ECOL 553L

Introduction to Formats, UNIX, and VIM

File Formats and Introduction to Unix

- “Today”s Topics:
  - Sequence File Formats
  - Unix Intro
    - Basic Commands
    - SSH
  - VIM (file editing)

A note about grades

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- The Syllabus has been on the (now down) server, is now temporarily at http://www.cs.arizona.edu/~deblasio/ECOL553/

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- Lab Grades:

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- Lab Grades:
  - Homework 40%

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    - Homework 40%
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  - Homework 40%
  - Quizzes 50%
  - Class Participation 10%
  - (lowest quiz grade and lowest homework grade dropped)

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  - This week is an exception

The Taxonomy of (Biological) File Formats

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- Raw Data

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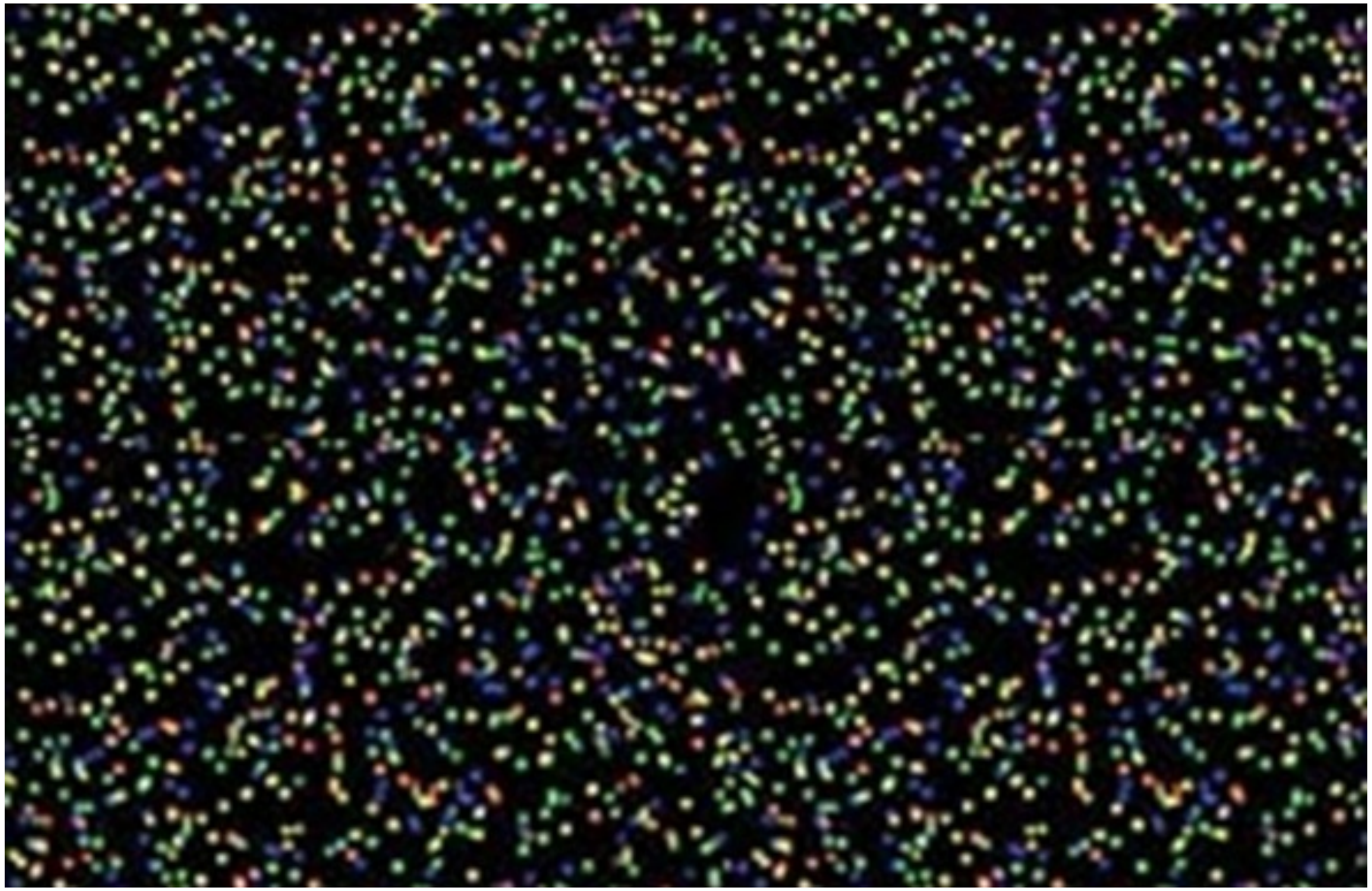
- Raw Data
  - sequencer images (think back to what Dr. Barker was talking about last week)



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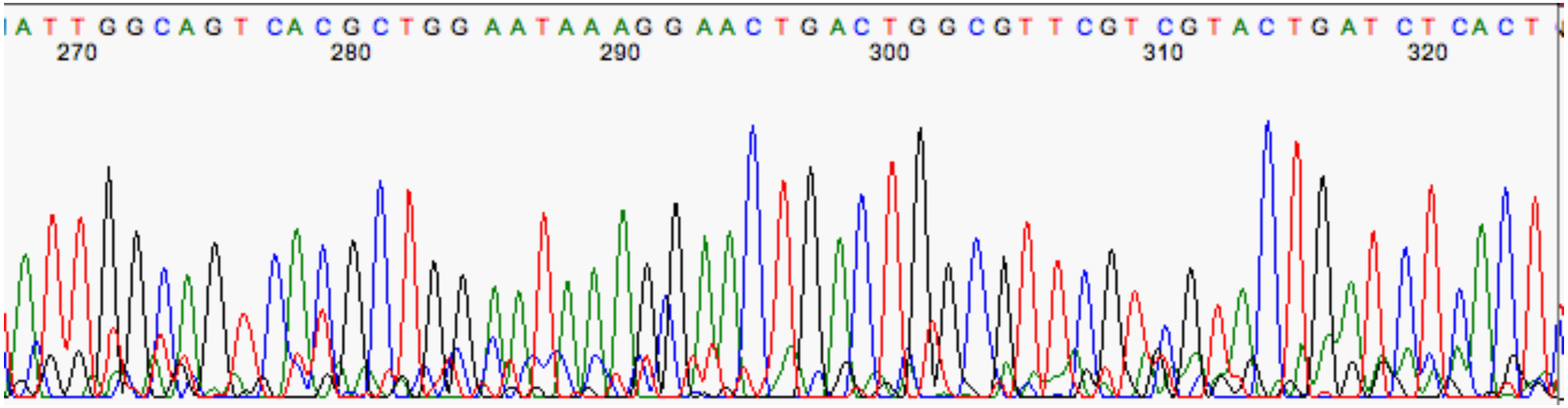

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  - chromatograph data
- Sequence Data

The Taxonomy of (Biological) File Formats

- Raw Data

```
>gi|5524211|gb|AAD44166.1| cytochrome b [Elephas maximus maximus]
LCLYTHIGRNIYYGSYLYSETWNTGIMLLLITMATAFMGYVLPWGQMSFWGATVITNLFSAIPYIGTNLV
EWIWGGFSVDKATLNRFFAFHFILPFTMVALAGVHLTFLHETGSNNPLGLTSDSDKIPFHPYYTIKDFLG
LLILILLLLLLALLSPDMLGDPDNHMPADPLNTPLHIKPEWYFLFAYAILRSVPNKLGGVLALFLSIVIL
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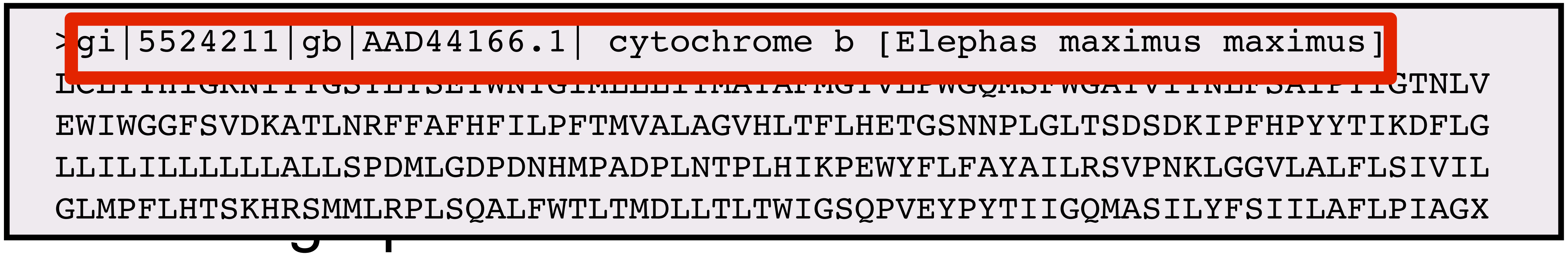

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  - 3 major components
    - sequence (nucleotide, amino acid, structure, quality...)
    - label (identifier, name)
    - meta-data [optional] (location, publication, species...)

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- Sequence Data
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```

Sometimes programs trim the name of sequences! Be Careful!

The Taxonomy of (Biological) File Formats

- Sequence Data
  - Fasta
  - Clustal

```
CLUSTAL W (1.82) multiple sequence alignment


FOSB_MOUSE      MFQAFPGDYDSGSRCSSSPSAESQYLSSVDSFGSPPTAAASQECAGLGEMPGSFVPTVTA 60
FOSB_HUMAN      MFQAFPGDYDSGSRCSSSPSAESQYLSSVDSFGSPPTAAASQECAGLGEMPGSFVPTVTA 60
                ************************************************************

FOSB_MOUSE      ITTSQDLQWLVQPTLISSMAQSQGQPLASQPPAVDPYDMPGTSYSTPGLSAYSTGGASGS 120
FOSB_HUMAN      ITTSQDLQWLVQPTLISSMAQSQGQPLASQPPVVDPYDMPGTSYSTPGMSGYSSGGASGS 120
                ********************************.***************:*.**:******

FOSB_MOUSE      GGPSTSTTTSGPVSARPARARPRRPREETLTPEEEEKRRVRRERNKLAAAKCRNRRRELT 180
FOSB_HUMAN      GGPSTSGTTSGPGPARPARARPRRPREETLTPEEEEKRRVRRERNKLAAAKCRNRRRELT 180
                ****** ***** .**********************************************

FOSB_MOUSE      DRLQAETDQLEEEKAELESEIAELQKEKERLEFVLVAHKPGCKIPYEEGPGPGPLAEVRD 240
FOSB_HUMAN      DRLQAETDQLEEEKAELESEIAELQKEKERLEFVLVAHKPGCKIPYEEGPGPGPLAEVRD 240
                ************************************************************

FOSB_MOUSE      LPGSTSAKEDGFGWLLPPPPPPPLPFQSSRDAPPNLTASLFTHSEVQVLGDPFPVVSPSY 300
FOSB_HUMAN      LPGSAPAKEDGFSWLLPPPPPPPLPFQTSQDAPPNLTASLFTHSEVQVLGDPFPVVNPSY 300
                ****:.******.**************:*:**************************.***

FOSB_MOUSE      TSSFVLTCPEVSAFAGAQRTSGSEQPSDPLNSPSLLAL 338
FOSB_HUMAN      TSSFVLTCPEVSAFAGAQRTSGSDQPSDPLNSPSLLAL 338
                ***********************:**************
```

The Taxonomy of (Biological) File Formats

- Sequence Data
  - Fasta
  - Clustal
  - GenBank

```
LOCUS       AB000263                368 bp    mRNA    linear   PRI 05-
FEB-1999
DEFINITION  Homo sapiens mRNA for prepro cortistatin like peptide, complete
            cds.
ACCESSION   AB000263
ORIGIN
        1 acaagatgcc attgtccccc ggcctcctgc tgctgctgct ctccggggcc acggccaccg
       61 ctgccctgcc cctggagggt ggccccaccg gccgagacag cgagcatatg caggaagcgg
      121 caggaataag gaaaagcagc ctcctgactt tcctcgcttg gtggtttgag tggacctccc
      181 aggccagtgc cgggcccctc ataggagagg aagctcggga ggtggccagg cggcaggaag
      241 gcgcaccccc ccagcaatcc gcgcgccggg acagaatgcc ctgcaggaac ttcttctgga
      301 agaccttctc ctcctgcaaa taaaacctca cccatgaatg ctcacgcaag tttaattaca
      361 gacctgaa
//
```

The Taxonomy of (Biological) File Formats

- Sequence Data
  - Fasta
  - Clustal
  - GenBank
  - SAM

```
@HD VN:1.3 SO:coordinate
@SQ SN:ref LN:45
r001 163 ref 7 30 8M2I4M1D3M = 37 39 TTAGATAAAGGATACTG *
r002 0 ref 9 30 3S6M1P1I4M * 0 0 AAAAGATAAGGATA *
r003 0 ref 9 30 5H6M * 0 0 AGCTAA * NM:i:1
r004 0 ref 16 30 6M14N5M * 0 0 ATAGCTTCAGC *
r003 16 ref 29 30 6H5M * 0 0 TAGGC * NM:i:0
r001 83 ref 37 30 9M = 7 -39 CAGCGCCAT *
```

The Taxonomy of (Biological) File Formats

- Sequence Data
  - Fasta
  - Clustal
  - GenBank
  - SAM
  - Variants

The Taxonomy of (Biological) File Formats

- Sequence Data
  - Fasta
  - Clustal
  - GenBank
  - SAM
  - Variants
    - FASTQ

