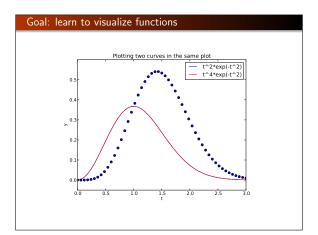
Ch.5: Array computing and curve Plotting

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We need to learn about a new object: array

- Curves y = f(x) are visualized by drawing straight lines between points along the curve
- Meed to store the coordinates of the points along the curve in lists or arrays x and y
- ullet Arrays pprox lists, but computationally much more efficient
- To compute the y coordinates (in an array) we need to learn about array computations or vectorization
- Array computations are useful for much more than plotting curves!

The minimal need-to-know about vectors

- Vectors are known from high school mathematics, e.g., point (x, y) in the plane, point (x, y, z) in space
- In general, a vector v is an n-tuple of numbers: $v = (v_0, \dots, v_{n-1})$
- Vectors can be represented by lists: v_i is stored as v[i], but we shall use arrays instead

Vectors and arrays are key concepts in this chapter. It takes separate math courses to understand what vectors and arrays really are, but in this course we only need a small subset of the complete story. A learning strategy may be to just start using vectors/arrays in programs and later, if necessary, go back to the more mathematical details in the first part of Ch. 5.

The minimal need-to-know about arrays

Arrays are a generalization of vectors where we can have multiple indices: $A_{i,j}$, $A_{i,j,k}$

Example: table of numbers, one index for the row, one for the column

$$\begin{bmatrix} 0 & 12 & -1 & 5 \\ -1 & -1 & -1 & 0 \\ 11 & 5 & 5 & -2 \end{bmatrix}$$

- $A = \begin{bmatrix} A_{0,0} & \cdots & A_{0,n-1} \\ \vdots & \ddots & \vdots \\ A_{m-1,0} & \cdots & A_{m-1,n-1} \end{bmatrix}$
- The no of indices in an array is the rank or number of dimensions
- $\bullet \ \ \mathsf{Vector} = \mathsf{one}\text{-}\mathsf{dimensional} \ \mathsf{array}, \ \mathsf{or} \ \mathsf{rank} \ 1 \ \mathsf{array}$
- In Python code, we use Numerical Python arrays instead of nested lists to represent mathematical arrays (because this is computationally more efficient)

Storing (x,y) points on a curve in lists

Collect points on a function curve y = f(x) in lists:

Turn lists into Numerical Python (NumPy) arrays:

```
>>> import numpy as np # module for arrays
>>> x2 = np.array(xlist) # turn list alist into array
>>> y2 = np.array(ylist)
```

The pro drops lists and makes NumPy arrays directly: >>> n = 5 >>> x2 = np.linspace(0, 1, n) # n points in [0, 1] >>> y2 = np.zeros(n) >>> for i in xrange(n): ... y2[i] = f(x2[i]) Note: • xrange is like range but faster (esp. for large n - xrange does not explicitly build a list of integers, xrange just lets you loop over the values) • Entire arrays must be made by numpy (np) functions

```
Arrays are not as flexible as list, but computational much more efficient
```

- List elements can be any Python objects
- Array elements can only be of one object type
- Arrays are very efficient to store in memory and compute with if the element type is float, int, or complex
- Rule: use arrays for sequences of numbers

```
We can work with entire arrays at once - instead of one element at a time

Typical code for taking the sine of a list (or array) x by working with one element at a time:

for i in xrange(len(x)):
 y[i] = sin(x[i])

However, if x is array, y can be computed by
 y = np.sin(x) # x: array, y: array

The loop is now inside np.sin and implemented in very efficient C code.
```

```
A function f(x) written for a number x usually works for array x too

from numpy import sin, exp, linspace

def f(x):
    return x**3 + sin(x)*exp(-3*x)

x = 1.2
    y = f(x)  # float object
    y = f(x)  # y is float

x = linspace(0, 3, 10001)  # 10000 intervals in [0,3]
    y = f(x)  # y is array

Note: math is for numbers and numpy for arrays.

>>> import math, numpy
>>> x = numpy linspace(0, 1, 11)
>>> math.sin(x[3])
0.2955202066613396
>>> math.sin(x)
...

TypeError: only length-1 arrays can be converted to Python scalars
>>> numpy.sin(x)
array([0, ..., 0.09983, 0.19866, 0.29552, 0.38941, 0.47942, 0.56464, 0.64421, 0.71735, 0.78332, 0.84147])
```

```
Array arithmetics is broken down to a series of
unary/binary array operations
    • Consider y = f(x), where f returns
      x**3 + sin(x)*exp(-3*x)
    • f(x) leads to the following set of vectorized
      sub-computations:
        for i in range(len(x)): r1[i] = x[i] **3 (but with
          loop in C)
        9 r2 = sin(x) (unary op, computed elementwise, but with loop
         in C)
        1 r4 = exp(r3) (unary op.)
        o r5 = r3*r4 (binary op.)
        o r6 = r1 + r5 (binary op.)
        0 y = r6
    • Note: this is the same set of operations as you would do with
      a calculator when x is a number
```

