Computational Astrophysics I: Introduction and basic concepts

Helge Todt

Astrophysics
Institute of Physics and Astronomy
University of Potsdam

SoSe 2025, 17.3.2025

Aims and contents I

Recommended prerequisites:

- basic knowledge of programming, especially in C/C++ $\rightarrow$ e.g., "Tools for Astronomers"
- basic knowledge in astrophysics

How to get a certificate of attendance / 6 CP/LP/ECTS ($\hat{=}$ 4 semester periods per week):

- without mark, e.g., Master of Astrophysics, module PHY-765: Topics in Advanced Astrophysics (this module has in total 12 CP! and an oral exam at the end):

  $\rightarrow$ at least 1./3. of the points of the exercises

Attention!

PULS is strict: It is absolutely necessary to enroll for this lecture until **10.05.2025**!

- with a mark (other Master courses):
  little programming project at the end of the semester

Please note that the focus for this course is on the exercises!

Aims and contents II

Specialization track "Computational Astrophysics"

the regulations for obtaining the computational astrophysics specialization *certificate* are as follows:

1. Computational Astrophysics I (4 SWS, SoSe) :
   Computational Astrophysics: Introduction
   Computational Astrophysics: Basic Concepts
2. Computational Astrophysics II (3 SWS, WiSe)
   Advanced Computational Astrophysics: Concepts and Applications
3. Seminar Computational Astrophysics (2 SWS)
   Advanced Computational Astrophysics: Seminar
4. a 4th course of the computational curriculum, e.g.,
   Computational Astrophysics: Advanced Programming (2 SWS)

Aims and contents III

Aims & Contents of CA I:

- enhance existing basic knowledge in programming (C/C++)
- brief introduction to Fortran → relatively common in astrophysics
- work on astrophysical topics which require computer modeling:
  - solving ordinary differential equations

    → from the two-body problem to N-body simulations
    → stellar structure, the Lane-Emden equation
  - solving equations: linear algebra, root finding, data fitting
  - data analysis

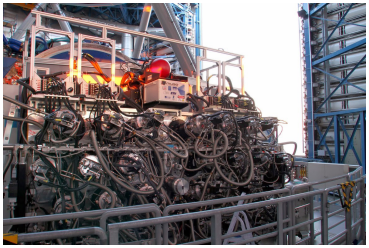
    → data analysis and simulations
  - simulation of physical processes

    → Monte-Carlo simulations and radiative transfer

\+ introduction to parallelization (e.g., OpenMP)

What are computers used for in astrophysics?

- control of instruments/telescopes/satellites:



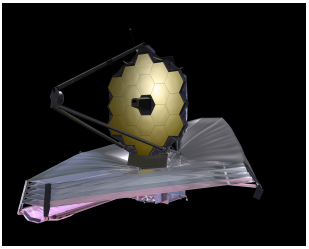
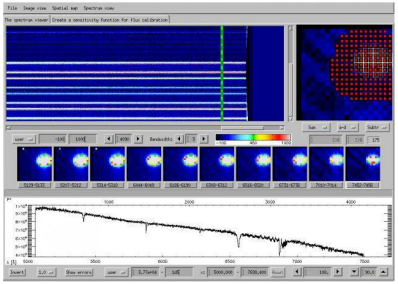
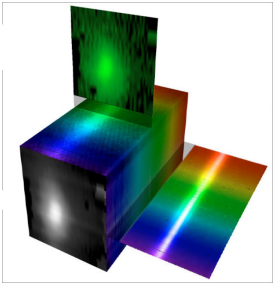


Figure: Multi Unit Spectroscopic Explorer (MUSE), Very Large Array (VLA), James Webb Space Telescope (JWST)

- data analysis / data reduction





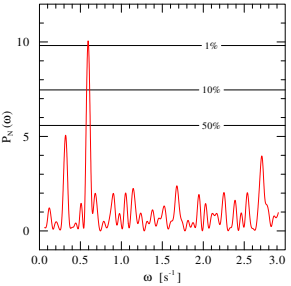
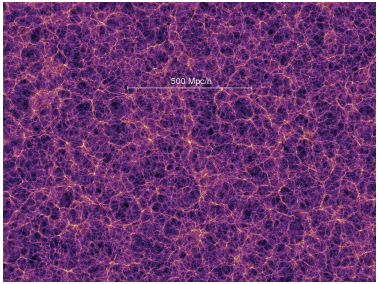
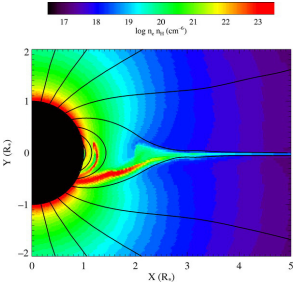