```
@NCYC361-11a03.q1k bases 1 to 1576
GCGTGCCCGAAAAAATGCTTTTGGAGCCGCGCGTGAAAT...
+NCYC361-11a03.q1k bases 1 to 1576
!)))))****(((***%%((((*(((+,**(((+***+,-...
```

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- Sequence Data
  - Fasta
  - Clustal
  - GenBank
  - SAM
  - Variants
    - FASTQ
    - Anootated Fasta

```
# STOCKHOLM 1.0

AL929536.7/77590-77911     GGAUGUGAGGGCGAUCUGGCUGCGACAUCUGUCACCCCAUUGAUCGCUAG
M63671.1/163-492           GGAUGUGAGGGCGAUCUGGCUGCGACAUCUGUCACCCCAUUGAUCGCCAG
K02909.1/1-330             GGAUGUGAGG.CGAUCUGGCUGCGACAUCUGUCACCCUAUUGAUCGCCAG
X05490.1/245-574           GGAUGUGAGG.CGAUCUGGCUGCGACAUCUGUCACCCCAUUGAUCGCCAG
X04236.1/2-328             .GAUGUGAGGGCGAUCUGGCUGCGACAUCUGUCACCCCAUUGAUCGCCAG
X04992.1/244-574           GGAUGUGAGGGCGAUCUGGCUGCGACAUCUGUCACCCCAUUGAUCGCCAG
#=GC SS_cons               <<<.<<<<<<<.<<...<<....<<<<<<<<<<.<<<<<..<<<<<<<..
```

The Taxonomy of (Biological) File Formats

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- Viewing

The Taxonomy of (Biological) File Formats

- Viewing
  - Single Alignments

The Taxonomy of (Biological) File Formats

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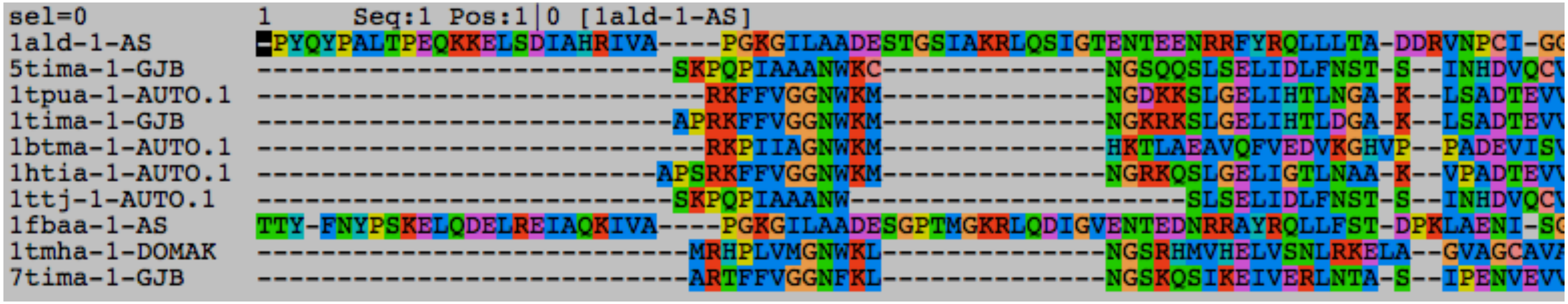
    - Seaview