Important application: vectorized code for computing points along a curve

$$f(x) = x^2 e^{-\frac{1}{2}x} \sin(x - \frac{1}{3}\pi), \quad x \in [0, 4\pi]$$

from numpy import * # Vectorized computation of 101 points along the curve x = 1 inspace(0, 4 *pi, 101) y = 2.5 + x**2*exp(-0.5*x)*sin(x-pi/3)

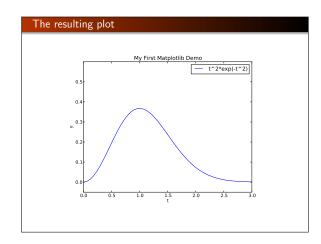
Vectorization

Terminology.

- Scalar: a number
- Vector or array: sequence of numbers (vector in mathematics)
- We speak about scalar computations (one number at a time) versus vectorized computations (operations on entire arrays, no Python loops)
- Functions that can operate on vectors (arrays) are called vectorized functions
- Vectorized functions are (usually) built of vectorized unary/binary operations
- Vectorization is the process of turning a non-vectorized algorithm with (Python) loops into a vectorized version without (Python) loops
- Mathematical functions in Python without if tests automatically work for both scalar and vector (array) arguments (i.e., no vectorization is needed by the

Plotting the curve of a function: the very basics Plot the curve of $y(t) = t^2 e^{-t^2}$: from scitools.std import * # import numpy and plotting # Make points along the curve t = linspace(0, 3, 5i) # 50 intervals in [0, 3] y = t**2*exp(-t**2) # wectorized expression plot(t, y) # make plot on the screen savefig('fig.pdf') # make PDF image for reports savefig('fig.png') # make PNG image for web pages

from scitools.std import * # import numpy and plotting def f(t): return t**2*exp(-t**2) t = linspace(0, 3, 51) # t coordinates y = f(t) # corresponding y values plot(t, y) xlabel('t') # label on the x axis ylabel('t') # label on the y axix legend('t^2*exp(-t^2)') # mark the curve axis([0, 3, -0.05, 0.6]) # [tmin, tmax, ymin, ymax] title('My First Easyviz Demo')



SciTools vs. NumPy and Matplotlib SciTools is a Python package with lots of useful tools for mathematical computations, developed here in Oslo (Langtangen, Ring, Wilbers, Bredesen, ...) Easyviz is a subpackage of SciTools (scitools.easyviz) doing plotting with Matlab-like syntax Easyviz can use many plotting engine to produce a plot: Matplotlib, Gnuplot, Grace, Matlab, VTK, OpenDx, ... but the syntax remains the same Matplotlib is the standard plotting package in the Python community - Easyviz can use the same syntax as Matplotlib from scitools.std import * # is ca equivalent to from numpy import * from matplotlib.pyplot import *


```
Plotting several curves in one plot

Plot t^2e^{-t^2} and t^4e^{-t^2} in the same plot:

from scitools.std import * # curve plotting + array computing

def f1(t):
    return t**2*exp(-t**2)

def f2(t):
    return t**2*f1(t)

t = linspace(0, 3, 51)
    y1 = f1(t)
    y2 = f2(t)
    plot(t, y1)
    hold('on') # continue plotting in the same plot
    plot(t, y2)
    xlabel('t')
    ylabel('t')
    ylabel('t'2*exp(-t*2)', 't*4*exp(-t*2)')
    title('Plotting two curves in the same plot')
    savefig('tmp2.png')
```

```
When plotting multiple curves in the same plot, the different lines (normally) look different. We can control the line type and color, if desired:

plot(t, y1, 'r-')  # red (r) line (-) hold('on') plot(t, y2, 'bo')  # blue (b) circles (a)

# or plot(t, y1, 'r-', t, y2, 'bo')

Documentation of colors and line styles: see the book, Ch. 5, or Unix> pydoc scitools.easyviz for
```

```
Quick plotting with minimal typing

A lazy pro would do this:

t = linspace(0, 3, 51)
plot(t, t**2*exp(-t**2), t, t**4*exp(-t**2))
```

Plot function given on the command line

Task: plot function given on the command line.