Figure: IDL, 3dCube / FITS, Fourier analysis

- modeling / numerical simulations





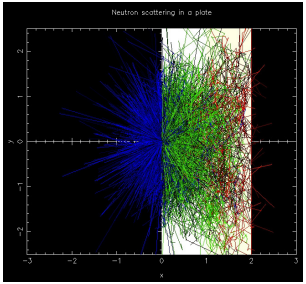


Figure: N-body simulation, hydrodynamics , Monte-Carlo

Conventions of used fonts

Meaning of the fonts / shapes

font/shape	meaning	example
`xvzf` (typewriter)	text to be entered literally (e.g., commands)	`man ls`
argument (italic)	place holder for own text	`file` *myfile*

The computer lab I

User accounts

useful for the lecture: your own account for this computer lab
(room 0.087 & 1.100)

Please, get your own account!
Sysad: Helge Todt, room 2.004

Guest account

$\rightarrow$ see left-hand side whiteboard
only valid per computer and in room 0.087

Attention: Unix/Linux is case sensitive!
Hint: You can choose the session type (e.g., Xfce, IceWM) at login screen.

The computer lab II

Security advice

As soon as you got your own account:

`passwd` Change the user password

(Enter the command in a terminal, Xterm, Konsole, or similar.)

Change your initial NIS password(!) to a strong password, use

- at least 9 characters, comprising of:
- capital AND lowercase letters, but not single words
- AND numbers
- AND special characters (Attention! Mind the keyboard layout!)

e.g., `$cPhT-25@comP2` or `tea4Pollen+Ahead`
But: prefer length over complexity!

The initial password expires after 14 days.

The computer lab III

Computers:

- 17 *NFS*[1] mounted Linux computers (openSUSE 15.4/15.5), several Intel Core i7-2600K, i7-4770, i7-7700, i7-8700 + 1 Xeon Gold 6152 *44*-core compute server
- home server (∼`user`) always-on:
  - bell
  - mahler
  - weber

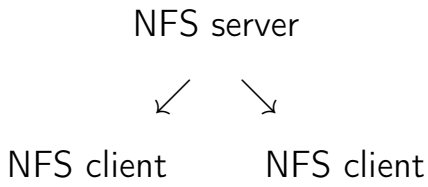
room 0.087:

- only for lectures
- Please, do not eat or drink in this room.

student's computer lab in room 1.100:

- open during the day
- b/w printer (500 pages / semester) and color printer (100 pages / semester)

NFS home directories



NFS server: provides (home) directories (physical on disk)

NFS clients: mount NFS (home) directories in their root directory

As also other users might have their home directory on your computer

Never switch off the computers!

Linux

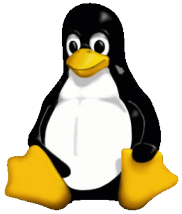
Operating system

Linux is a derivative of the operating system UNIX. It is a multi-user and multitasking operating system.

It was written in 1991 as a UNIX for PCs, now available for (almost) every platform, e.g., as Android or in Wireless routers and under permanent development.

Linux is ...

- for free
- open source (program code can also be modified)
- the combination of a *monolithic*[1] kernel and (GNU) software
- dominant in supercomputers (more than 90%)



[1] i.e., kernel contains also hardware driver

Important X-Window based environments under Linux: GNOME and KDE,
here: Xfce

Desktop environment (session type) can be chosen during local login, e.g., Xfce (nice) or IceWM (simple)

Desktop environment $\neq$ Linux

Desktop environment:	KDE	Xfce	GNOME	...
Linux distributions:	Ubuntu (Debian)		openSUSE	...

Important tools/programs

xterm or terminal: input of Linux shell commands, e.g., `cd`, `ls`

emacs or kate: editor for ASCII text files, e.g., `hello.cpp`

g++ or gfortran: gcc compilers, e.g., `g++ -o hello hello.cpp`

Shell and shell commands

Shell and shell commands I

Unix provides by the *shell* (command line) an extremely powerful tool. Within the shell Unix commands are executed.

Unix command syntax

`command [-option] [argument] <ENTER>`

Attention! Mind the blanks!

Open an xterm or similar terminal/console and enter following: (finish each line with <ENTER>):

```
echo hello
```

and

```
echo -n hello
```

What's the difference?

Tip 1:

Command history

By ↑ (arrow key up) you can repeat the last commands entered in the shell.

