Physics 329: Introduction to Computational Physics: Software Availability and Usage Hints

This document will be updated throughout the course

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X Windows: As the man page says, X is a "portable, network-transparent window system". It is the main windowing system used in most Unix environments. You will *automatically* use **X** when you login to one of the Phys. Dept. linux machines, or one of the Center for Relativity SGI machines. To use X on the PCs in the PMCL follow these instructions:

- login
- double click on the *Internet Applications* icon
- in the *Internet Applications* panel, double click on the *XServer* icon
- an *Xapplication Starter* window should pop up. **IGNORE OR CLOSE THIS WINDOW**.
- Put the cursor on *eXodus* in the tool bar on the bottom of the screen. Click the right mouse button to bring up a menu and select *Login using XDM*
- In the *XDM Login* window which appears, type in the name of the host to which you wish to connect using X (`einstein, linux1,` etc.), then type or click *CONNECT*
- The remote host's login window should appear; login as usual. (You will have to put the cursor in the login window and click with a mouse button before you can start typing in the window.) If the login is successful, in a few seconds you should see the usual components of an X-session on the remote machine. (These components will be superimposed on the usual Windows screen.) For example, on `einstein` you should see a "toolchest" labelled *Desk 1* in the upper left of the screen, as well as an **xterm** window. At this point you can start additional X-applications (**xmaple**, more **xterm**s etc.) from the **xterm** window, or from the toolchest.
- Once you have established a session on the remote host via X, you can also connect to other hosts (using the **telnet** icon in *Network Applications* for example), set the `DISPLAY` environment variable appropriately, e.g.

  ```
  einstein % setenv DISPLAY pmcl-pc8.ph.utexas.edu:0.0
  ```

  and start X-applications from there. Note that the Internet address of each machine should be taped to the system's monitor.
- Don't forget to log out of the remote X-session when you are through. For example, if logged into `einstein`, choose *Log out* from the *Desktop* menu of the toolchest. A notifier asking you to confirm the log out should appear---click *Yes* to log out. A less graceful way to exit is to choose *Close* from the *eXodus* menu.

Maple: One of the two major general-purpose "symbolic manipulation" packages (also general-purpose *programming* environments), and the one that we will study in this course. On the SGIs type

```
% xmaple
```

for the GUI version (in which case make sure your DISPLAY environment variable is set correctly if running on a remote machine), or

```
% maple
```

for a terminal-based (text) session. In the latter instance you should see something like this.

```
% maple
    |\^/|     Maple V Release 5 (University of Texas at Austin)
._|\|   |/|_. Copyright (c) 1981-1997 by Waterloo Maple Inc. All rights
 \  MAPLE  /  reserved. Maple and Maple V are registered trademarks of
 <____ ____>  Waterloo Maple Inc.
      |       Type ? for help.
>
```

If there is any sequence of `Maple` commands that you find yourself typing at the beginning of each session (`maple` or `xmaple`) you can put them in a file `.mapleinit` in your home directory, whereafter they will automatically be executed each time you use `Maple`.

Fortran 77: A general purpose programming language which is particularly well-suited to numerical (scientific/engineering) applications. On Unix systems, such as SGI IRIX, the Fortran 77 compiler is often called **f77**.

Typical usage (on the SGIs):

```
% f77 -n32 -g mypgm.f mysubs.f -o mypgm
```

See the on-line notes describing the use of Fortran and C in the Unix environment for additional information.

C: Another general purpose programming language which is also widely-used for scientific and engineering applications. On Unix systems the C compiler is often called **cc**.

Typical usage (on the SGIs):

```
% cc -n32 -g mypgm.c myfcns.c -o mypgm
```

See the on-line notes describing the use of Fortran and C in the Unix environment for additional information.

---

libp329fa: Utility library for Fortran 77 programs. Available on SGIs and Crays. Sample driver for utility routines: `p329fsa.f`. See source code and course notes for further information.

Typical usage:

```
   % f77 pgm.f -L/usr/localn32/lib -lp329 -o pgm
```

---

ghostview: Available on SGIs and Linux machines. Use for viewing Postscript documents. This is an X-application. As with any X-application, if you are running `ghostview` on a remote machine, be sure to set your DISPLAY environment variable so that your local display is used.

Typical usage (assuming a remote login to einstein from one the Physics Linux machines):

```
   einstein% set DISPLAY linux1.ph.utexas.edu:0
   einstein% ghostview somefile.ps
```

Note: Not all Postscript files will have `.ps` extensions, but many do by convention.