Terminal> python plotf.py expression xmin xmax
Terminal> python plotf.py "exp(-0.2*x)*sin(2*pi*x)" 0 4*pi

Should plot $e^{-0.2x}\sin(2\pi x)$, $x\in[0,4\pi]$. plotf.py should work for "any" mathematical expression.

Solution

```
Complete program:
    from scitools.std import *
    # or alternatively
    from numpy import *
    from matplotlib.pyplot import *

    formula = sys.argv[1]
    xmin = eval(sys.argv[2])
    xmax = eval(sys.argv[3])

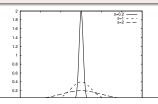
x = linspace(xmin, xmax, 101)
    y = eval(formula)
    plot(x, y, title=formula)
```

Let's make a movie/animation

The Gaussian bell function:

$$f(x; m, s) = \frac{1}{\sqrt{2\pi}} \frac{1}{s} \exp \left[-\frac{1}{2} \left(\frac{x - m}{s} \right)^2 \right]$$

- m is the location of the peak
- s is a measure of the width of the function
- Make a movie (animation) of how f(x; m, s) changes shape as s goes from 2 to 0.2



Movies are made from a (large) set of individual plots

- Goal: make a movie showing how f(x) varies in shape as s decreases
- Idea: put many plots (for different s values) together (exactly as a cartoon movie)
- How to program: loop over s values, call plot for each s and make hardcopy, combine all hardcopies to a movie
- Very important: fix the *y* axis! Otherwise, the *y* axis always adapts to the peak of the function and the visual impression gets completely wrong

The complete code for making the animation

How to combine plot files to a movie (video file)

We now have a lot of files:

tmp_0000.png tmp_0001.png tmp_0002.png ...

We use some program to combine these files to a video file:

- convert for animted GIF format (if we have just a few plot files)
- avconv for MP4, WebM, Ogg, and Flash formats

Make and play animated GIF file Tool: convert from the ImageMagick software suite. Unix command: Terminal> convert -delay 50 tmp_*.png movie.gif Delay: 50/100 s, i.e., 0.5 s between each frame. Play animated GIF file with animate from ImageMagick: Terminal> animate movie.gif or insert this HTML code in some file tmp.html loaded into a browser:

Making MP4, Ogg, WebM, or Flash videos Tool: avconv or ffmpeg Terminal> avconv -r 5 -i tmp_%04d.png -vcodec flv movie.flv where • -r 5 specifies 5 frames per second • -i tmp_%04d.png specifies filenames (tmp_0000.png, tmp_0001.png, ...) Different formats apply different codecs (-vcodec) and video filenamet extensions: Format Codec and filename Flash -vcodec flv movie.flv MP4 -vcodec flv movie.flv Webm -vcodec libvpx movie.webm Ogg -vcodec libtheora movie.ogg

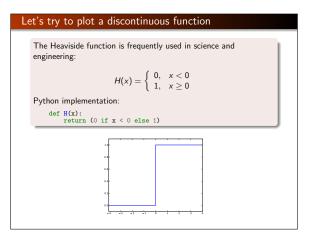
```
How to play movie files in general

Terminal> vlc movie.flv
Terminal> vlc movie.evem
Terminal> vlc movie.webm
Terminal> vlc movie.flv
```

```
HTML PNG file player

Terminal> scitools movie output_file=mymovie.html fps=4 tmp_*.png
makes a player of tmp_*.png files in a file mymovie.html (load into a web browser), 4 frames per second
```

```
    Plots are stored in image files of type PDF, PNG, JPEG, or GIF
    Sometimes you want a plot to be included in your program, e.g., to prove that the curve looks right in a compulsory exercise where only the program (and not a nicely typeset report) is submitted
    scitools.aplotter can then be used for drawing primitive curves in pure text (ASCII) format
    >>> from scitools.aplotter import plot
    >>> from numpy import linspace, exp, cos, pi
    >>> x = linspace(-2, 2, 8i)
    >>> y = exp(-0.5x**2)*cos(pi*x)
    >>> plot(x, y)
    Try these statements out!
```