A list of the last commands can be shown via the command

```
history
```

Tip2:

Moreover, you can save typing by using the TAB key, it completes commands or file names:

`ech` TAB is completed to `echo`

Copying text with the mouse

Tip 3:
Linux: Copy by Selection

mark the text with the mouse:

press left mouse button, keep it pressed

move mouse cursor until end of the region you want to mark

$\rightarrow$ marked region will be highlighted

marked text was copied to the *clipboard*

paste the copied text:

move cursor to the intended position

press the middle(!) mouse button (or wheel)

$\rightarrow$ the previously copied text was inserted

Directories

The filesystem tree

```
/
|
|-- /home/
|      |
|      |-- /home/weber/
|             |
|             |--/home/weber/htodt/
|
|
|-- /etc/
|
|
|-- /dev/
```

→ root of the FS tree

→ Home directories

→ Homes on weber

→ Helge's home

→ et cetera (config)

→ devices

Navigation through directories I

`pwd`	shows the current directory path (absolute) e.g., `/home/weber/htodt`
`cd` *name*	change to directory *name*
`.`	means the current directory
`..`	the parent directory, e.g., `cd ..`
/	root of the FS tree
~	the home directory, e.g., `cd ~` or just `cd`
~*user*	the home directory of *user*

Navigation through directories II

`mkdir` *name*	create directory *name*
`rmdir` *name*	remove directory *name*
`ls`	show (list) the content of the directory

Navigation through directories III

`ls` show the content of the current directory

`ls -a` also show hidden files (starting with a `.`)

`ls -l` show the file attributes, owner, creation time

File attributes

```
drwxr-xr-x  2 htodt users    4096 14. Oct 13:35 Documents
```

`d` = directory `r` = readable
`w` = writeable `x` = executable
`htodt` = owner `users` = group
`4096` = size in byte `14. Oct 13:35` = creation time
`Documents` = name of the file (here: of the directory)

Hint: `ls -lc` → time of last modification ; `ls -lu` → time of last access

Navigation through directories IV

`man ls`	Manual pages (help for the command ls)
`info ls`	Info pages (alternative help for the command ls)
`ls --help`	Help for the command ls
`ls --help | less`	if more than one screen page

man page navigation – also `less`, `more`

`q`	quit		
`<SPACE>`	next page	`b`	previous page
`/`	forward search	`?`	backward search
`n`	next occurrence	`N`	previous occurrence
`>`	jump to the end	`<`	jump to the beginning

→ to create pure ASCII files (e.g., as input for g++)

`emacs` *file* `&`

Starting programs in background:

The ampersand & at the end of a command let the command run in the background (bg) of the shell.

Hence, the input line of the shell can be still used.

If forgotten: <CTRL>+z followed by bg <ENTER>.

The text editor emacs

`emacs` available on almost every system (must be installed),
window- or terminal-based (`emacs -nw`)

`<STRG>` + `x` `<STRG>` + `c`	close (quit/exit)
`<STRG>` + `x` `<STRG>` + `s`	save
`<STRG>` + `k`	kill (cut, from cursor to end of line)
`<STRG>` + `y`	yank (paste)
`<STRG>` + `<SPACE>`	mark
`<STRG>` + `w`	cut marked region
`<ESC>` `w`	copy marked region
`<STRG>` + `a`	go to beginning of line
`<STRG>` + `e`	go to end of line

Files

Remark: In Linux almost everything is a file (also directories and devices, see `ls -l /dev/`).

`mv` *source target*	move (rename) files
`cp` *source target*	copy files
`rm` *file*	remove file
`rm -rf` *directory*	remove directory

Compress files and directories

`tar` *action archive files* — use *action* on *archive*

tar actions

`c`	create archive from file/directory
`x`	extract archive
`v`	show executed actions (verbose)
`z`	zipp archive
`t`	show content of archive
`f`	archive is a file (default: tape device)

Example: Untar a tarball

```
tar xvzf muCommander.tar.gz
```

Connecting to other hosts (computers)

Login on other hosts (computers) I

`hostname`

this command shows the name of the host you're currently logged in

Login on other hosts (computers) II

Connection to another host (*remote host*) under Linux/Unix with the *secure shell*, within the same domain (e.g., within the computer lab cluster)

`ssh` *host name*

After successful *login*, in the same terminal/window a shell is shown that runs on the remote host.

Login on other hosts (computers) III

The SecureSHell

Client-server system for establishing a secure connection (encrypted), login on the remote host (remote host = SSH server)

if SSH client and SSH server support X11:

```
ssh host name -Y
```

allows the SSH server to open a graphical window (e.g., for `evince` or `kate`) on the SSH client

Besides the interactive use of the SSH one can also just let a program run on the remote host via ssh:

```
ssh hostname "ls -l"
```

The connection will be automatically closed after program/command is finished.