---

gnuplot: X-application available on SGIs and Linux machines. Use for generating X-Y (2D) and some surface plots. Has extensive on-line documentation: type `help` at the `gnuplot` prompt for help.

Typical usage:

```
einstein% gnuplot
          .
          .
          .
Terminal type set to 'x11'
gnuplot> help
          .
          .
          .
gnuplot> quit
```

---

sm: Supermongo plotting package. Available on SGIs. An alternative to `gnuplot` which is somewhat quirkier but generally produces more professional-looking (i.e. publication-quality) plots. See on-line postscript documentation and on-line help (type `help` at the the sm command prompt) for further details. Supermongo runs as an X-application provided the `device` is set to `x11`. Ignore the `"Can't find entry for iris-ansi-net ..."` message at start-up.

Typical usage:

```
einstein% sm
Can't find entry for iris-ansi-net in /usr/local/lib/sm/termcap
Hello Matt, please give me a command
: device x11
: help
          .
          .
          .
: quit
```

---

vsxynt: A Fortran- and C-callable routine which was specifically designed for the output and subsequent visualization of data generated in the solution of time-dependent problems in one spatial dimension.

Use of this routine in **Fortran** is illustrated by the code **vswave.f** which generates a time-series of waveforms, and, at each time step, outputs the data using **vsxynt**. Note that this program is essentially identical to the **gpwave.f** example discussed in class, we're just changing the "output interface".

Depending on which library is linked-to, data which is output via **vsxynt** will be sent to special-purpose files, or sometimes directly to a visualization server such as **scivis**. I strongly recommend that you use the following libraries when using the **vsxynt** interface:

```
    -lsvs -lrnpl -lmfhdf -ldf -ljpeg -lz -lsv -lm
```

I further recommend that you communicate these libraries to **make** using the following **setenv** command which should be placed in your **.cshrc**:

```
    setenv LIBVS '-lsvs -lrnpl -lmfhdf -ldf -ljpeg -lz -lsv -lm'
```

If you do this, then Makefiles such as this one will work properly.

Assuming that your executable has linked to the libraries given above, calls to **vsxynt** will direct data to files with the extension **.sdf**. Thus, in the **vswave.f** example, the call

```
     call vsxynt('wave',t,x,y,nx)
```

will send data to

```
     wave.sdf
```

.sdf files can then be sent to **scivis** using the **sdftosv** command, as discussed in more detail below.

Important: Note that **.sdf** files are *not* ‘‘human-readable’’, so *please* don’t try to edit them or, worse, to print them!

---

scivis (jser): A package for interactive & collaborative visualization developed at NPAC in Syracuse. Some documentation is available from the Scivis home page and the User’s Guide, but the following should help get you going.

PLEASE SEND ME E-MAIL IMMEDAITELY IF YOU HAGE PROBLEMS WITH THIS SOFTWARE.

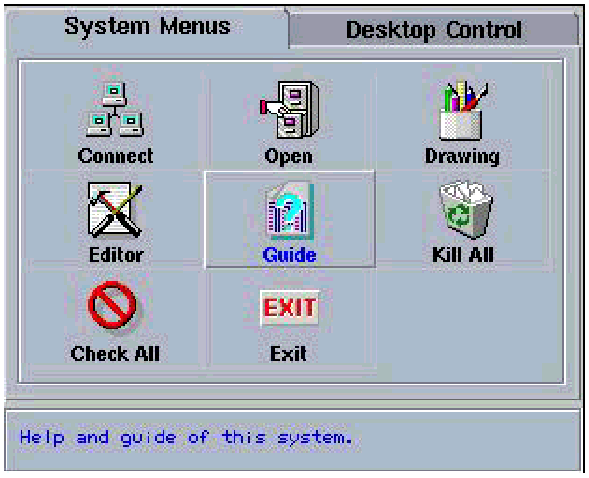
Assuming that you have established an **X** session to **einstein**, you should be able to start the **scivis** visualization server (also known as **jser**) by selecting *jser* from the *Tools* sub-menu of the toolchest in the upper left corner of the screen.

Alternatively, you can start **jser** from the command-line:

```
   einstein% jser &
```

Note, that we start **jser** in the background so that we can continue to type commands at the shell prompt. Note that **jser** is an X-application, so be sure that the **DISPLAY** environment variable points to your local screen.

Whichever way you start **jser**, the following window should pop up on your screen in a few seconds:



Help and guide of this system.