```
sel=0           1     Seq:1 Pos:1|0 [1ald-1-AS]
1ald-1-AS       -PYQYPALTPEQKKELSDIAHRIVA----PGKGILAADESTGSIAKRLQSIGTENTEENRRFYRQLLLTA-DDRVNPCI-GG
5tima-1-GJB     --------------------------SKPQPIAAANWKC--------------NGSQQSLSELIDLFNST-S--INHDVQCV
1tpua-1-AUTO.1  ----------------------------RKFFVGGNWKM--------------NGDKKSLGELIHTLNGA-K--LSADTEVV
1tima-1-GJB     --------------------------APRKFFVGGNWKM--------------NGKRKSLGELIHTLDGA-K--LSADTEVV
1btma-1-AUTO.1  ----------------------------RKPIIAGNWKM--------------HKTLAEAVQFVEDVKGHVP--PADEVISV
1htia-1-AUTO.1  -------------------------APSRKFFVGGNWKM--------------NGRKQSLGELIGTLNAA-K--VPADTEVV
1ttj-1-AUTO.1   --------------------------SKPQPIAAANW---------------------SLSELIDLFNST-S--INHDVQCV
1fbaa-1-AS      TTY-FNYPSKELQDELREIAQKIVA----PGKGILAADESGPTMGKRLQDIGVENTEDNRRAYRQLLFST-DPKLAENI-SG
1tmha-1-DOMAK   ---------------------------MRHPLVMGNWKL--------------NGSRHMVHELVSNLRKELA--GVAGCAVA
7tima-1-GJB     ---------------------------ARTFFVGGNFKL--------------NGSKQSIKEIVERLNTA-S--IPENVEVV
```

The Taxonomy of (Biological) File Formats

- Viewing
  - Single Alignments
    - Seaview
    - ClustalW

The Taxonomy of (Biological) File Formats

- Viewing
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        - Seaview
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    - Genome Browsers

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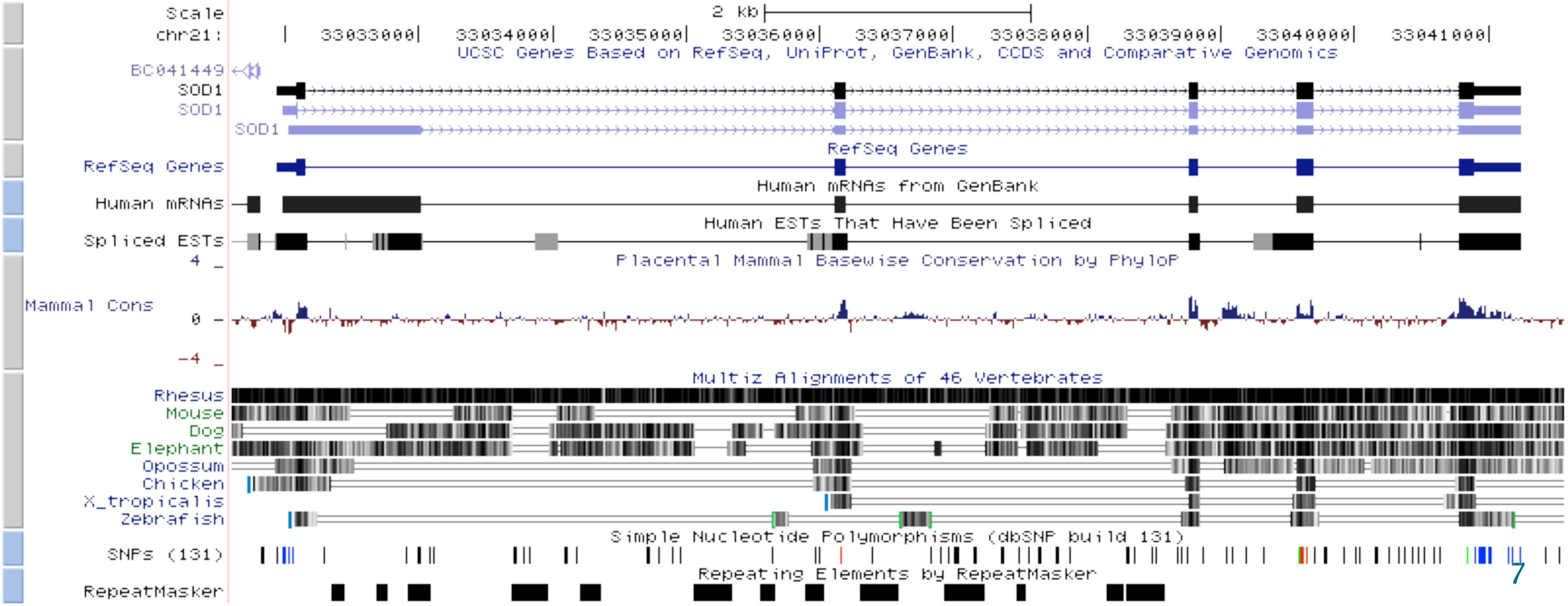
    - UCSC



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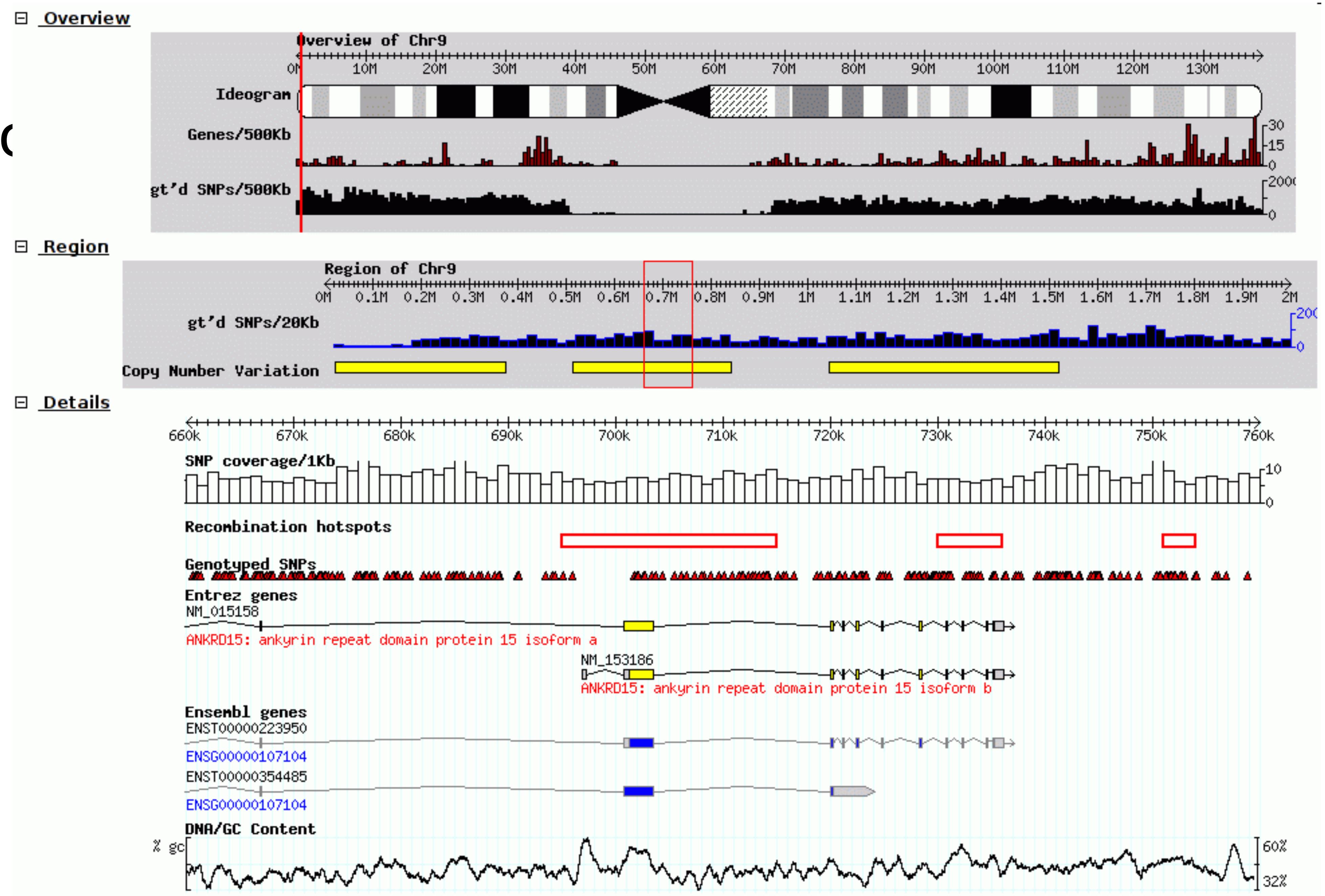

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Phylogeny File Formats

- NEWICK/NHX (phylip)
    - Rooted or unrooted tree representation

      `(A:0.1,B:0.2,(C:0.3,D:0.4):0.5);`
- Nexus (PAUP, MacClade, NDE)
