, if you specified an output filename of “osurf.png”, as above, the output files would be “osurf.png.1”, “osurf.png.2”, and so forth. When you are finished plotting, you need to call the done routine to clean up the storage, finish the plotting, and close open files.

call plt%done

6. Interpolation

We use the pspline library to create bicubic splines for interpolation. The EZSpline Fortran90 interface is the easiest to use.

use EZspline_obj
use EZspline

type(EZspline2_r8) :: spl ! 2-D real*8 interpolation object

To create a double precision bicubic spline, create a type to store it as follows.

type(EZspline2_r8) :: spl ! 2-D real*8 interpolation object

Since we have a periodic, FFT generated, surface. Periodic boundary conditions are a good choice. In the example program, these are stored in the two arrays, bcs1 and bcs2. The first array has the boundary conditions for the x axis and the second for the y axis.

integer:: bcs1(2), bcs2(2), ier, i, j

! Set periodic boundary conditions
bcs1 = -1
bcs2 = -1

Next, call the initialization routine to allocate storage and initialize variables.

call EZspline_init(spl, nx, ny, bcs1, bcs2, ier)
call EZspline_error(ier)

The ier variable is returned as 0 if there is no error. Otherwise it has an error code. If there is an error code, EZspline_error prints an error message. After filling the f array with the data to be interpolated, a call to EZspline_setup prepares the spline for future interpolations.

call EZspline_setup(spl, f, ier)
call EZspline_error(ier)

There are three kinds of interpolation possible:

• using individual points (point interpolation)
• using an array of randomly spaced points (cloud interpolation)
• using an array of equally spaced points on a grid (array interpolation)

I think the cloud interpolation is the most helpful for us.

```cpp
real(real64)::zx(2),zy(2),fz(2)
...
! cloud interpolation
zx(1)=1.1d0
zx(2)=1.3d0
zy(1)=0.8d0
zy(2)=0.9d0
call EZspline_interp(spl, 2, zx, zy, fz, ier)
call EZspline_error(ier)
```

There are also routines for computing the derivative. The interface for cloud interpolation is as follows.

```cpp
call EZspline_derivative(spl, 1, 0, 2, zx, zy, dp, ier)
call EZspline_error(ier)
call EZspline_derivative(spl, 0, 1, 2, zx, zy, dp, ier)
call EZspline_error(ier)
call EZspline_gradient(spl, 2, zx, zy, gp, ier)
call EZspline_error(ier)
```

The first call to `EZspline_derivative` computes the partial derivative with respect to \( x \) (the first coordinate). The second call to `EZspline_derivative` computes \( \partial/\partial y \). The final call computes the gradient. The first index of the gradient `gp` is the point number in the cloud. The second index is 1 for \( \partial/\partial x \) and 2 for \( \partial/\partial y \).

### 7. CMake File

In order to link to the MKL library, you'll need something like the following in your `CMakeLists.txt` file. First you need to specify the directories where the libraries are found.

```cpp
# Intel libraries on nystrom
set(MKL_ROOT /opt/intel/mkl)
set(LAPACK_LIB ${MKL_ROOT}/lib/intel64_lin)
link_directories(${LAPACK_LIB} /usr/local/lib/intel64)
```

Next you need to specify where to find the include files.

```cpp
set(MKL_INCLUDE /opt/intel/compilers_and_libraries_2017.1.132/linux/mkl/include)
includedirectories(${MKL_INCLUDE})
```

Finally, you need to specify the appropriate libraries to link the program. If you are using slatec in your program, be sure to list the MKL libraries before the slatec libraries.
Otherwise it will use the slower slatc routines that have the same names as the MKL routines.

```cpp
add_executable(surface surface.f95 gplotc.c gplot.f90)
target_link_libraries(surface mkl_gf_lp64 mkl_sequential
    mkl_core pthread m dl)
```

The libraries pthread, m, and dl are actually system libraries that are needed by the MKL library.