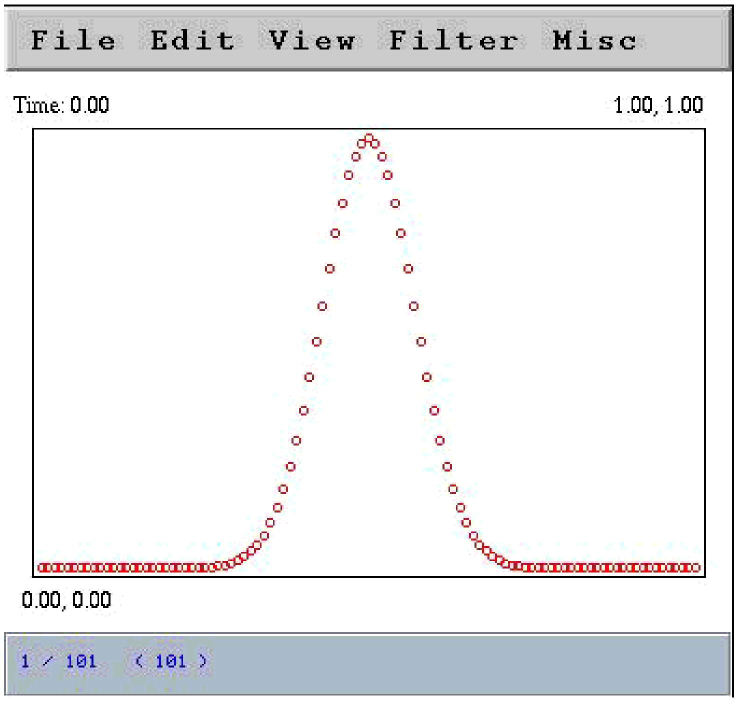
Note that, with the exception of the *Exit* button---which shuts the server down---you will probably find little use for the various selections on the server panel. Rather, you will primarily interact with the server through additional windows which display data sets which are sent to the server after it is started. For example, assume that we have previously generated an **.sdf** file using, for example, a Fortran program which calls **vsxynt**:

```
einstein% pwd
/usr2/people/phy329/fd/new_wave

einstein% ls
Makefile   gpwave.f   vswave.f

einstein% make vswave
   f77 -g -n32 -c vswave.f
   f77 -g -n32 -L/usr/localn32/lib vswave.o -lp329f \
       -lsvs -lrnpl -lmfhdf -ldf -ljpeg -lz -lsv -lm -o vswave
ld32: WARNING 84: /usr/localn32/lib/libjpeg.a is not used for ...

einstein% vswave
 usage: vswave

einstein% vswave 101

einstein% ls *.sdf
wave.sdf
```

Then, once we have started the **scivis** server, we can send the data in this **.sdf** file to the server using the **sdftosv** command:

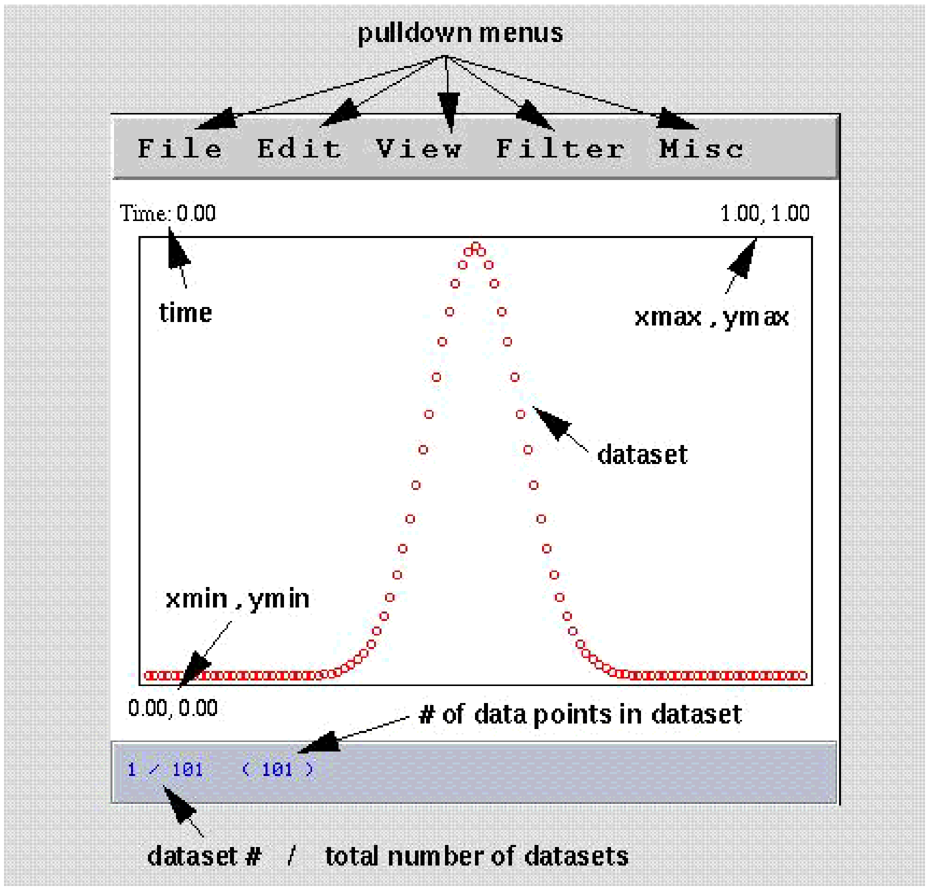
```
einstein% sdftosv wave
```

In a few seconds you should see a window such as the following pop-up:



Observe that the new window displays one time step (dataset) of the data at a time. Using the pull down menus and/or keyboard accelerators, you can step through the data, zoom-in or or, play (animate) the data, and perform many other functions, many of which are fairly self-explanatory.

Here is a guide to the annotations on the above **scivis** data window:



Note that the server's main function in the context of this course, is to provide you with a useful tool to develop and analyze programs which solve time-dependent partial differential equations (or time dependent particle motion in 2 dimensions). In particular, you should not expect to use it to produce ‘‘quality’’ hardcopy output.

scivis (jser) keyboard-accelerators

Important Note: *Due to a bug in SGI's implementation of Java, you must first RESIZE any window that* ***scivis*** *creates in order for the following keyboard accelerators to work. All accelerators are Ctrl-key based; for example,* ***C-a*** *means depress the* ***ctrl*** *key and then the* ***a*** *key (without releasing the* ***ctrl*** *key).*

Keystroke	Mnemonic	Function
C-q	Quit	Closes window
C-a	Animate	Starts animation
C-s	Stop	Stops animation
C-n	Next	Displays next dataset
C-p	Previous	Displays previous dataset
C-g	Goto	Goto specific dataset

sdftosv: Sends data in **.sdf** files to the **Scivis** server (also known as **jser**). Here is the full usage for the command

```
   % sdftosv
sdftosv version: 1.0
  Copyright (c) 1997 by Robert L. Marsa
  sends .sdf files to the scivis visualization server
Usage:
  sdftosv [ -i ivec ]
          [ -n oname ]
          [ -s ]
          input_file [ input_file [ ... ] ]

  -i ivec  -- use ivec (0 based) for output control
  -n oname -- name all data sets oname
  -s       -- send data sets one at a time
              useful for large or nonuniform data
  input_file is an .sdf file
```

*Beware that there is a command **sdftovs** which sends an **.sdf** file to a different server---if you get an error message such as*

```
  assign_Server: Could not communicate with einstein
  assign_Server: Ensure that server is running on einstein and/or
  assign_Server: check/reset value of environment variable VSHOST.
```

*you have typed **sdftovs** instead of **sdftosv**.*

A typical invocation will be:

```
   % ls
   wave.sdf

   % sdftosv wave
```

Note that you do not have to specify the **.sdf** extension explicitly.

If we wanted to send only every second time step of **wave.sdf** to the server we could use

```
   % sdftosv -i ’0-*/2’ wave
```

In this example, the construct

```
   0-*/2
```

is an example of an **index-vector** (or **ivec**), which is just a shorthand for a regular sequence of integers:

```
   min-max/step  ===>  min, min + step, min + 2 step, ... min + n step
```

where `n` is the largest integer such that

```
   min + n step <= max
```

Index 0 refers to the first time level of data stored in the file, and an asterisk (`*`) can be used in place of `min` and/or `max` to denote "first time-level" or "last time-level" respectively. When using `*` in an index-vector specfication, such as in the above example, be sure to enclose the index-vector in single quotes to inhibit the shell from interpreting `*` in its own special way.