    - Data/descriptor blocks plus analysis commands
    - http://www.paup.csit.fsu.edu/nfiles.html
- phyloXML (forester-atv)
    - Taxonomy, sequence, confidence, events
    - http://www.phyloxml.org/
    - http://sourceforge.net/projects/forester-atv/

- Format converter: http://www.phylogeny.fr/version2_cgi/data_converter.cgi

Converting Sequence File Formats

- http://hcv.lanl.gov/content/sequence/FORMAT_CONVERSION/form.html
  - Online tool for conversion
- http://mybio.wikia.com/wiki/Sequence_format_conversion
  - Links to conversion tools
- BioPerl (we'll use this later), BioPython, BioRuby, BioJava, …
- Galaxy (Penn State)
  - Tools, history, basic workflow, data libraries, sharing
  - Wiki and screencasts
  - http://galaxy.psu.edu/

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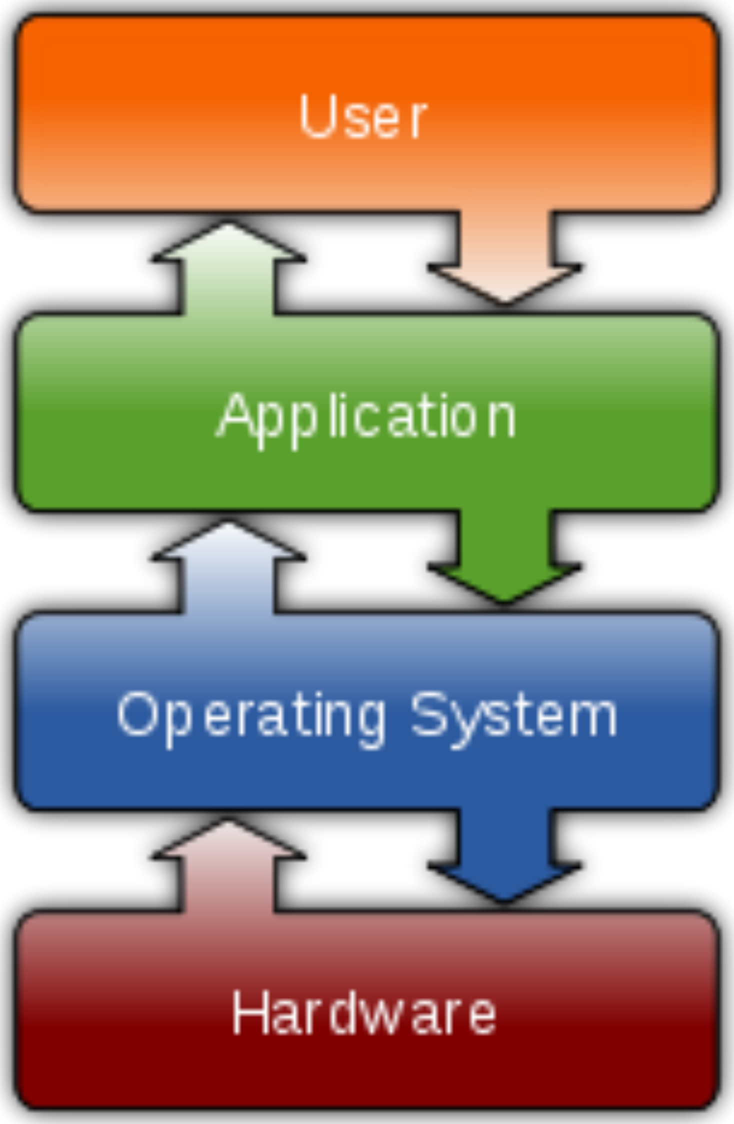
    - http://www.unixtools.com/tutorials.html

- There are some short Quicktime movies accessible from the UA Computer-Based Training Site (type UNIX in the 'Find a Course' box): http://uacbt.arizona.edu/default.htm
  - (you do not need to purchase these!)

- BCF Unix Tutorials: http://bcf.arl.arizona.edu
  - Follow the 'Site Navigation' and 'Resources' links

- Google is often a good method of finding helpful material.

What is Unix?



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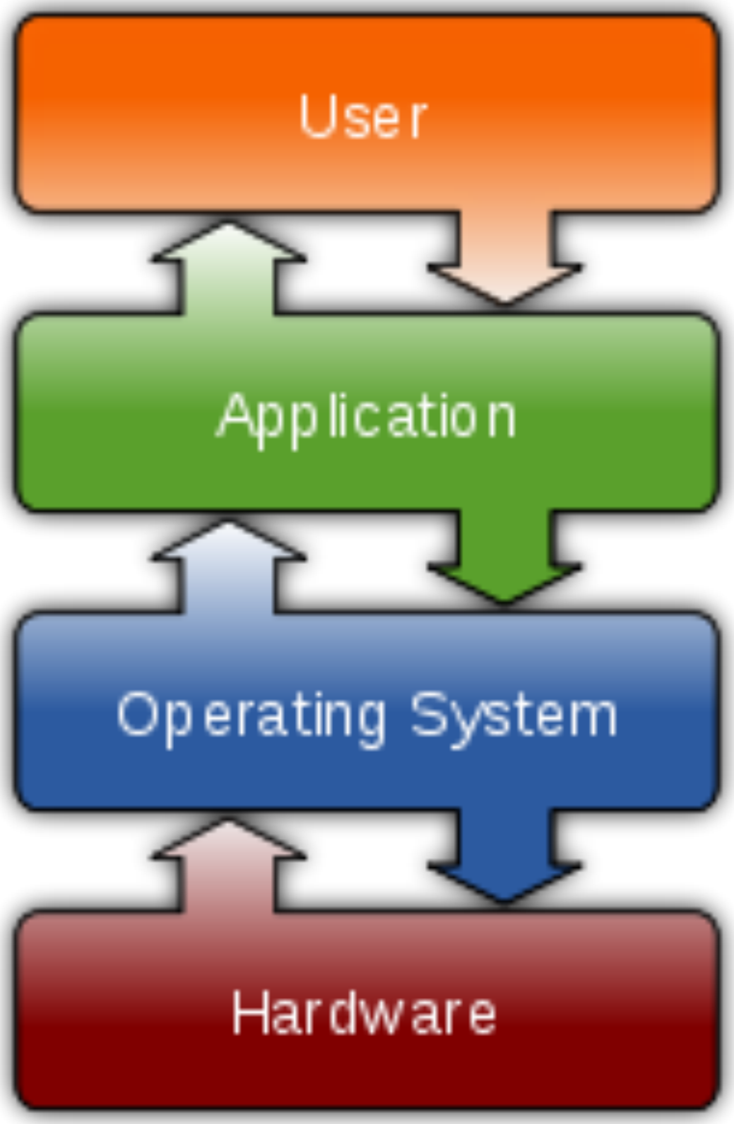

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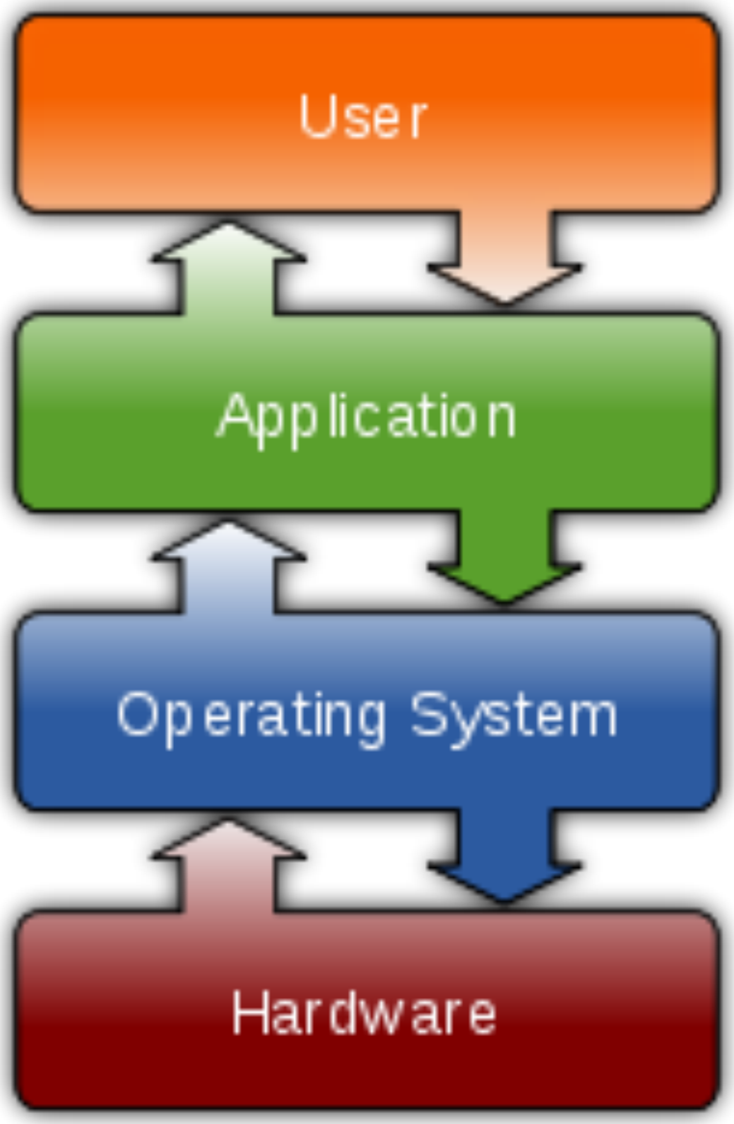

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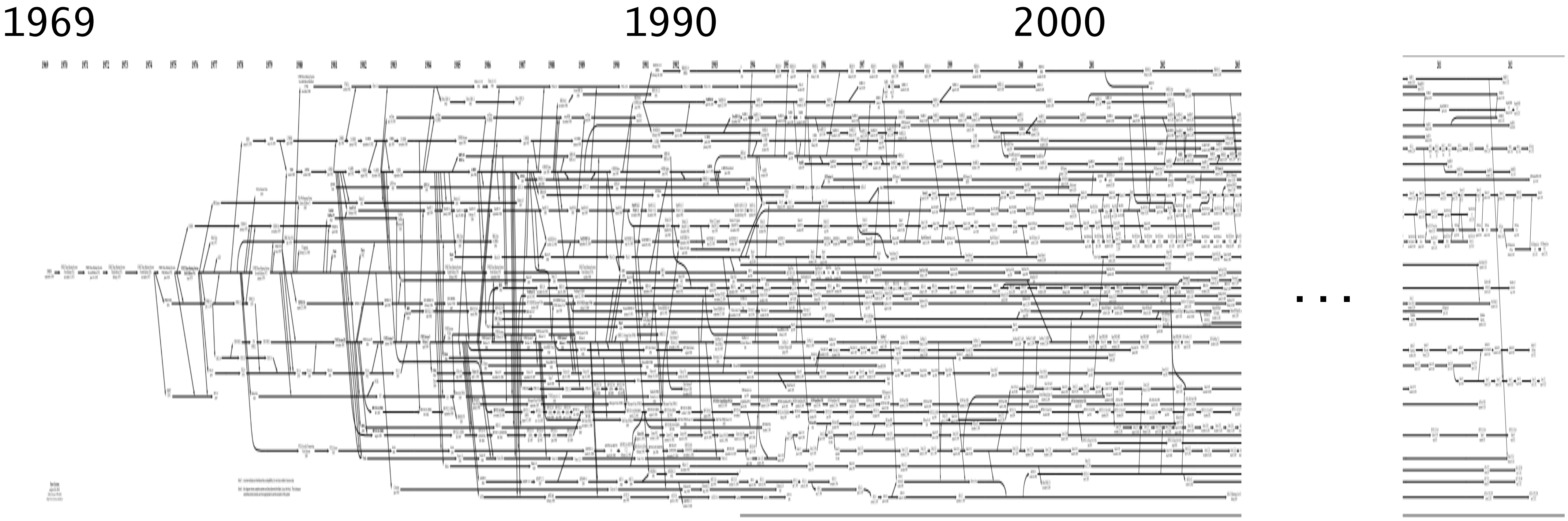

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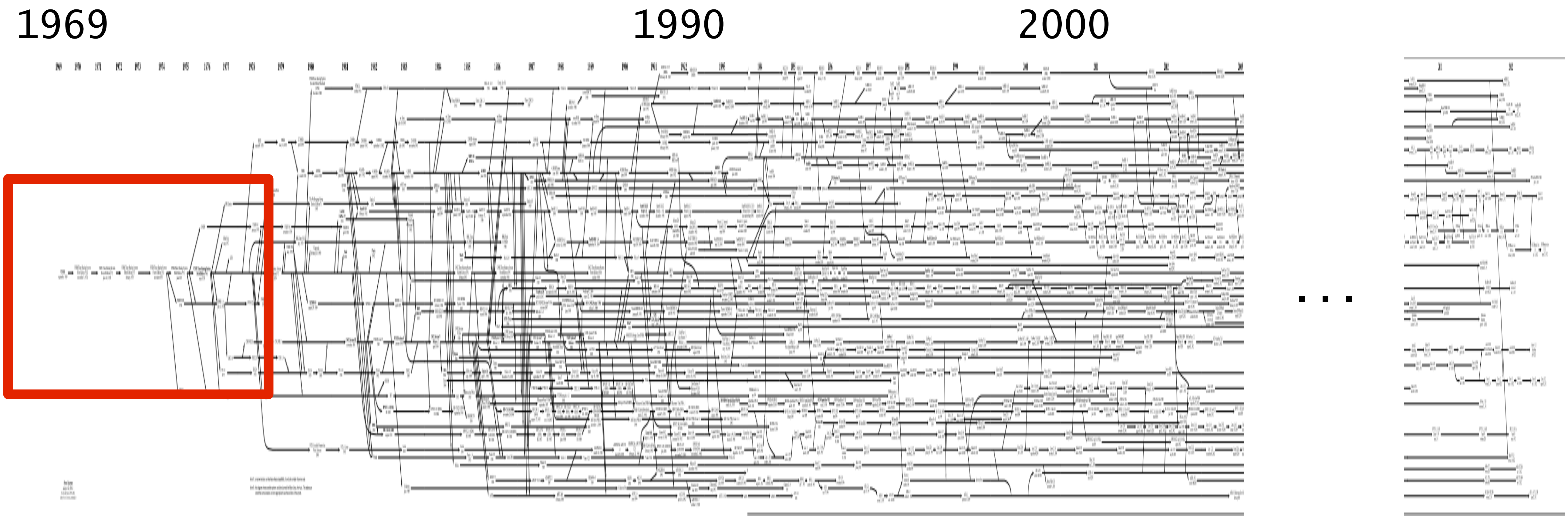

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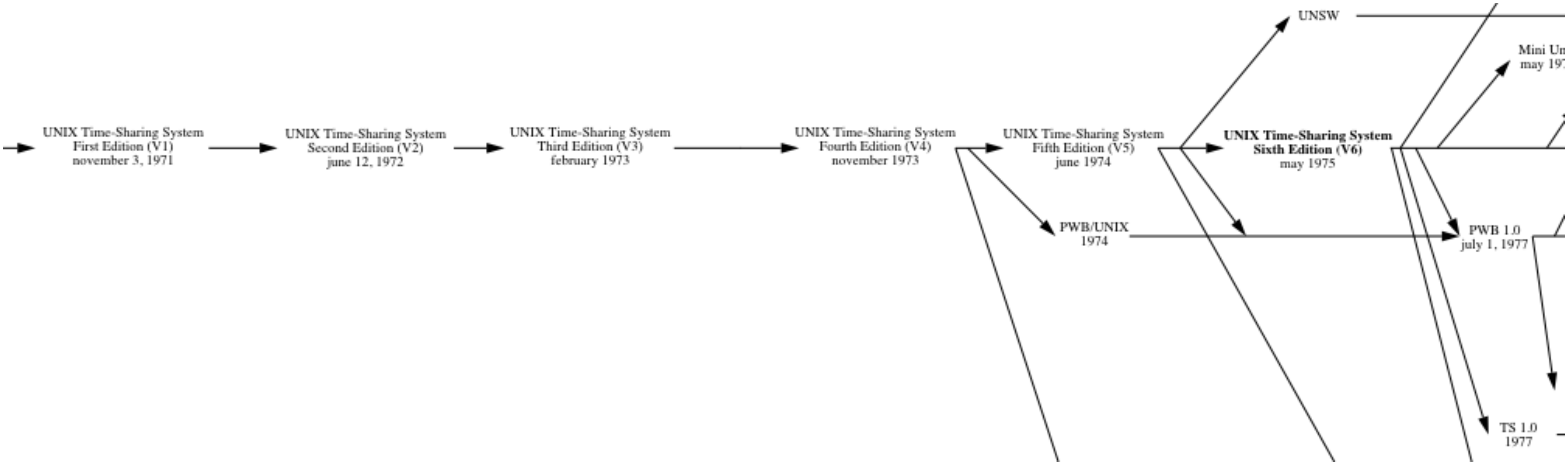