### A. CMakeLists.txt

```
# Specify the minimum version for CMake
# It might work with earlier ones, but specify my current
# version for now.
cmake_minimum_required(VERSION 2.8.12)

# Project’s name
project(fft)

set(PSPLINE "/usr/local")
set(PSPLINE_LIB ${PSPLINE}/lib)
set(PSPLINE_MOD ${PSPLINE}/mod)

set(CMAKE_BINARY_DIR ${CMAKE_SOURCE_DIR}/bin)
set(EXECUTABLE_OUTPUT_PATH ${CMAKE_BINARY_DIR})
set(LIBRARY_OUTPUT_PATH ${CMAKE_BINARY_DIR})
set(PROJECT_BINARY_DIR ${PROJECT_SOURCE_DIR}/bin)
set(MODULE_DIRECTORY ${CMAKE_BINARY_DIR}/mod)
set(CMAKE_Fortran_MODULE_DIRECTORY ${MODULE_DIRECTORY})
include_directories(${MODULE_DIRECTORY} ${PSPLINE_MOD})
link_directories(${PSPLINE_LIB})
set(SPLINE_LIBS pspline)

set(PLPLOT_MOD "/usr/lib/x86_64-linux-gnu/fortran/modules/plplot")
if(EXISTS ${PLPLOT_MOD})
    include_directories(${PLPLOT_MOD})
endif(EXISTS ${PLPLOT_MOD})

set(MKL_ROOT /opt/intel/mkl)
set(LAPACK_LIB ${MKL_ROOT}/lib/intel64_lin)
link_directories(${LAPACK_LIB} /usr/local/lib/intel64)
set(MKL_INCLUDE /opt/intel/compilers_and_libraries_2017.1.132/linux/mkl/include)
include_directories(${MKL_INCLUDE})
```
set(MKL_MOD ${MKL_INCLUDE}/intel64/lp64)
include_directories(${MKL_MOD})

enable_language(Fortran)
set(CMAKE_Fortran_FLAGS "-g -Wall" ${CMAKE_Fortran_FLAGS})

add_subdirectory(doc)

set(LIB_SOURCES plot_template.f95 gplot.c gplot.f90 fft_surface.f95 surface.f90
    normal.f95 simple_plot.f95)
add_library(fftlib ${LIB_SOURCES})

set(MKL_ROOT $ENV{MKLROOT})
if(EXISTS ${MKL_ROOT}/interfaces)
  # This is marylou
  message("This is Marylou")
  set(LAPACK_LIB ${MKL_ROOT}/lib/intel64)
  set(LAPACK_INC ${MKL_ROOT}/include/intel64/lp64)
  link_directories(${LAPACK_LIB})
  include_directories(${LAPACK_INC})
  set(FFT_LIBS fftlib mkl_intel_lp64 mkl_core mkl_intel_thread pthread m iomp5)
else (EXISTS ${MKL_ROOT}/interfaces)
  # Not marylou, assume ubuntu
  message("Not Marylou, assuming ubuntu")
  set(FFT_LIBS fftlib mkl_gf_lp64 mkl_sequential
             mkl_core pthread dl m)
endif(EXISTS ${MKL_ROOT}/interfaces)
set(PLOT_LIBS plplotf95d plplotf95cd)

add_executable(fft_example fft_example.f95)
target_link_libraries(fft_example ${FFT_LIBS} ${PLOT_LIBS})

add_executable(twod_example twod_example.f95)
target_link_libraries(twod_example ${FFT_LIBS})

add_executable(surfplot surfplot.f95)
target_link_libraries(surfplot fftlib)

add_executable(deriv deriv.f95)
target_link_libraries(deriv ${FFT_LIBS})

add_executable(surface_test surface_test.f95)
target_link_libraries(surface_test ${FFT_LIBS})
add_executable(pspline_test pspline_test.f95)
target_link_libraries(pspline_test ${SPLINE_LIBS})

add_executable(reshapex reshapex.f95)

target_link_libraries(reshape ${PLOT_LIBS})

add_executable(tplt tplt.f95)
target_link_libraries(tplt ${PLOT_LIBS})

add_executable(tplt3d tplt3d.f95)
target_link_libraries(tplt3d ${PLOT_LIBS})

B. simple_plot.f90

module simple_plot
  use plplot
  use iso_fortran_env, only: real64
  implicit none
  private
  type plot
    private
    contains
      procedure :: splot
      procedure :: done
  end type plot
  public splot, done, plot
! Constructors
interface plot
  module procedure :: init
  module procedure :: init_file
end interface plot
contains

function init()
  type(plot):: init
! Select qtwidget output, otherwise it will prompt
  call plsdev("qtwidget") ! window on workstation; could be hardcopy file
  call plinit()
  call cmapl_init(0) ! color instead of gray
end function init

function init_file(filename)
  type(plot):: init_file
  character(*):: filename


call plsfam(1,1,16000000)
call plsdev("pngqt") ! use png graphics
call plsfnam(trim(filename))
call plinit()
call cmap1_init(0) ! color instead of gray
end function init_file