---

libbbhutil.a: Fortran- and C-callable output utility routines written for the Binary Black Holes Grand Challenge Project. Available on SGIs and HPCF Cray machines. Postscript ‘‘man-style’’ documentation for the `C` routines is available here. Fortran routines have the same names (`gft_out_bbox` etc.) and can be either `call`ed, or invoked as `integer` functions. For output of 2- and 3-D arrays on uniform finite-difference meshes, the routines

```
      gft_out_bbox
```

should suffice. Here is a usage example:

```
      integer      nx,         ny
      parameter  ( nx = 65,    ny = 33 )

      real*8       gfcn(nx,ny)
      real*8       xmin,       xmax,     ymin,     ymax,
     &             time

      integer      shape(2),   rank
      real*8       bbox(4)
               .
               .
               .
c-------------------------------------------------------
c     'bbox' defines 'bounding box' of coords.
c     associated with the data:
c
c     bbox := ( xmin, xmax, ymin, ymax )
c-------------------------------------------------------
      bbox(1) = xmin
      bbox(2) = xmax
      bbox(3) = ymin
      bbox(4) = ymax

      rank = 2
      shape(1) = nx
      shape(2) = ny

      do it = 1 , nt
              .
              .
              .
c-------------------------------------------------------
c     The first (string) arg. to 'gft_out_bbox'
c     is stripped of non alphanumeric/underscore
c     characters (including punctuation) if necessary,
c     and then used as the 'stem' for a filename of
c     the form 'stem.sdf'.  All calls to 'gft_out_bbox'
c     with the same string result in output to the
c     same file.
c-------------------------------------------------------
         time = it * 1.0d0
         call gft_out_bbox('gfcn',time,shape,rank,
     &                     bbox,gfcn)
      end do
              .
              .
              .
```

The `gft_` routines use a *machine-independent* binary format; thus data output using `gft_out_bbox` on a Cray, for example, can be processed on an SGI. On the SGIs, 2- and 3-D data is best visualized using *IRIS Explorer*. A locally developed module, called **ReadSDF_GFT0**, is available for Explorer input of data written using the `gft_` routines. Here's an image of an Explorer map which uses this module.

IRIS Explorer: A powerful scientific visualization system available on the Center SGI machines, including `einstein`. *You need to be logged into `einstein` via the graphics console to use the software*. Complete documentation for the system is available via the *Online Books* selection of the pull-down *Help* menu which should appear in the "Toolchest" located in the upper right corner of the screen when you login. To use, simply type

```
      % explorer
```

Here are links to the IRIS Explorer Center and Postscript versions of the User's Guide with graphics and without graphics.

---

latex and **tex**: Available on SGIs. Scientific typesetting software. Converts `.tex` source files to `.dvi` files which can then be previewed using `xdvi`, or converted to postscript using `dvips`.

Typical usage:

```
   % ls
   document.tex

   % latex document.tex
   This is TeX, Version 3.14159 (C version 6.1)
   (document.tex
   LaTeX2e <1996/06/01>
   Hyphenation patterns for english, german, loaded.
            .
            .
            .
   No file document.aux.
   [1] (document.aux) )
   Output written on document.dvi (1 page, 696 bytes).
   Transcript written on document.log.

   % ls
   document.aux   document.dvi   document.log   document.tex
```

---

xdvi: X-application for previewing `.dvi` files (output from Latex-ing or tex-ing of `.tex` files). You don’t have to explicitly specify the `.dvi` extension.

Typical usage:

```
% ls
document.aux   document.dvi   document.log   document.tex

% xdvi document
```

---

dvips: Utility for converting `.dvi` files to postscript.

Typical usage:

```
% ls
document.aux   document.dvi   document.log   document.tex

% dvips document
Got a new papersize
This is dvips 5.58 Copyright 1986, 1994 Radical Eye Software
’ TeX output 1997.01.22:1442’ -> document.ps
. [1]

% ls
document.aux   document.dvi   document.log   document.ps    document.tex
```

---

pp2d: OpenGL/X Graphics program for animating two dimensional particle motion. Currently available *only* on Center for Relativity SGI machines, but should display on any workstation running X (and X-terms).

Typical usage (second form is for monochrome displays):

```
% nbody 2.0 0.01 < nbody_input | pp2d
% nbody 2.0 0.01 < nbody_input | pp2d -m
```

Help is available via

```
% pp2d -h
```

The source code, pp2d.c and pp2d.h, may be of interest to those of you interested in using OpenGL for graphics programming. Makefile for `pp2d`.

GLUT: OpenGL Utility Toolkit Programming Interface. Facilitates construction of OpenGL programs which manipulate windows, handle user-initiated events etc. Available PS documentation: Overview and Specification/Programmer’s Guide.

Typical usage (not all Mesa and X libraries will be required for all applications):

```
% cc -n32 -I/usr/local/include pp2d.c -L/usr/localn32/lib -lglut \
      -lMesaaux -lMesatk -lMesaGLU -lMesaGL -lXmu -lXi -lXext -lX11 \
      -lm -o pp2d
```