Standard approach: x = linspace(-10, 10, 5) # few points (simple curve) y = H(x) plot(x, y) First problem: ValueError error in H(x) from if x < 0 Let us debug in an interactive shell: >>> x = linspace(-10,10,5) >>> x array([-10., -5., 0., 5., 10.]) >>> b = x < 0 >>> b array([True, True, False, False, False], dtype=bool) >>> bool(b) # evaluate b in a boolean context ... ValueError: The truth value of an array with more than one element is ambiguous. Use a.any() or a.all()

```
Remedy 1: use a loop over x values.

def H_loop(x):
    r = zeros(len(x)) # or r = x.copy()
    for i in xrange(len(x)):
        r[i] = H(x[i])
    return r

n = 5
    x = linspace(-5, 5, n+1)
    y = H_loop(x)

Downside: much to write, slow code if n is large
```

```
Remedy 2: use vectorize.

from numpy import vectorize

# Automatic vectorization of function H

Hv = vectorize(H)

# Hu(x) works with array x

Downside: The resulting function is as slow as Remedy 1
```

```
Remedy 3: code the if test differently.

def Hv(x):
    return where(x < 0, 0.0, 1.0)

More generally:

def f(x):
    if condition:
        x = <expression1>
    else:
        x = <expression2>
    return x

def f_vectorized(x):
    def f_vectorized(x):
    x1 = <expression1>
    x2 = <expression1>
    x2 = <expression2>
    return x

def f_vectorized(x):
    x1 = <expression1>
    x2 = <expression2>
    r = np. where(condition, x1, x2)
    return r
```

```
With a vectorized Hv(x) function we can plot in the standard way

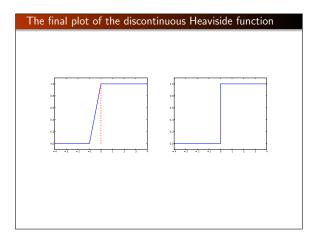
x = linspace(-10, 10, 5) # linspace(-10, 10, 50)

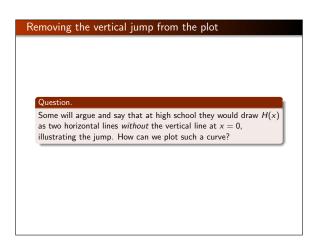
y = Hv(x)
plot(x, y, axis=[x[0], x[-1], -0.1, 1.1])
```

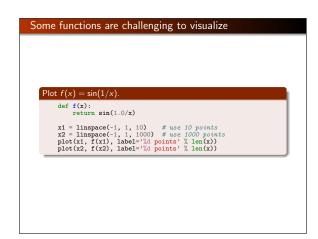
```
How to make the function look discontinuous in the plot?

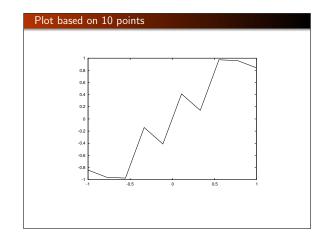
• Newbie: use a lot of x points; the curve gets steeper
• Pro: plot just two horizontal line segments one from x=-10 to x=0, y=0; and one from x=0 to x=10, y=1

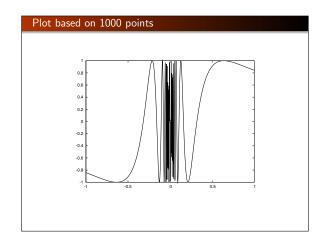
plot([-10, 0, 0, 10], [0, 0, 1, 1], axis=[x[0], x[-1], -0.1, 1.1])
Draws straight lines between (-10,0), (0,0), (0,1), (10,1)
```











```
Assignment of an array does not copy the elements!

a = x
a[-1] = q

Is x[-1] also changed to q?

Yes, because a refers to the same array as x.

Avoid changing x by letting a be a copy of x:
a = x.copy()

The same yields slices:

a = x[r:] # a refers to a part of the x array
a[-1] = q # changes x[-1]!

a = x[r:].copy()
a[-1] = q # does not change x[-1]
```

In-place array arithmetics The two following statements are mathematically equivalent: a = a + b # a and b are arrays a += b However, a = a + b is computed as (extra array needed) of 1 = a + b a = r1 a += b is computed as a[i] += b[i] for i in all indices (i.e., not extra array) a += b is an in-place addition, because we change each element in a, rather than letting the name a refer to a new array, the result of a+b