Login on other hosts (computers) IV

Login from outside (e.g., from home):

```
ssh username@bell.stud.physik.uni-potsdam.de
```

There are SSH clients for Windows that are for free, e.g., PuTTY. Moreover, MobaXterm, Xming, X2Go (requires also installation on the server) or with help of the Windows Subsystem for Linux (requires the installation of Linux distribution) it is also possible to perform a graphical SSH login from Windows to Unix/Linux.

Hint:

With help of the graphical login you can, e.g., use Mathematica on the computer lab cluster at home.

Login on other hosts (computers) V

For login without password:

1. run `ssh-keygen` on the client, answer all question just with `<ENTER>`
2. add the resulting `~/.ssh/id_rsa.pub` from the client host to `~/.ssh/authorized_keys` on the *remote host*

Remote copy I

With help of the SSH protocol it is also possible to transfer files between different computers:

`scp` *document.txt* *username@bell.stud.physik.uni-potsdam.de:*
: secure copy to the remote host

`scp` *username@bell.stud.physik.uni-potsdam.de:document.txt* **.**
: secure copy from the remote host (mind the dot!)

After the colon `:` is a path given, either absolute or relative to the home directory

Remote copy II

To copy only files that have been modified (comparison of source and target):

`rsync -rtvz` *username@host.domain:directory/* `.`

secure copy from the remote host, only modified files

some useful options:

`-r`	recursive: also directories
`-t`	time: keep time stamps of transferred files
`-v`	verbose: print information during transfer
`-z`	zip: compressed file transfer (faster for slow connections)
`-c`	checksum: use check sums (instead of time stamps) for comparison

Copy files via `konqueror` from other hosts

`konqueror` allows to show directories of remote hosts with help of the `fish` protocol. So, enter in the address bar, e.g.,

```
fish://user@weber.stud.physik.uni-potsdam.de
```

More Unix commands

`df -h`	shows free space on hard drive
`du -hs`	shows total size of current directory
`ps ux`	shows running processes of the current user
`top`	shows load and running processes (interactive)
`htop`	
`kill -9` *PID*	"kills" the process with the given process ID (PID)

Computing jobs on the stud cluster I

The ressources of the stud cluster (CPUs, RAM, disk space) can be used by all users, the users share these ressources.

→ Therefore, please, think of other users:

- Log out, when leaving the computer, do not just lock the screen. Never switch off/shutdown the computer.
- Have an eye on the disk usage of you home directory (see below), delete regularly data that are no longer required.
- If you intend to start a job that will run a bit longer, then *nice* this job (see below).

Nice and renice jobs/processes

The command `top` shows the priority and the consumption of ressources of running processes:

```
  PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
26054 htodt     39  19 1103308 179636   8648 R 100,0 0,552   0:28.93 53_steal.exe
14763 htodt     20   0 1749032 358808  74328 S 3,322 1,102  12:23.34 Xvnc
```

Jobs that might run longer than just a few minutes and put some load on the CPU, should be niced when started, e.g.:

`nice -19 ./53_steal.exe`

→ The priority is decreased from 20 (default) by 19 to 39 (higher values mean actually lower priority).

A job can also be niced when already running with help of `renice` and the process ID (PID), e.g.:

`renice +19 26054`

The program `top` in its interactive mode can also renice a process by pressing the key `r`.

Checking disk space

The command `df -hT` shows an overview of the available and used disk space on the current host:

```
weber/htodt> df -hT
Filesystem          Type      Size    Used Avail  Use% Mounted on
/dev/sdb1           xfs       3,7T    981G  2,7T   27% /home
bell:/home/bell     nfs4      1,8T    1,1T  702G   60% /nfs/bell
```

Moreover, the command `du -hs ~` displays the disk usage of your own home directory.

```
weber/htodt> du -hs ~
30G /home/weber/htodt
```

Instead of the tilde ~ you can also use other (own) subdirectories as an argument, to check their disk usage.

→ If a disk shows a use of 100%, you cannot longer write on this disk or copy data to it.

Computing jobs on the stud cluster IV

Show CPU performance

The type, its parameters, and its current clock rate(s) of the installed CPU are shown in the file `/proc/cpuinfo`, which you can read with help of `cat` or `less` (info is duplicated for each thread/logical core):

```
weber/htodt>cat /proc/cpuinfo
model name      : Intel(R) Core(TM) i7-4770 CPU @ 3.40GHz
cpu MHz         : 3491.946
```

The number of logical cores/threads (= either number of physical cores or number of physical cores $\times 2$ for Hyperthreading) can be also seen in the program `top`, if you press the key $\boxed{1}$.

Show available RAM

The command `free -h` shows the amount of free/available RAM:

```
weber/htodt> free -h
              total        used        free      shared  buff/cache   available
Mem:          187Gi        66Gi        51Gi       3,2Gi        69Gi       116Gi
```