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First Edition (V1)
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Second Edition (V2)
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Fifth Edition (V5)
june 1974

PWB/UNIX
1974

UNSW

UNIX Time-Sharing System
Sixth Edition (V6)
may 1975

Mini Un
may 19

PWB 1.0
july 1, 1977

TS 1.0
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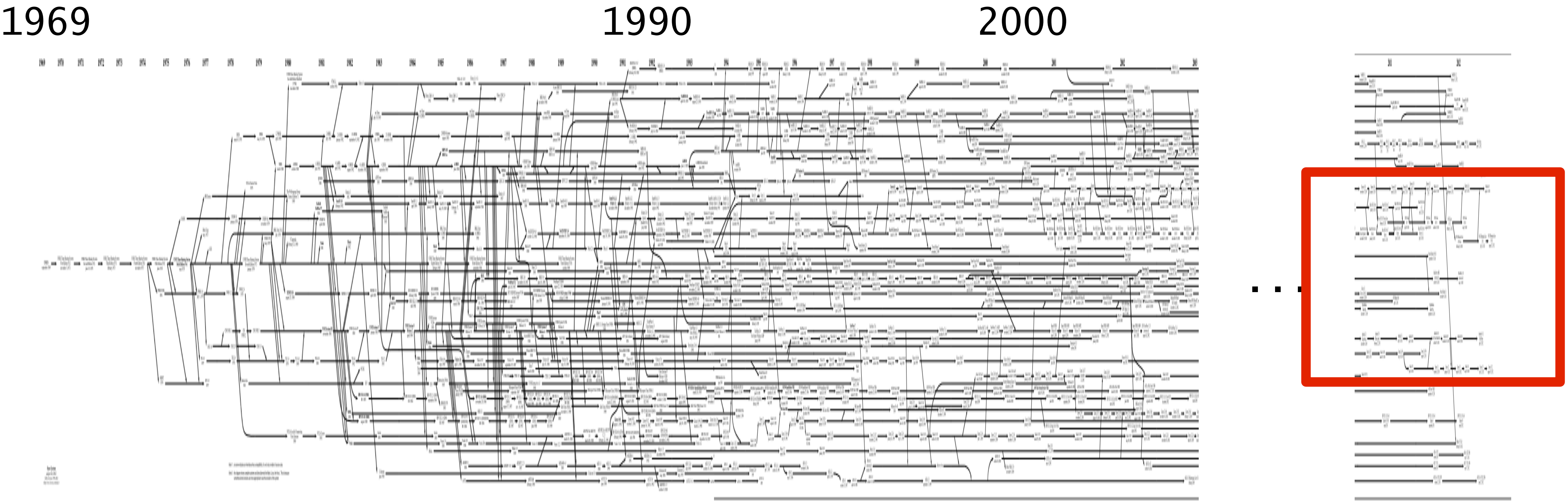

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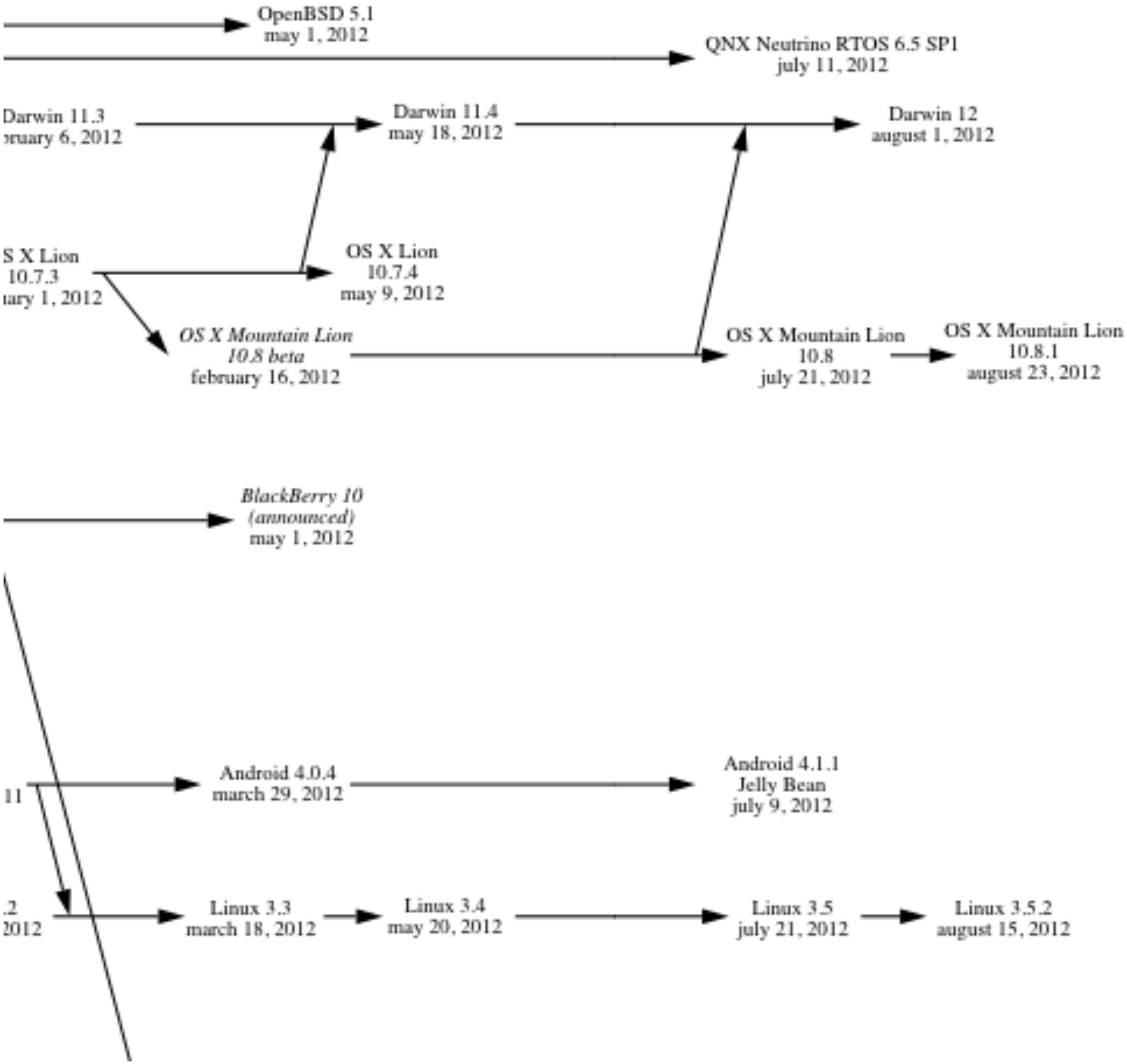
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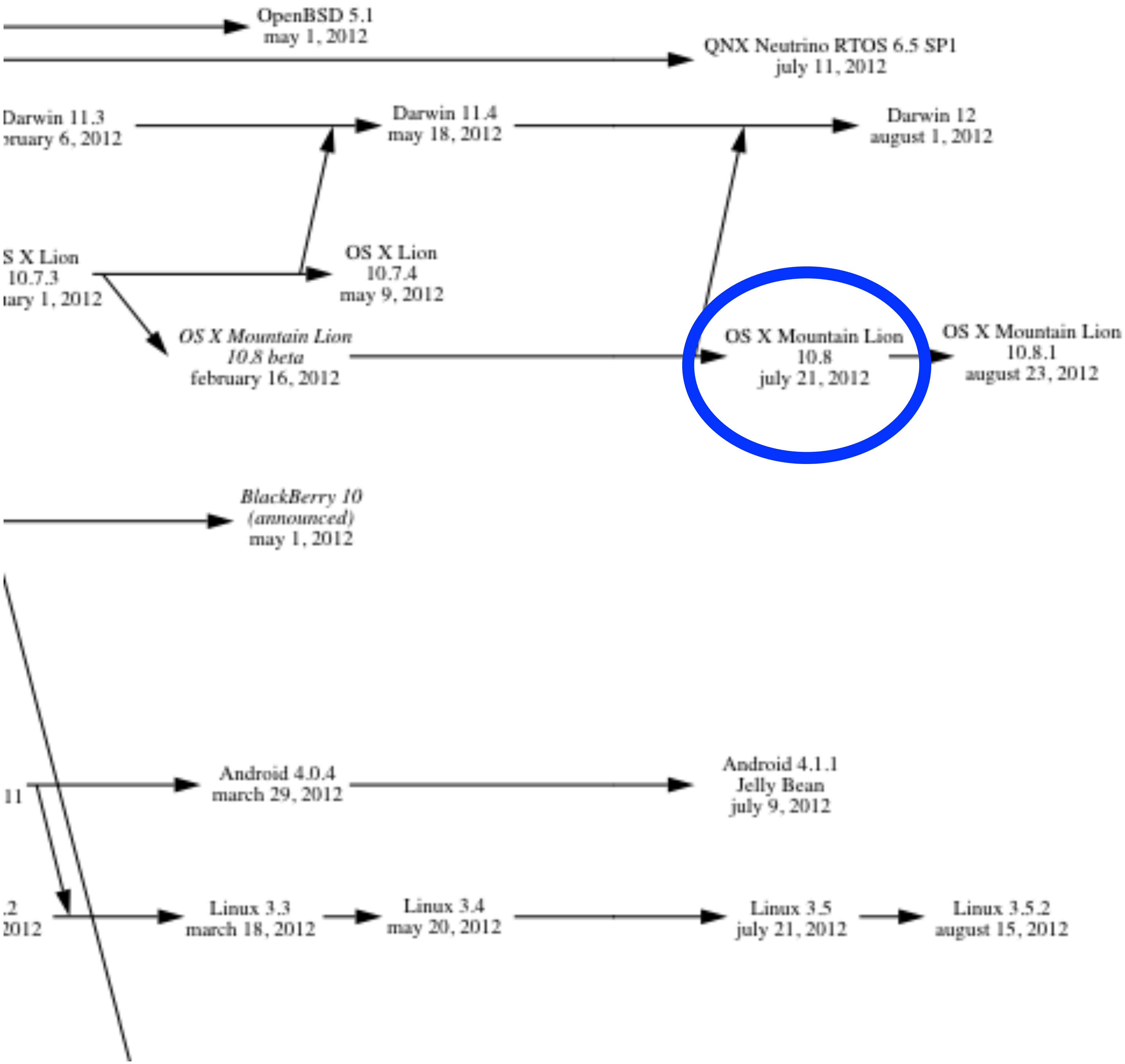

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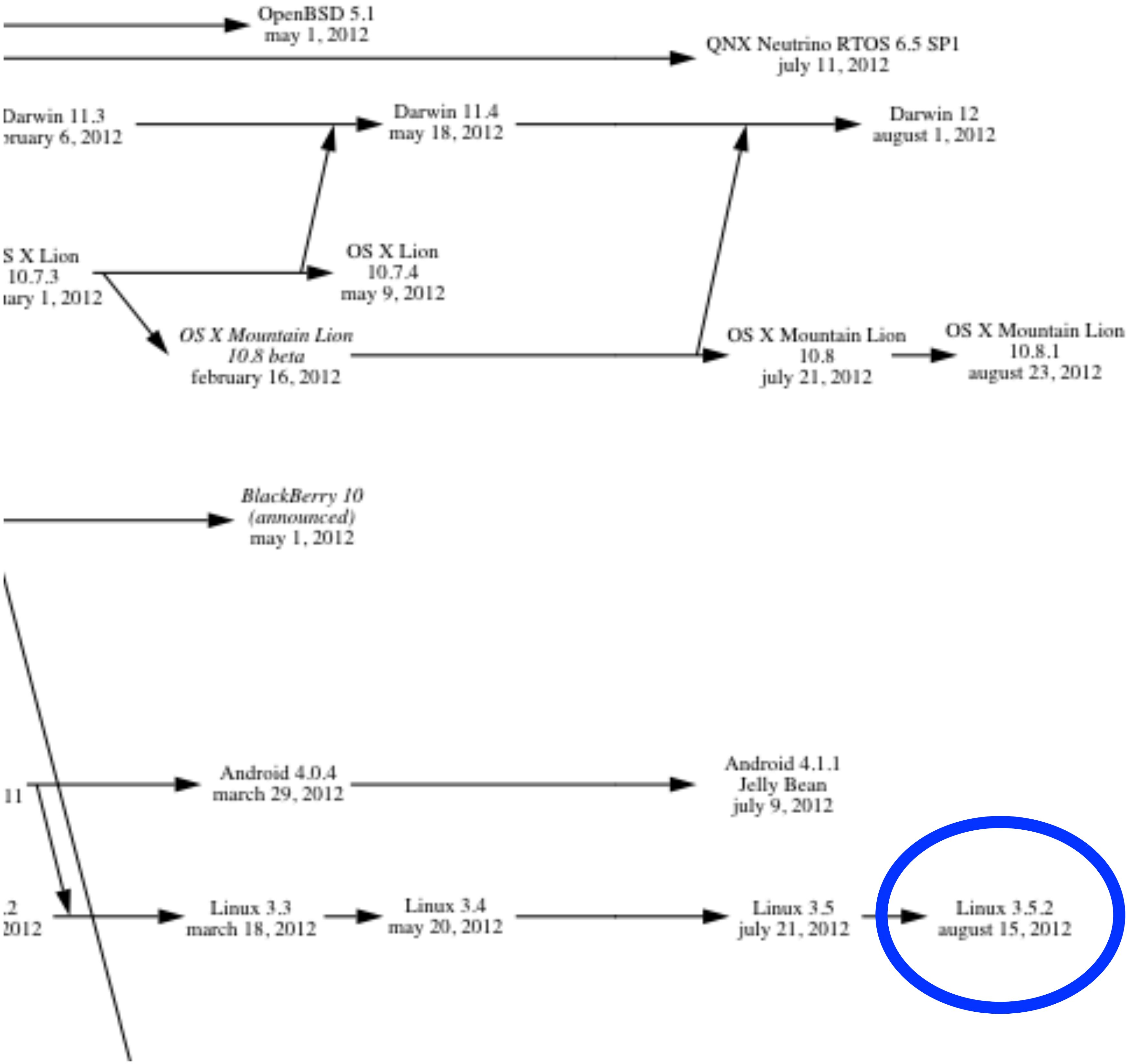
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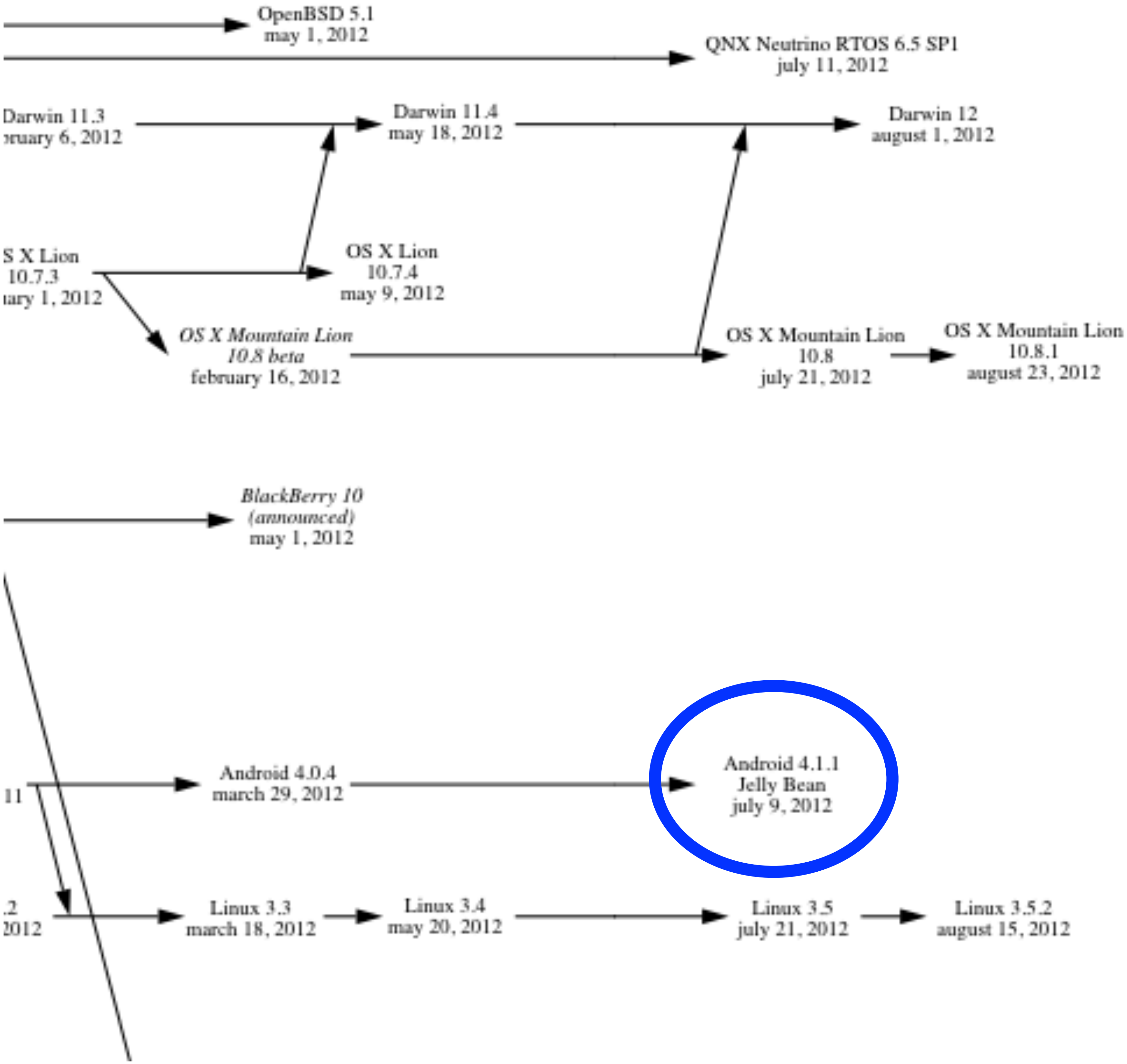

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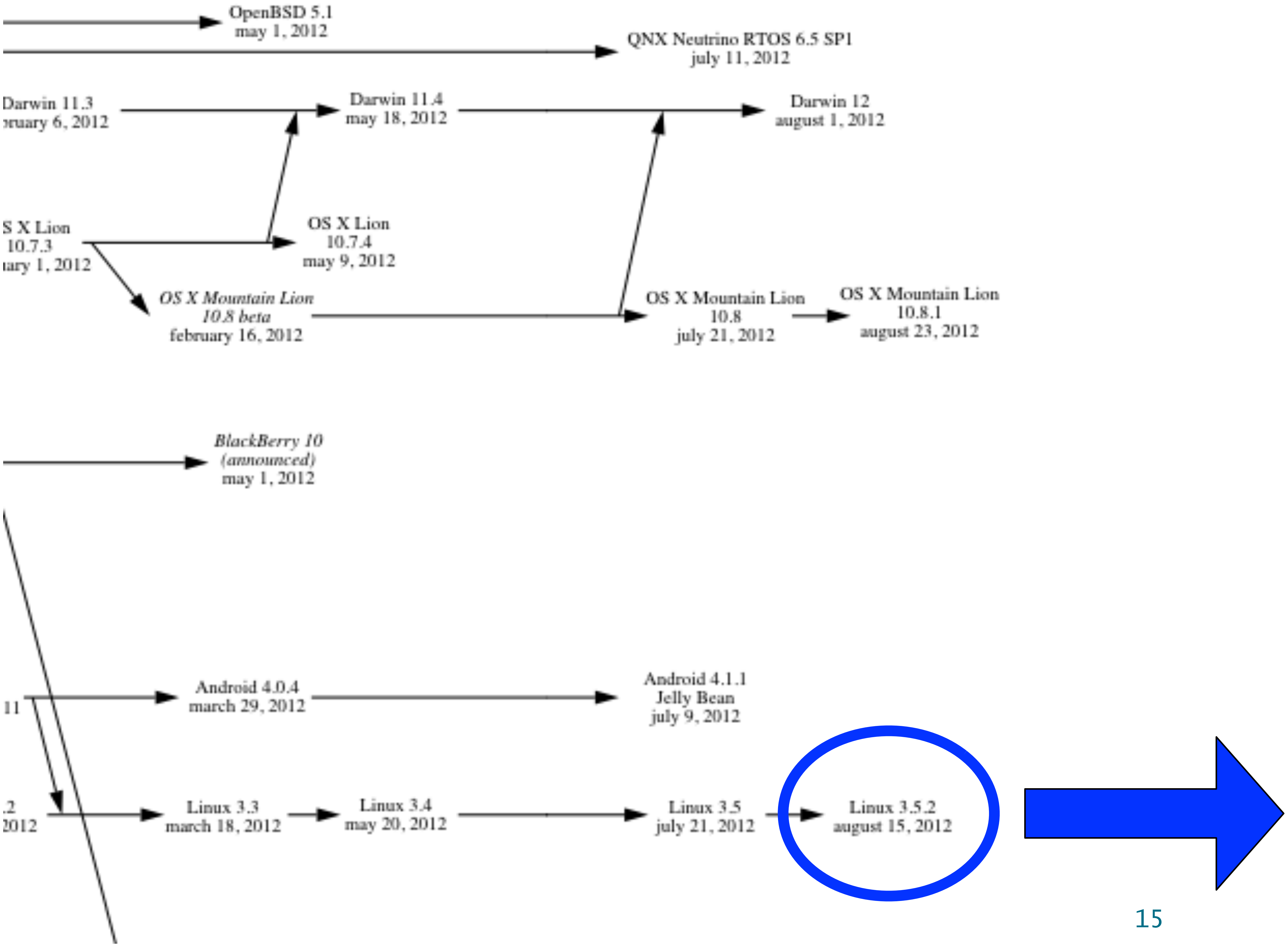
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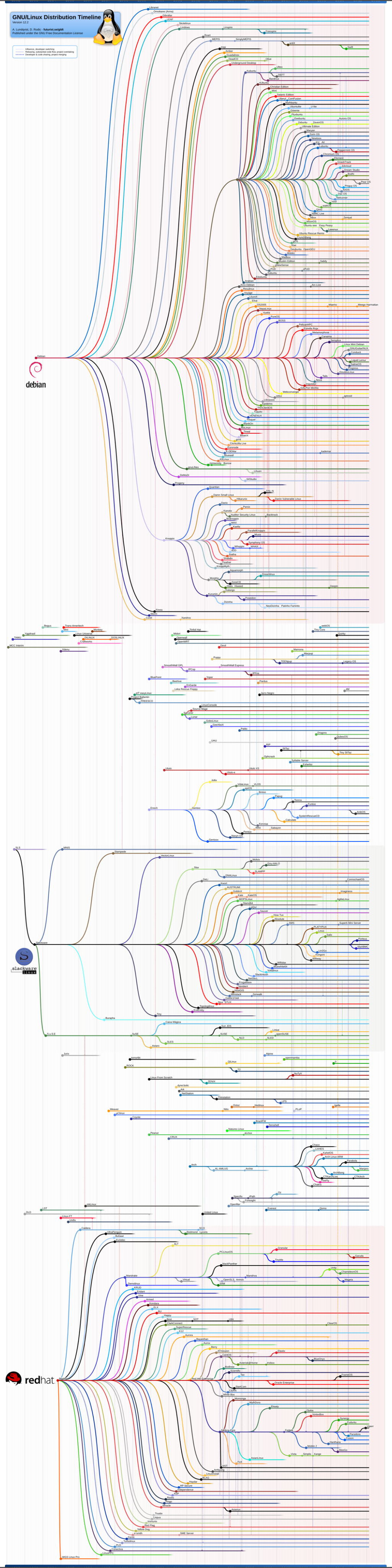
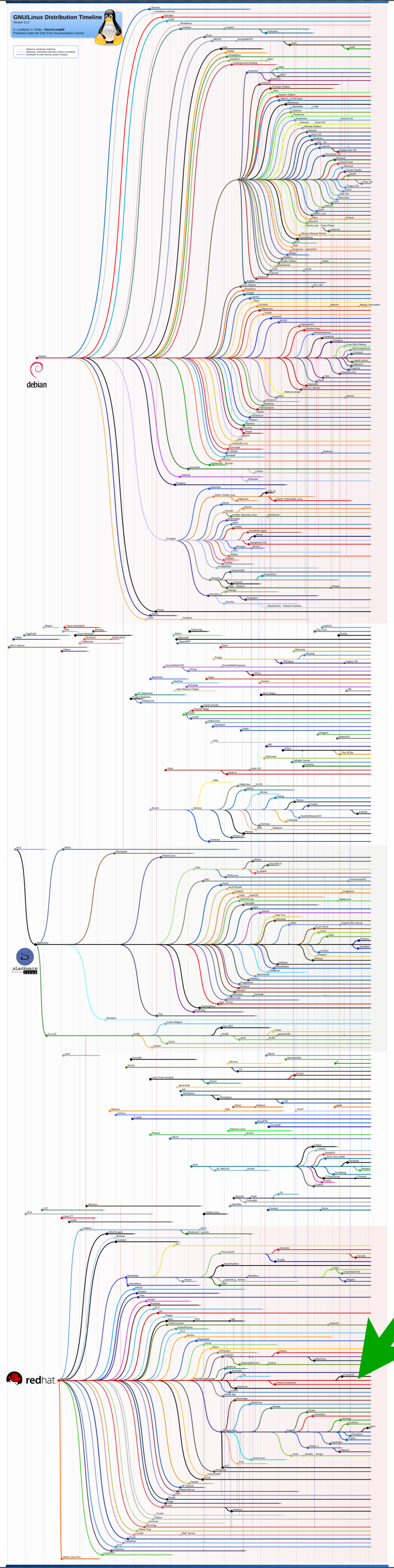

GNU/Linux Distribution Timeline
Version 12.2
A. Lundqvist, D. Rodic - futurist.se/gldt
Published under the GNU Free Documentation License
Influence, developer switching
Rebasing, substantial code flow, project overtaking
Developer & code sharing, project merging
Libranet
debian
slackware
redhat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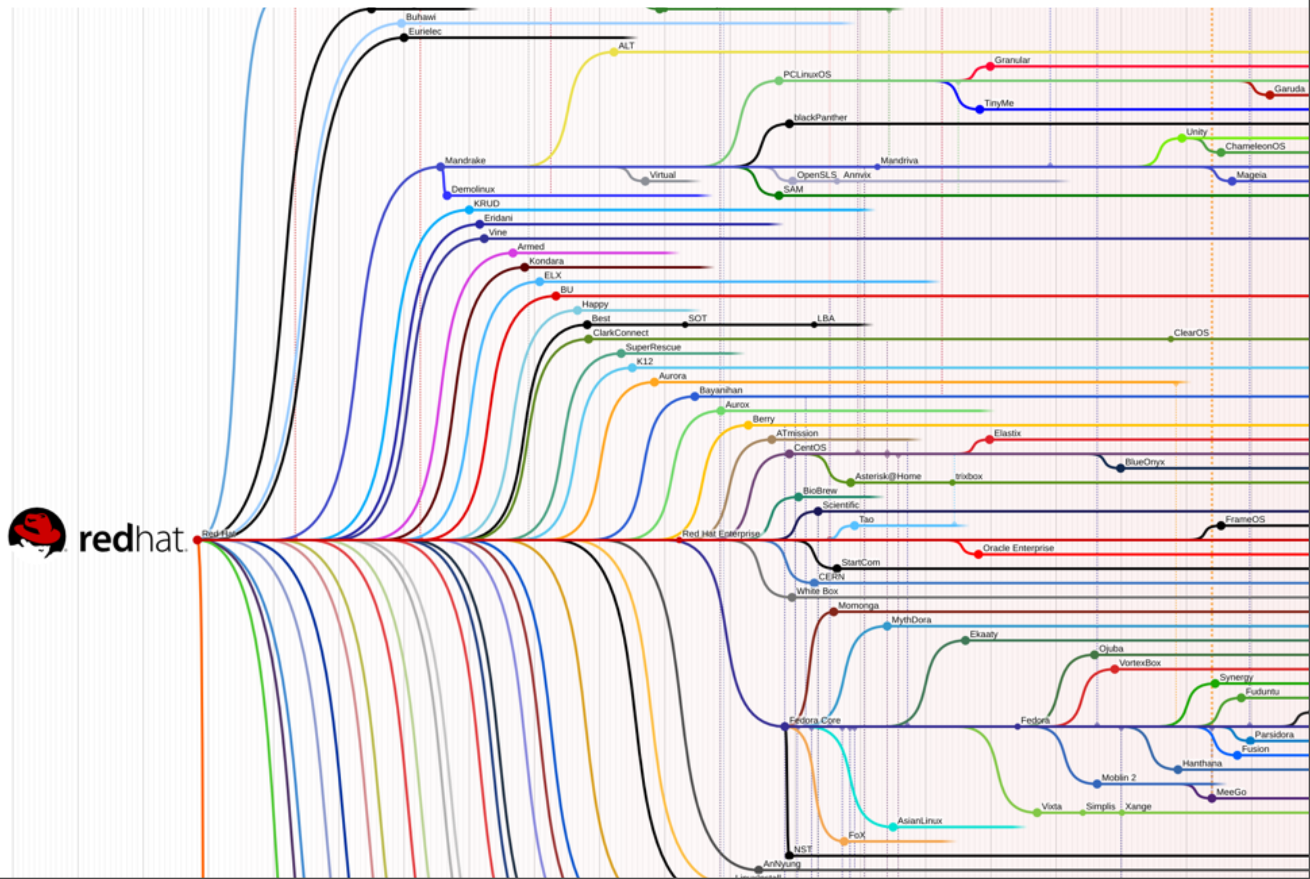
debian
redhat

UA HPC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Eurielec
ALT
PCLinuxOS
Granular
Garuda
TinyMe
blackPanther
Unity
ChameleonOS
Mandrake
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OpenSLS
Annvix
Mageia
Demolinux
SAM
KRUD
Eridani
Vine
Armed
Kondara
ELX
BU
Happy
Best
SOT
LBA