subroutine splot(this,x,y,z)
class(plot)::this
real(real64), intent(in)::x(:,),y(:,),z(:,:)
real(real64), parameter::basex=1.d0, basey=1.d0, height=1.d0
real(real64)::xmin, xmax, ymin, ymax, zmin, zmax
real(real64), parameter::altitude=30.d0, azimuth=30.d0
integer, parameter::nlevel=10
real(real64)::cmin, cmax, cstep, clevel(nlevel)
integer::i
! bounds check
if(size(x) /= size(z,1)) call error("X dimension mismatch in splot")
if(size(y) /= size(z,2)) call error("Y dimension mismatch in splot")

! contour levels for surface plot
cmin = minval(z)
cmax = maxval(z)
cstep = (zmax−zmin)/(nlevel+1)
clevel = cmin + cstep * (/ (i, i=1, nlevel) /)

  call pladv(0) ! advance to next subframe (window in plot)
call plcol0(1) ! color selection for axes and labels
call plvpor(0.0d0, 1.0d0, 0.0d0, 0.9d0) ! viewport
call plwind(-1.0d0, 1.0d0, -1.0d0, 1.5d0) ! window
! bounds
xmin = minval(x)
xmax = maxval(x)
ymin = minval(y)
ymax = maxval(y)
zmin = cmin
zmax = cmax
call plw3d(basex, basey, height, xmin, xmax, ymin, ymax, zmin, zmax,&
  altitude, azimuth)
call plbox3('bnstu', 'x axis', 0.0d0, 0, &
  'bnstu', 'y axis', 0.0d0, 0, &
  'bcdmnstuv', 'z axis', 0.0d0, 0) ! axis labels
call plcol0(2) ! color for surface
call plbox3('bnstu', 'x axis', 0.0d0, 0, &
    'bnstu', 'y axis', 0.0d0, 0, &
    'bcdmstuv', 'z axis', 0.0d0, 0) ! axis labels

call plc010(2) ! color for surface
! possible options: MAG_COLOR (contour colors), FACETED,
! BASE_CONT (contour at base), SURF_CONT (contour on surface),
! DRAW_SIDES. You can add these instead of doing an ior

call plsrf3d(x,y,z,ior(MAG_COLOR, FACETED),clevel) ! clevel are contour l
end subroutine splot

subroutine done(this)
    class(plot) :: this
    call plend
end subroutine done

subroutine error(msg)
    character(*), intent(in) :: msg
    write(*,*) msg
    stop
end subroutine error

subroutine cmap1_init(gray)
! For gray.eq.1, basic grayscale variation from half–dark
! to light. Otherwise, hue variations around the front of the
! colour wheel from blue to green to red with constant lightness
! and saturation.

    integer, intent(in) :: gray
    real(real64) i(0:1), h(0:1), l(0:1), s(0:1)

    ! left boundary
    i(0) = 0._plfllt
    ! right boundary
    i(1) = 1._plfllt
    if (gray == 1) then
        ! hue — low: red (arbitrary if s=0)
        h(0) = 0.0 _plfllt
        ! hue — high: red (arbitrary if s=0)
        h(1) = 0.0 _plfllt
        ! lightness — low: half–dark
        l(0) = 0.5 _plfllt
        ! lightness — high: light
        l(1) = 1.0 _plfllt
        ! minimum saturation
This combination of hues ranges from blue to cyan to green to yellow to red (front of colour wheel) with constant lightness = 0.6 and saturation = 0.8.

hue — low: blue
h(0) = 240._plflt
hue — high: red
h(1) = 0.0._plflt
lightness — low:
l(0) = 0.6._plflt
lightness — high:
l(1) = 0.6._plflt
saturation
s(0) = 0.8._plflt
minimum saturation
s(1) = 0.8._plflt
endif
call p1scmap1n(256)
call p1scmap11(.false., i, h, l, s)
end subroutine cmap1_init