Consider a = (3*x**4 + 2*x + 4)/(x + 1) Here are the actual computations in the computer: r1 = x**4; r2 = 3*r1; r3 = 2*x; r4 = r1 + r3 r5 = r4 + 4; r6 = x + 1; r7 = r5/r6; a = r7 With in-place arithmetics we can save four extra arrays, though at the cost of much less readable code: a = x.copy() a **= 4 a *= 3 a += 2*x a += 4 a /= x + 1

```
In-place arithmetics only saves memory, no significant speed-up

Let's use IPython to measure the computational time:

In [1]: def expression(x):
...: return (3*x**4 + 2*x + 4)/(x + 1)
...:

In [2]: def expression_inplace(x):
...: a = x.copy()
...: a **= 4
...: a **= 3
...: a **= 4
...: a **= 4
...: a /*= x + 1
...: return a
...:

In [3]: import numpy as np
In [4]: x = np.linspace(0, 1, 10000000)

In [5]: %timeit expression(x)
1 loops, best of 3: 771 ms per loop

In [6]: %timeit expression_inplace(x)
1 loops, best of 3: 728 ms per loop
```

Generalized array indexing with boolean expressions

Two-dimensional arrays; math intro

When we have a table of numbers,

$$\begin{bmatrix} 0 & 12 & -1 & 5 \\ -1 & -1 & -1 & 0 \\ 11 & 5 & 5 & -2 \end{bmatrix}$$

(called matrix by mathematicians) it is natural to use a two-dimensional array $A_{i,j}$ with one index for the rows and one for the columns:

$$A = \begin{bmatrix} A_{0,0} & \cdots & A_{0,n-1} \\ \vdots & \ddots & \vdots \\ A_{m-1,0} & \cdots & A_{m-1,n-1} \end{bmatrix}$$

Two-dimensional arrays; Python code

Making and filling a two-dimensional NumPy array goes like this:

```
A = zeros((3,4)) # 3x4 table of numbers
A[0,0] = -1
A[1,0] = 1
A[2,0] = 10
A[0,1] = -5
...
A[2,3] = -100
# can also write (as for nested lists)
A[2][3] = -100
```

From nested list to two-dimensional array

```
Let us make a table of numbers in a nested list:

>>> Cdegrees = [-30 + i*10 for i in range(3)]
>>> Fdegrees = [9./5*C + 32 for C in Cdegrees]
>>> table = [[C, F] for C, F in zip(Cdegrees, Fdegrees)]
>>> print table
[[-30, -22.0], [-20, -4.0], [-10, 14.0]]

Turn into NumPy array:

>>> table2 = array(table)
>>> print table2
[[-30, -22.]
[-20, -4.]
[-10. 14.]]
```

```
How to loop over two-dimensional arrays

>>> table2.shape  # see the number of elements in each dir.
(3, 2)  # 3 rows, 2 columns

A for loop over all array elements:

>>> for i in range(table2.shape[0]):
... for j in range(table2.shape[i]):
... print 'table2[%d, %d] = %g' % (i, j, table2[i,j])

... table2[0,0] = -30
table2[0,1] = -22
... table2[2,1] = 14

Alternative single loop over all elements:

>>> for index_tuple, value in np.ndenumerate(table2):
... print 'index %s has value %g' % \
... (index_tuple, table2[index_tuple])
...
index (0,0) has value -30
index (0,1) has value -22
...
index (2,1) has value 14
>>> type(index_tuple)
<type 'tuple'>
```

How to take slices of two-dimensional arrays

Time for a question Given >>> t([1., 2., 3., 4., 5., 6.], [7., 8., 9., 10., 11., 12.], [13., 14., 15., 16., 17., 18.], [19., 20., 21., 22., 23., 24.], [25., 26., 27., 28., 29., 30.]]) What will t[1:-1:2, 2:] be? Slice 1:-1:2 for first index results in [7., 8., 9., 10., 11., 12.] [19., 20., 21., 22., 23., 24.] Slice 2: for the second index then gives [9., 10., 11., 12.] [21., 22., 23., 24.]