ClarkConnect
ClearOS
SuperRescue
K12
Aurora
Bayanihan
Aurox
Berry
ATmission
Elastix
CentOS
BlueOnyx
Asterisk@Home
trixbox
BioBrew
Scientific
Tao
FrameOS
redhat
Red Hat
Red Hat Enterprise
Oracle Enterprise
StartCom
CERN
White Box
Momonga
MythDora
Ekaaty
Ojuba
VortexBox
Synergy
Fuduntu
Fedora Core
Fedora
Parsidora
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Vixta
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FoX
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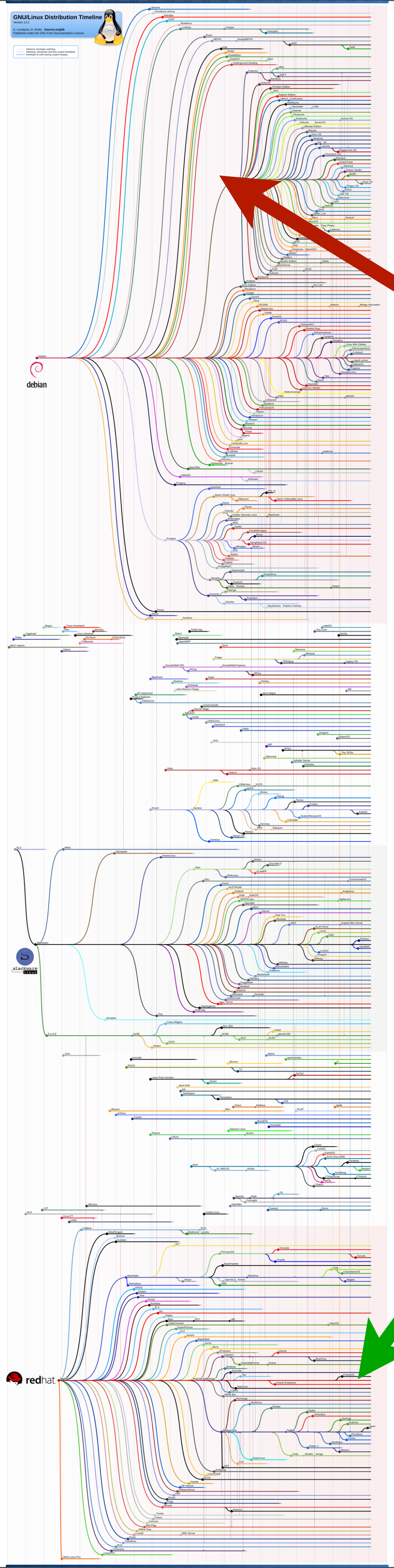

Ubuntu

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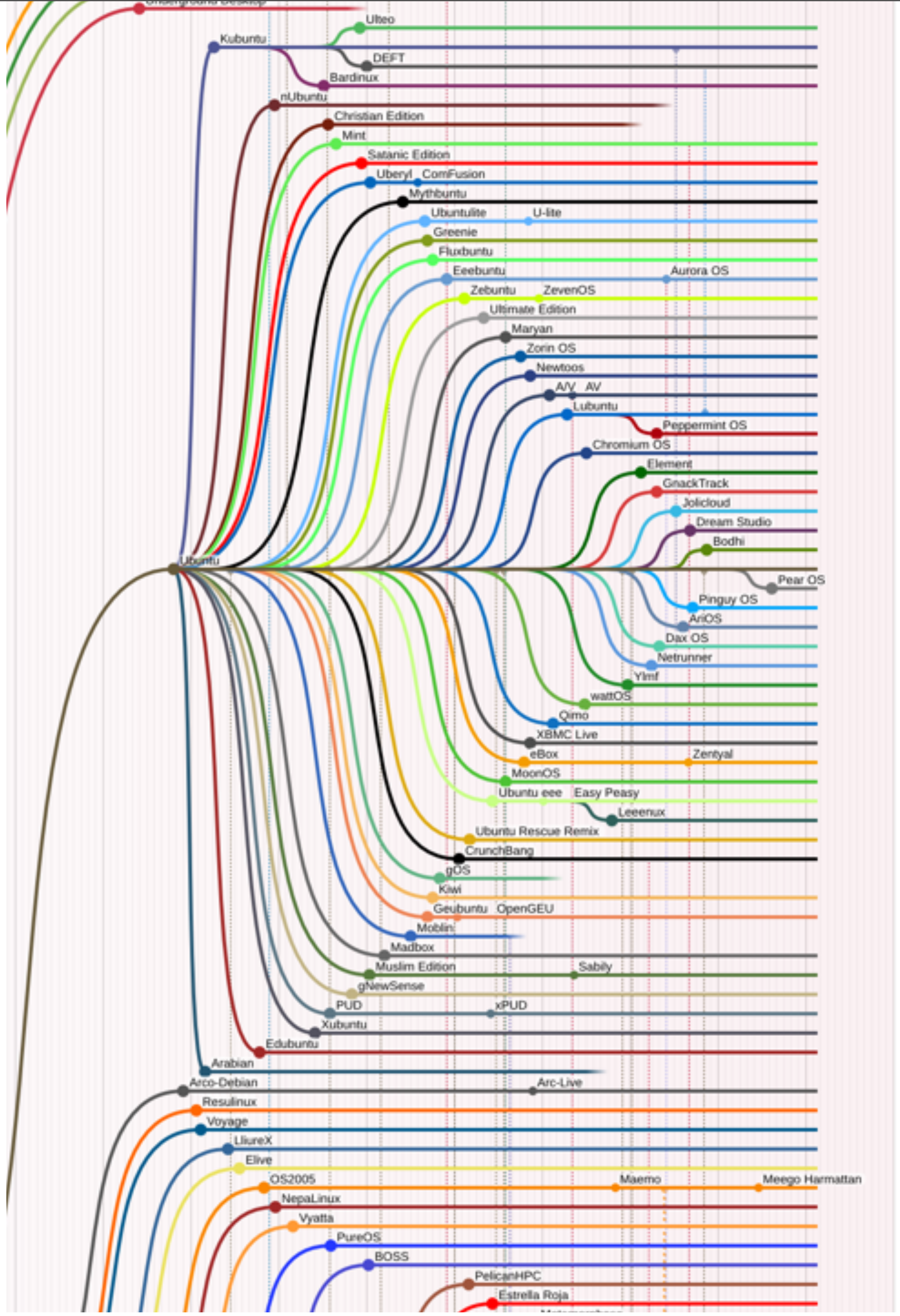

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- On top of the Unix operating system kernel is a Unix shell (sh, csh, tcsh, ksh, bash, etc.) The shell interprets the commands you type and interacts with the appropriate operating system components

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- Examples:
  - /
  - /home
  - /home/plantsci/sam/data/samples
  - /usr
  - /usr/local/bin
  - data/links
  - data/samples

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- The pwd (present working directory) command will tell you which directory you are in. On some computer systems the command prompt reflects the working directory.

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  - `sampleData.22.02.07`
  - `my_demo.txt`
  - `A01_JR165_T7.ab1`
  - `index.html`

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- If you do not see an error message, the command executed without a problem (Unix is not chatty!)

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- Open the Terminal application
  - On Mac/Linux, Terminal is in Applications-->Utilities
  - On Windows, use PuTTY (find it on google)

- Type:

```
ssh <myUANetID>@login.hpc.arizona.edu
```

- You should see a command prompt such as:

```
[service0][~]>
```

OR

```
/uNN/netid>
```

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    - `ls  -l`
    - `ls  -ltr`

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  - Examples:
    - `ls   -l`
    - `ls   -ltr`
    - `ls   -l   chromat_dir`

Getting help for UNIX commands

The man command (short for manual) can be used to see documentation for any UNIX command (even man itself!) To do a keyword search of the documentation, use man –k keyword

Example: `man man`

```
User Commands                                         man(1)

NAME
     man - find and display reference manual pages

SYNOPSIS
     man [ - ]  [ -adFlrt ]  [ -M path ]  [ -T macro-package ]  [
     -s section ]  name ...

     man [ -M path ]  -k keyword ...

DESCRIPTION
     The man command  displays  information  from  the  reference
     manuals.  It  displays complete manual pages that you select
     by name, or one-line summaries selected  either  by  keyword
     (-k),  or  by  the  name  of  an associated file (-f). If no
     manual page is located, man prints an error message.   …
```

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- There are three different supercomputers. The shared memory system is '`smp`', and the cluster system is '`cluster`', and the high throughput cluster is ‘`htc`’. All of these can be accessed from “`login`” (`login.hpc.arizona.edu`)

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- FAQs and User Guides are available here:
  http://rc.arizona.edu/hpc-htc/using-systems

Copying files

Copying files

- The `cp` command copies files or directories from one place to another. The files you want to copy are called "sources" and the place you want to copy them to is called the "destination". To copy an entire directory, use the `–r` option.
- Examples:
  - `cp   fileA   filA.backup`
  - `cp   fileA   fileB   recycle_bin/`
  - `cp –r   recycle_bin/   backup_dir/`

- Remember that `cp` ALWAYS requires *at least* two arguments: the source files/directories and the destination file/directory (often this will be .)

- Use the `cp` command to copy a directory of files to work with:
  - `cp –r /genome/student/data playground`

Exercise: practice with `man`, `pwd`, and `ls`

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When finished, type `logout`

UNIX Basic Command Recap

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man *<command>*	Output a manual page for the specified command
pwd	Display the present working directory
mkdir *<dirname>* …	Make new directory/directories named dirname …
ls *[<dirname> …]* ls -l	List directory contents (of dirname(s)) Show a long listing of directory contents
cp *<srcfile>* … *<dest>* cp –r *<srcdir>* … *<dest>*	Copy source file(s) to destination Recursively copy source dir(s) to destination
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- How many arguments does each of these commands take?

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A **line** is defined as the characters before a newline (i.e. the line count is the number of newlines)

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A **byte** is 8 *bits*, or the amount of space necessary to store one character. So the byte count of a text file is the number of characters (including newlines, tabs, and spaces)

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tab-delimited, or **tab-separated** format is a way of representing data where each record is on a new line, and entry related to that record is separated by a tab (‘\t’). An alternate is **comma-separated (csv).**

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- a useful option is:
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- to get to insert mode just type and *i*
- to write the current file and exit type *:wq*

Useful VIM commands

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```
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These two commands can take *Regular Expressions* which we will talk about later

Useful VIM commands

- to search a file

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/<search>
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- to find/replace

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:%s/<search>/<replace>/[g]
```

- to go to a line number

```
:<number>
```

Using `grep`

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Using `grep`

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```
grep [<options>] <search> <fileList>
```

- some useful options are:
  - `-c` counts the number of occurrences of search
  - `-v` returns lines **without** search

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  - `chsh -s /bin/bash`
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    - `export PATH=~deblasio/bin/553:~/bin:$PATH`
    - `export PATH=/genome/ICEbin/:$PATH`

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- try running `turnin --verify`

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- logout then log back into HPC
- try running `turnin --verify`
- You should see

```
deblasio@service0(login):~> turnin --verify
You are: deblasio
and you are good to go
```

Other helpful things for your `.profile`

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- `export PS1="\u@\h(login):\w> "`

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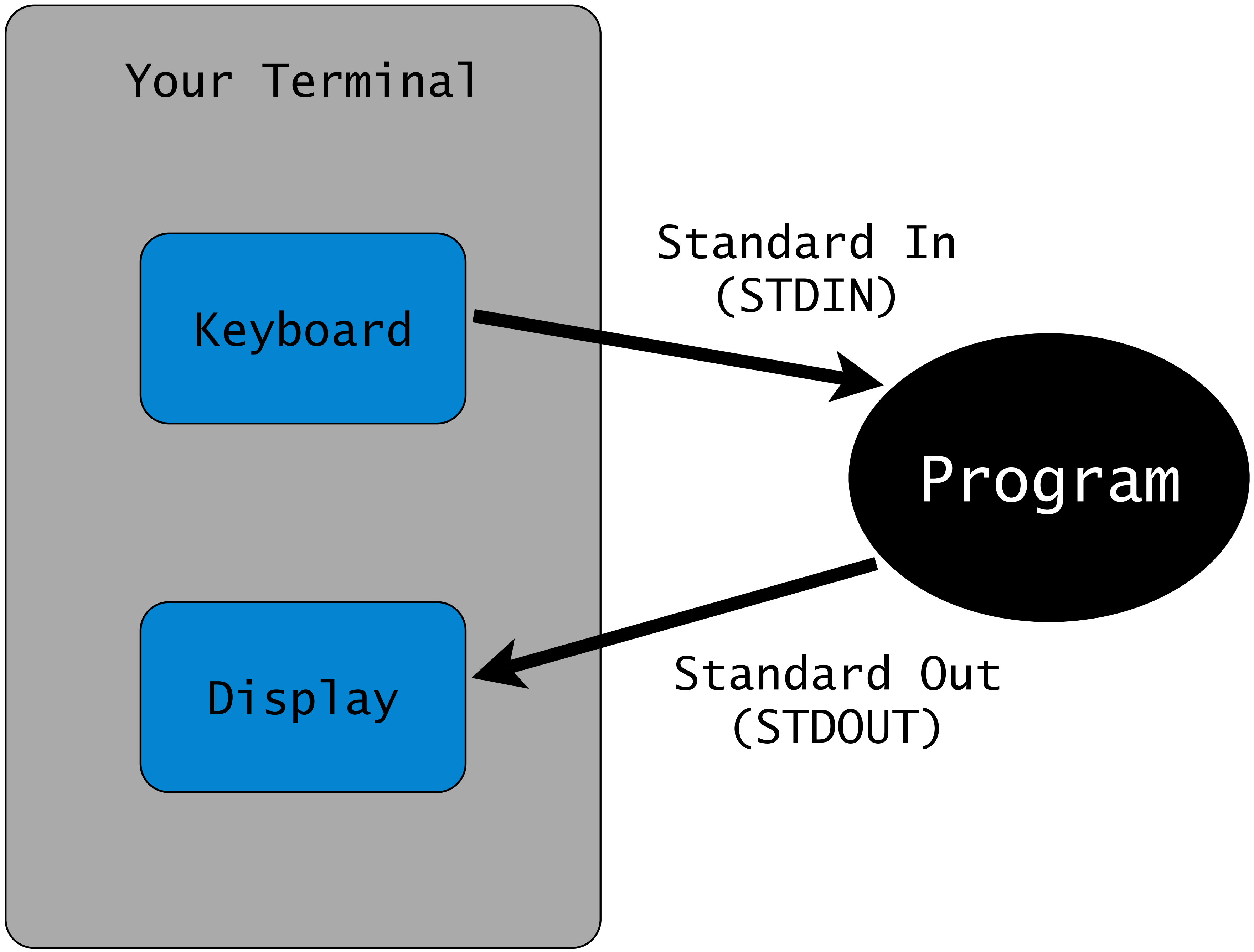
- `export LS_COLORS=ow\=01\;34\:tw\=01\;34\;`

Program input and output

```
>Program
```



Your Terminal

Keyboard

Display

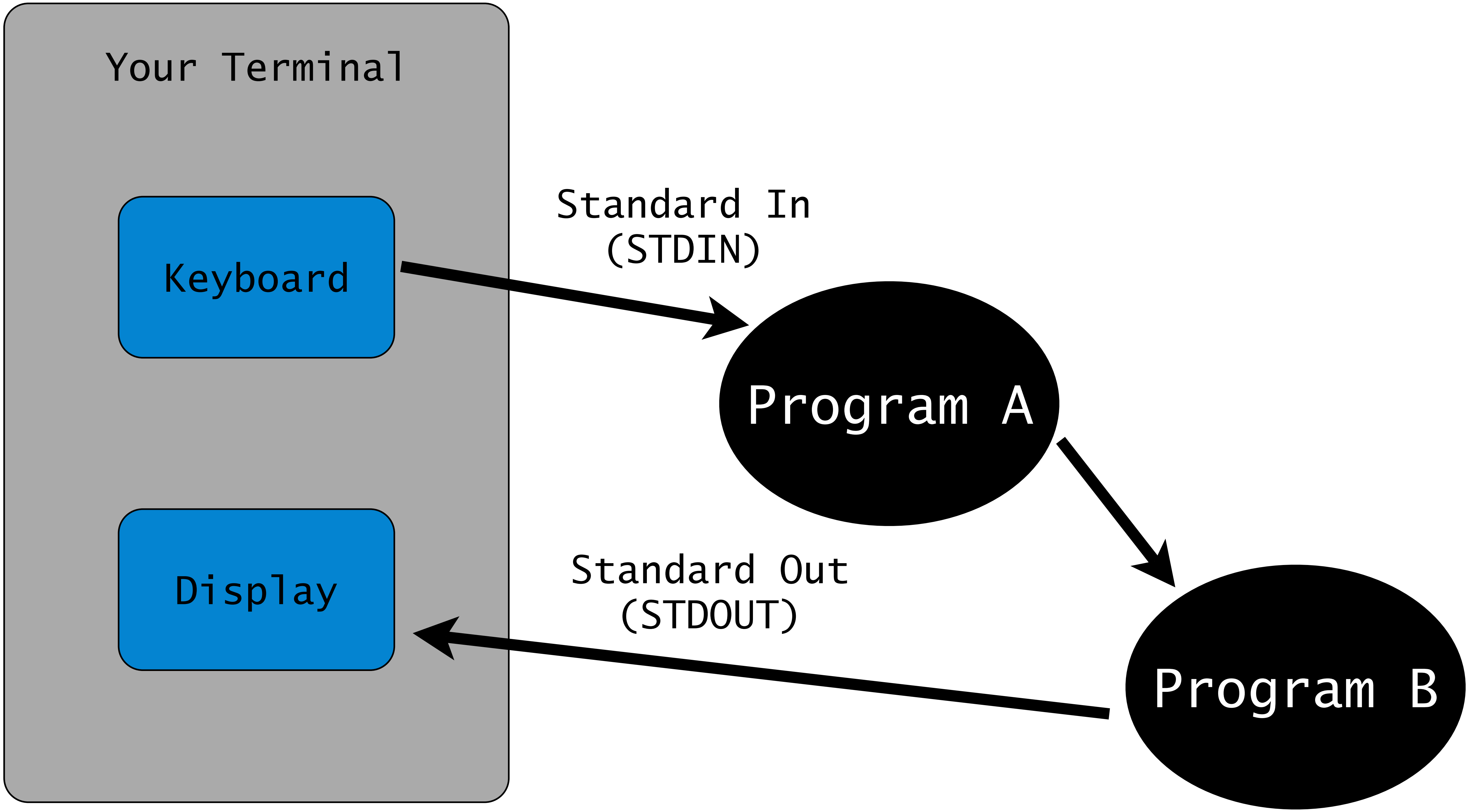
Standard In
(STDIN)

Program

Standard Out
(STDOUT)

Program input and output