C. fft_surface.f95

module fft_surface
  use iso_fortran_env
  use MKL_DFTI
  implicit none
type(DFTI_DESCRIPTOR), POINTER :: handle
integer :: stat
integer :: nx, ny

private
public create_surface

contains

subroutine create_surface(sigma, rms, s)
  use iso_fortran_env, only: real64
implicit none
real(real64), intent(out) :: s(:,)
real(real64), intent(in) :: sigma, rms
complex(real64), allocatable :: z(:)
real(real64), allocatable :: s1(:)
integer :: shape1(1)
nx = size(s,1)
y = size(s,2)
allocate(z(nx*ny),s1(nx*ny))
call fft_init(stat)
call random_surface(s)
shape1(1)=nx*ny
z = RESHAPE(s,shape1) - 0.5d0
! write(*,*), original surface z(1:4)=" , real(z(1:4))
call fft_forward(z,stat)
! write(*,*), FFT of surface z(1:4)=" , z(1:4)
call filter(z,sigma)
! write(*,*), filtered surface z(1:4)=" , z(1:4)
s1 = fft_backward(z,stat)
! write(*,*), reversed transform s1(1:4)=" , s1(1:4)
s = RESHAPE(s1,shape(s))
! write(*,*), reversed transform s(1:4,1)=" , s(1:4,1)
deallocate(z,s1)
call setrms(s, rms)
call fft_cleanup
end subroutine create_surface

subroutine setrms(s, sigma)
use iso_fortran_env
implicit none
real(real64), intent(inout) :: s(:,)
real(real64), intent(in) :: sigma
real(real64) :: sm, smsq, rms

sm = sum(s)/(nx*ny)
smsq = sum(s**2)/(nx*ny)
rms = sqrt(smsq-sm**2)
s = s*sigma/rms
end subroutine setrms

subroutine filter(z,sigma)
use iso_fortran_env
implicit none
complex(real64), intent(inout) :: z(nx,ny)
real(real64), intent(in) :: sigma
integer :: i, j
real(real64)::kx, ky, ksq, zf

! Assume even number of points
do i=1,nx
  if(i <= nx/2+1) then
    kx=i-1
  else
    kx=i-nx-1
  end if
  ! if j = 1, do nothing, we are multiplying by 1
  do j=1,ny
    if(j <= ny/2+1) then
      ky = j-1
    else
      ky = j-ny-1
    end if
    ksq=kx**2+ky**2
    zf = exp(-ksq/(2*sigma**2))
    z(i,j)=z(i,j)*zf
  end do
end do
end subroutine filter

subroutine fft_init(status)
  use MKL_DFTI
  use iso_fortran_env
  integer, intent(out) :: status
  integer :: l(2)

  ! Initialize data descriptors
  l(1)=nx
  l(2)=ny
  status = DftiCreateDescriptor(handle, DFTI_DOUBLE,& DFTI_COMPLEX, 2, l)
  status = DftiCommitDescriptor(handle)
end subroutine fft_init

subroutine fft_cleanup
  implicit none
  integer :: status

20


```fortran
status = DftiFreeDescriptor(handle)
end subroutine fft_cleanup

function fft_backward(z, status) result(s)
  use iso_fortran_env
  implicit none
  integer, intent(out) :: status
  complex(real64), intent(inout) :: z(:)
  real(real64), dimension(size(z)) :: s

  status = DftiComputeBackward(handle, z)
  s = real(z)/(nx*ny)
end function fft_backward

subroutine fft_forward(z, status)
  use iso_fortran_env
  implicit none
  integer, intent(out) :: status
  complex(real64), intent(inout) :: z(:)

  status = DftiComputeForward(handle, z)
end subroutine fft_forward

subroutine random_surface(s)
  use normal
  real(real64), intent(out) :: s(:, :)
  integer :: nx, ny, i, j

  nx=size(s,1)
  ny=size(s,2)
  do i=1,nx
    do j=1,ny
      s(i,j)=nrand()
    end do
  end do
end subroutine random_surface
end module fft_surface

D. fft_example.f95

program fft_example
  use fft_surface
  use iso_fortran_env, only: real64
  use simple_plot
  
  21
```
implicit none
integer, parameter :: NPTS=128
real(real64):: y(NPTS,NPTS), xp(NPTS), yp(NPTS)
real(real64), parameter:: sigma=NPTS/6d0, rms=0.1
real(real64), parameter:: dx=4.0/NPTS, dy=4.0/NPTS
integer :: i
type(plot) :: plt

write(*,*) '2d FFT Example Program'
call create_surface(sigma*1000, rms, y)
! plt = plot('osurf.png')
plt = plot()
xp = (/ (dx*i, i=0,NPTS-1) /)
yp = (/ (dy*i, i=0,NPTS-1) /)
call plt%splot(xp,yp,y)
call create_surface(sigma/2, rms, y)
call plt%splot(xp,yp,y)
call plt%done()
end program fft_example