Summary of plotting y = f(x) curves Curve plotting (unified syntax for Matplotlib and SciTools): from matplotlib.pyplot import * #from scitools.std import * plot(x, y) # simplest command plot(t1, y1, 'r', # curve 1, red line t2, y2, 'b', # curve 2, blue line t3, y3, 'o') # curve 3, circles at data points axis([t1[0], t1[-1], -1.1, 1.1]) legend(['model 1', 'model 2', 'measurements']) xlabel('time'); ylabel('force') savefig('myframe_%04d.png' % plot_counter) Note: straight lines are drawn between each data point

```
Summary of making animations
    • Make a hardcopy of each plot frame (PNG or PDF format)
    • Use avconv or ffmpeg to make movie
      Terminal> avconv -r 5 -i tmp_%04d.png -vcodec flv movie.flv
```

Summary of vectors and arrays • Vector/array computing: apply a mathematical expression to every element in the vector/array (no loops in Python) • Ex: sin(x**4)*exp(-x**2), x can be array or scalar for array the i'th element becomes sin(x[i]**4)*exp(-x[i]**2)• Vectorization: make scalar mathematical computation valid for vectors/arrays • Pure mathematical expressions require no extra vectorization • Mathematical formulas involving if tests require manual work for vectorization: scalar_result = expression1 if condition else expression2 vector_result = where(condition, expression1, expression2)

```
Alternativ plotting of y = f(x) curves
     Single SciTools plot command with keyword arguments:
            from scitools.std import *
             plot(t1, y1, 'r', # curve 1, red line
                      (t1, y1, 'r', " curve 2, blue line t2, y2, 'b', # curve 2, blue line t3, y3, 'o', # curve 3, circles at data points axis=[t1[0], t1[-1], -1.1, 1.1], legend=('model 1', 'model 2', 'measurements'), xlabel='time', ylabel='fore', savefig='myframe_%04d.png' % plot_counter)
```

```
Array functionality
           Construction
                                                     Meaning
    array(ld)
                                 copy list data 1d to a numpy array
    asarray(d)
                                make array of data d (no data copy if already array)
    zeros(n)
                                make a float vector/array of length n, with zeros
    zeros(n, int)
                                make an int vector/array of length n with zeros
                                make a two-dimensional float array with shape (m,'n
    zeros((m,n))
    zeros like(x)
                                make array of same shape and element type as x
                                uniform sequence of m numbers in [a, b]
    linspace(a,b,m)
    a.shape
                                tuple containing a's shape
                                total no of elements in a
    a.size
                                length of a one-dim. array a (same as a.shape[0])
    len(a)
    a.dtype
                                the type of elements in a
    a.reshape(3,2)
                                return a reshaped as 3 × 2 array
    a[i]
                                vector indexing
                                two-dim. array indexing
    a[i,j]
                                slice: reference data with indices 1,..., 'k-1'
    a[1:k]
    a[1:8:3]
                                slice: reference data with indices 1, 4,..., '7'
    b = a.copy()
                                copy an array
                                numpy functions applicable to arrays
    sin(a), exp(a), ...
    c = concatenate((a, b)) c contains a with b appended
    c = where(cond, a1, a2) c[i] = a1[i] if cond[i], else c[i] = a2[i]
    isinstance(a, ndarray) is True if a is an array
```

Summarizing example: animating a function (part 1)

 Goal: visualize the temperature in the ground as a function of depth (z) and time (t), displayed as a movie in time:

$$T(z,t) = T_0 + Ae^{-az}\cos(\omega t - az), \quad a = \sqrt{\frac{\omega}{2k}}$$

• First we make a general animation function for an f(x, t):

Summarizing example: animating a function (part 2)

```
# remove old plot files:
import glob, os
for filename in glob.glob('tmp*.png'): os.remove(filename)

def T(z, t):
    # TO, A, k, and omega are global variables
    a = sqrt(omega/(2*k))
    return TO + A*exp(-a*z)*cos(omega*t - a*z)

k = 1E-6    # heat conduction coefficient (in m*m/s)
P = 24*60*60.# oscillation period of 24 h (in seconds)
omega = 2*pi/P
dt = P/24    # time lag: 1 h
tmax = 3*P    # 3 day/night simulation
TO = 10    # mean surface temperature in Celsius
A = 10    # amplitude of the temperature variations (in C)
a = sqrt(omega/(2*k))
D = -(1/a)*log(0.001) # max depth
n = 501    # no of points in the z direction

z = linspace(0, D, n)
animate(tmax, dt, z, T, TO-A, TO+A, 0, 'z', 'T')
# make movie files:
movie('tmp*.png', encoder='convert', fps=2,
    output_file='tmp_heatwave.gif')
```