```
>Program_A | Program_B
```



Your Terminal

Keyboard

Display

Standard In
(STDIN)

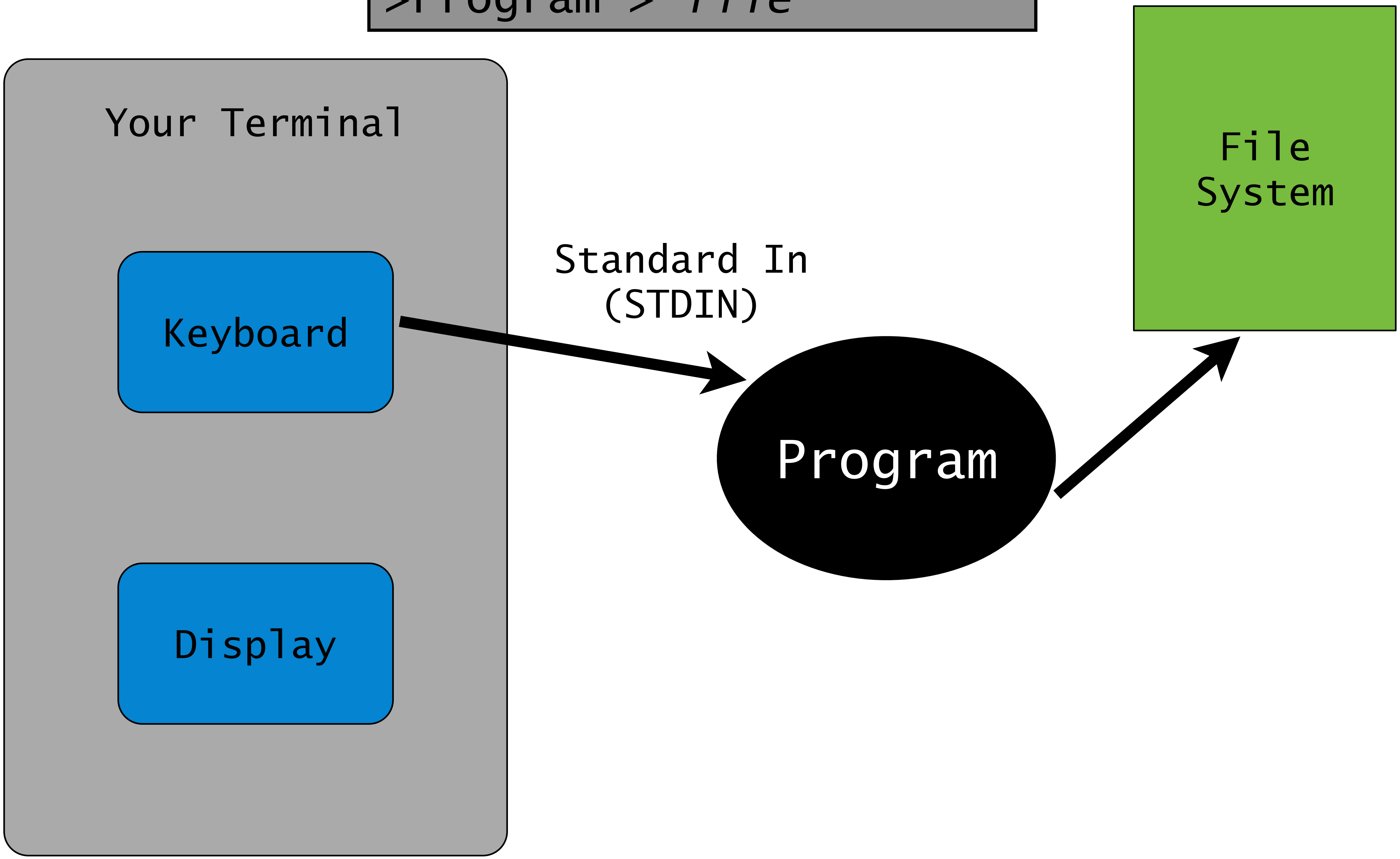
Program A

Program B

Standard Out
(STDOUT)

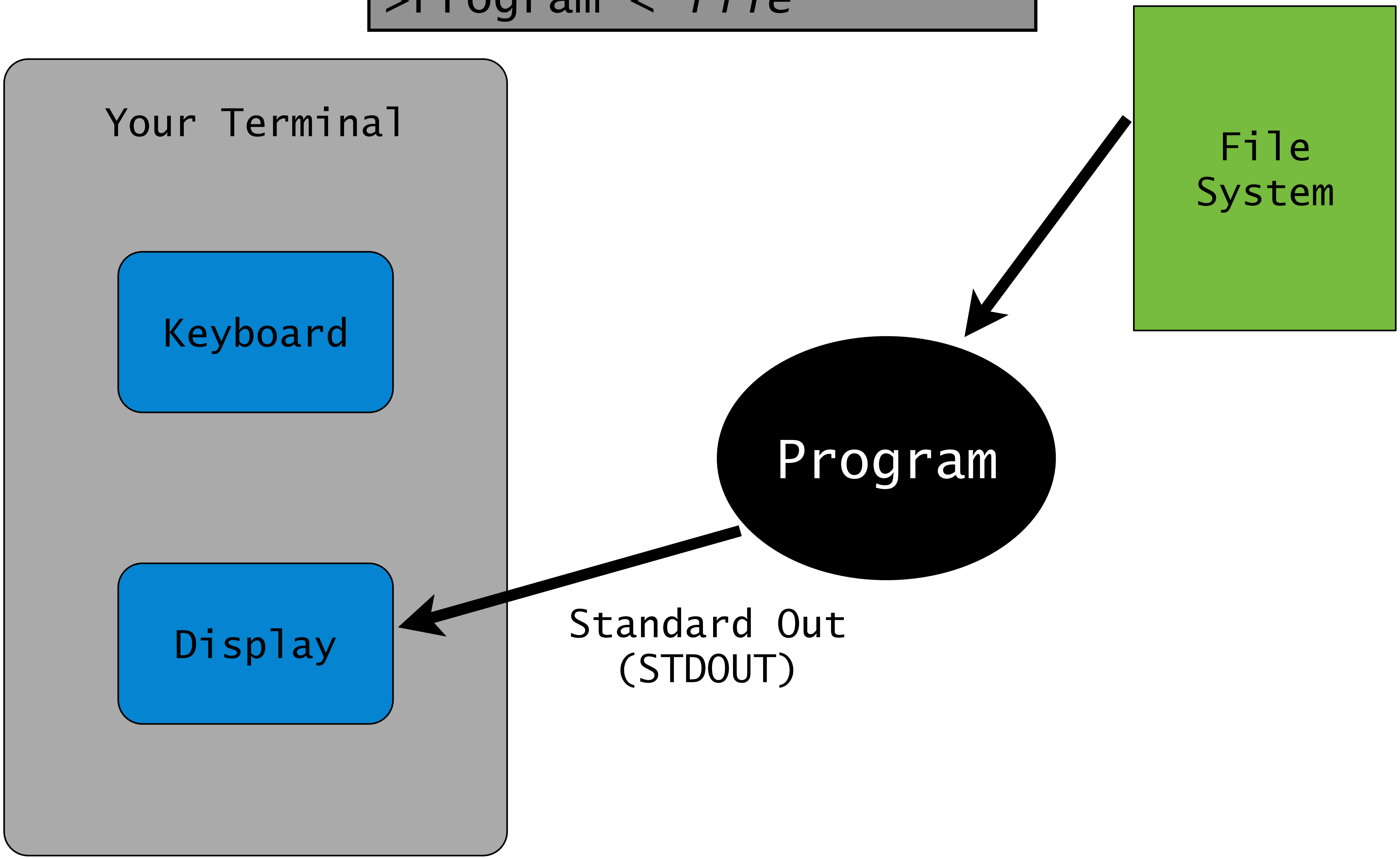
Program input and output

```
>Program > file
```



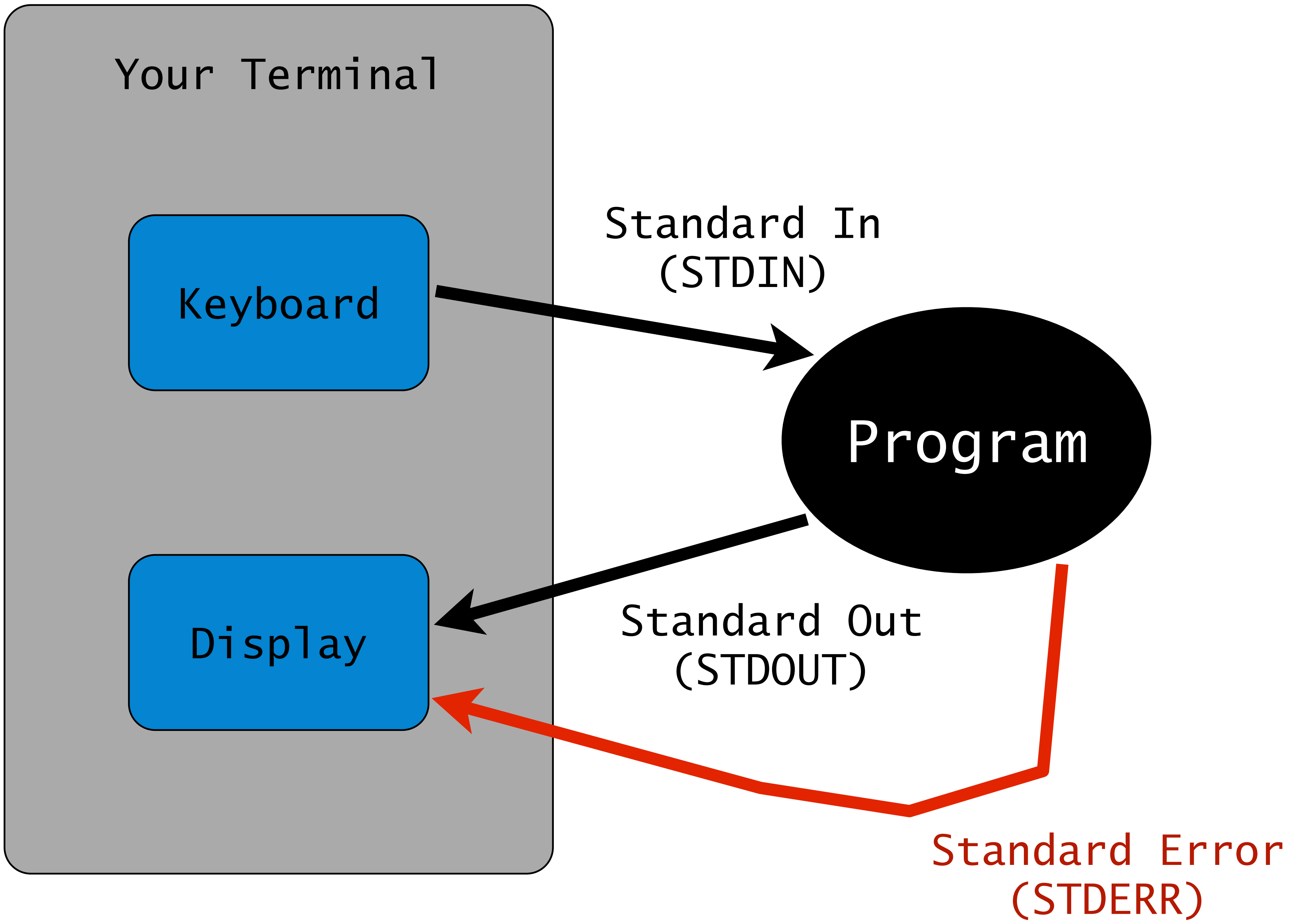
Program input and output

```
>Program < file
```



Program input and output

```
>Program
```



Your Terminal

Keyboard

Display

Standard In
(STDIN)

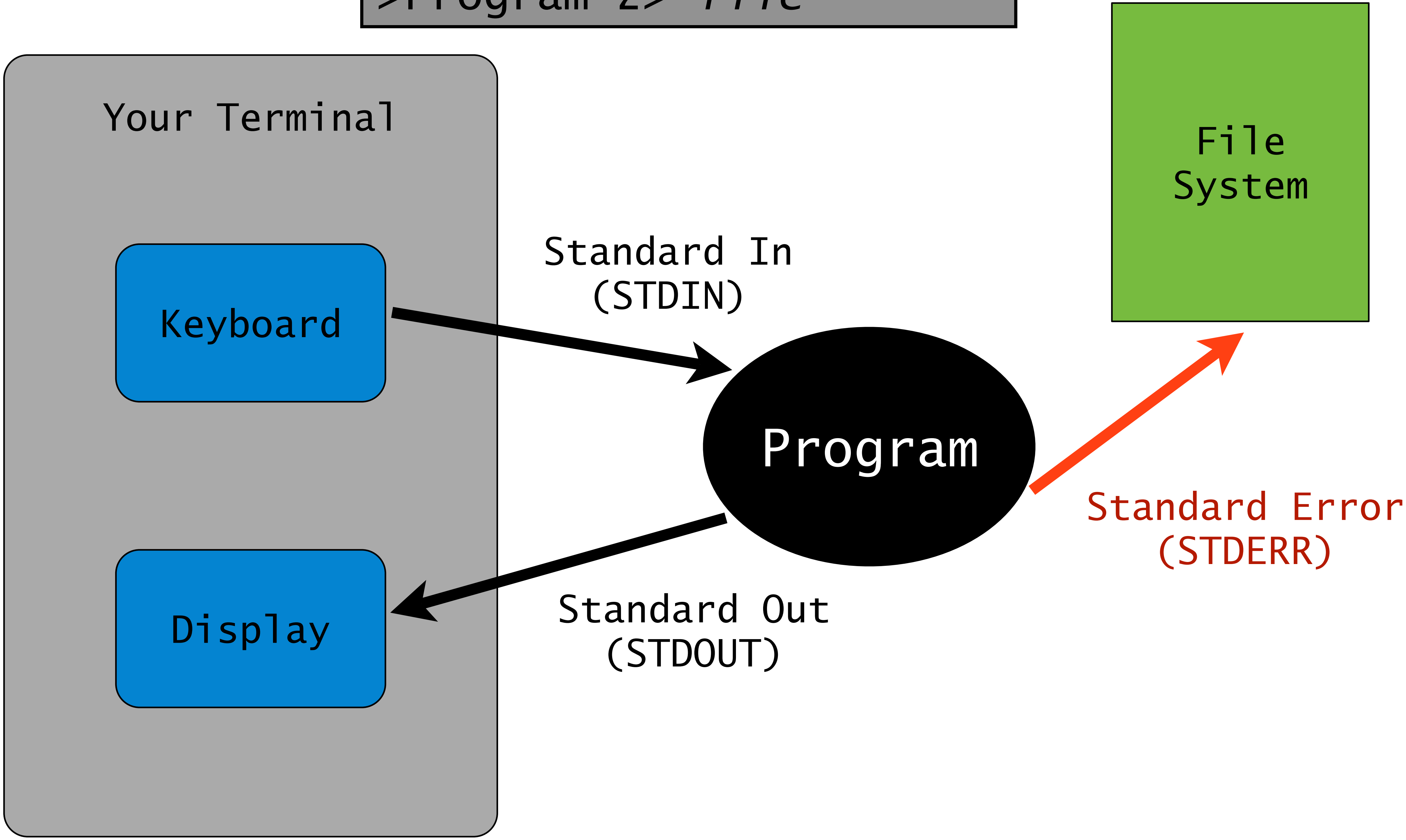
Program

Standard Out
(STDOUT)

Standard Error
(STDERR)

Program input and output

```
>Program 2> file
```



Your Terminal

Keyboard

Display

Standard In
(STDIN)

Program

Standard Out
(STDOUT)

File
System

Standard Error
(STDERR)

SCP/SFTP

SCP/SFTP

- Transferring files to/from the server

SCP/SFTP

- Transferring files to/from the server
- Mac

SCP/SFTP

- Transferring files to/from the server
- Mac
  - in terminal `SCP`

SCP/SFTP

- Transferring files to/from the server
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    - `scp <NetID>@login.hpc.arizona.edu:<path>/<fil> ./`

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  - Fugu (see links file from the first day)

SCP/SFTP

- Transferring files to/from the server
- Mac
  - in terminal `SCP`
    - `scp <NetID>@login.hpc.arizona.edu:<path>/<fil> ./`
    - `scp <fil> <NetID>@login.hpc.arizona.edu:<path>`
  - Fugu (see links file from the first day)
- PC

SCP/SFTP

- Transferring files to/from the server
- Mac
  - in terminal `SCP`
    - `scp <NetID>@login.hpc.arizona.edu:<path>/<fil> ./`
    - `scp <fil> <NetID>@login.hpc.arizona.edu:<path>`
  - Fugu (see links file from the first day)
- PC
  - WinSCP

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- We will have a short Quiz on ***next thursday 13 September*** by the beginning of class