CDE: A tool for automatically creating reproducible experimental software packages

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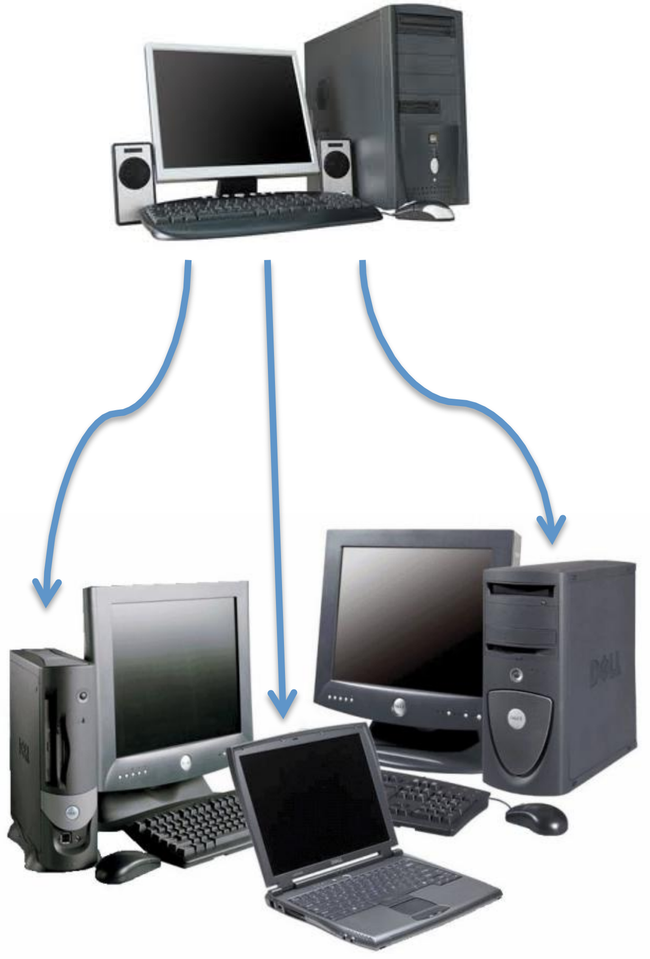
http://www.stanford.edu/~pgbovine/cde.html

Barriers to reproducible research

Cultural, Political, Behavioral, Institutional, Sociopsychological



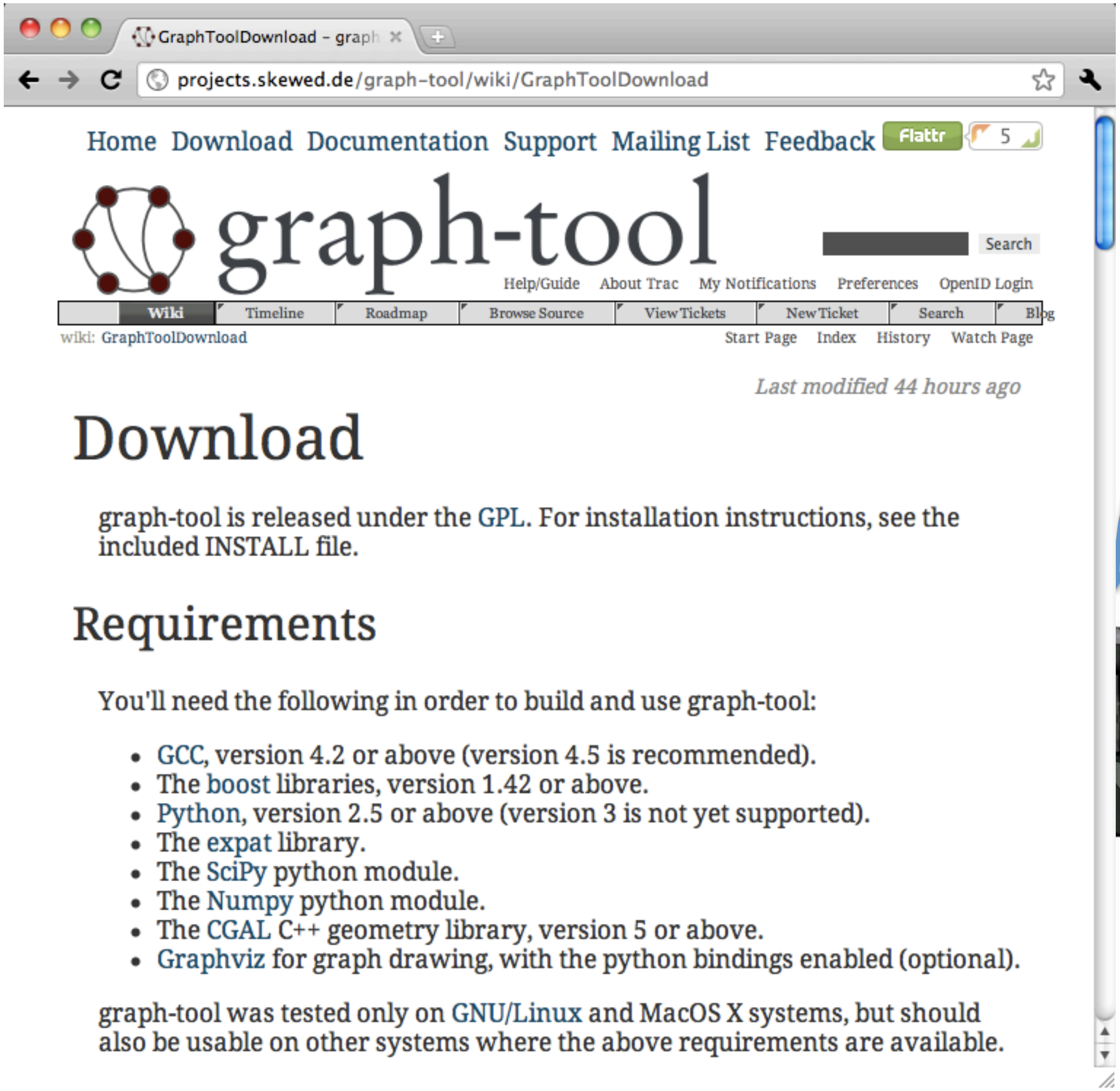
Technical

Barriers to reproducible research

It’s really hard to take research code that runs on your machine and get it to run on someone else’s machine, even one with the same OS as yours.

Technical

Barriers to reproducible research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Download

graph-tool is released under the GPL. For installation instructions, see the included INSTALL file.

Requirements

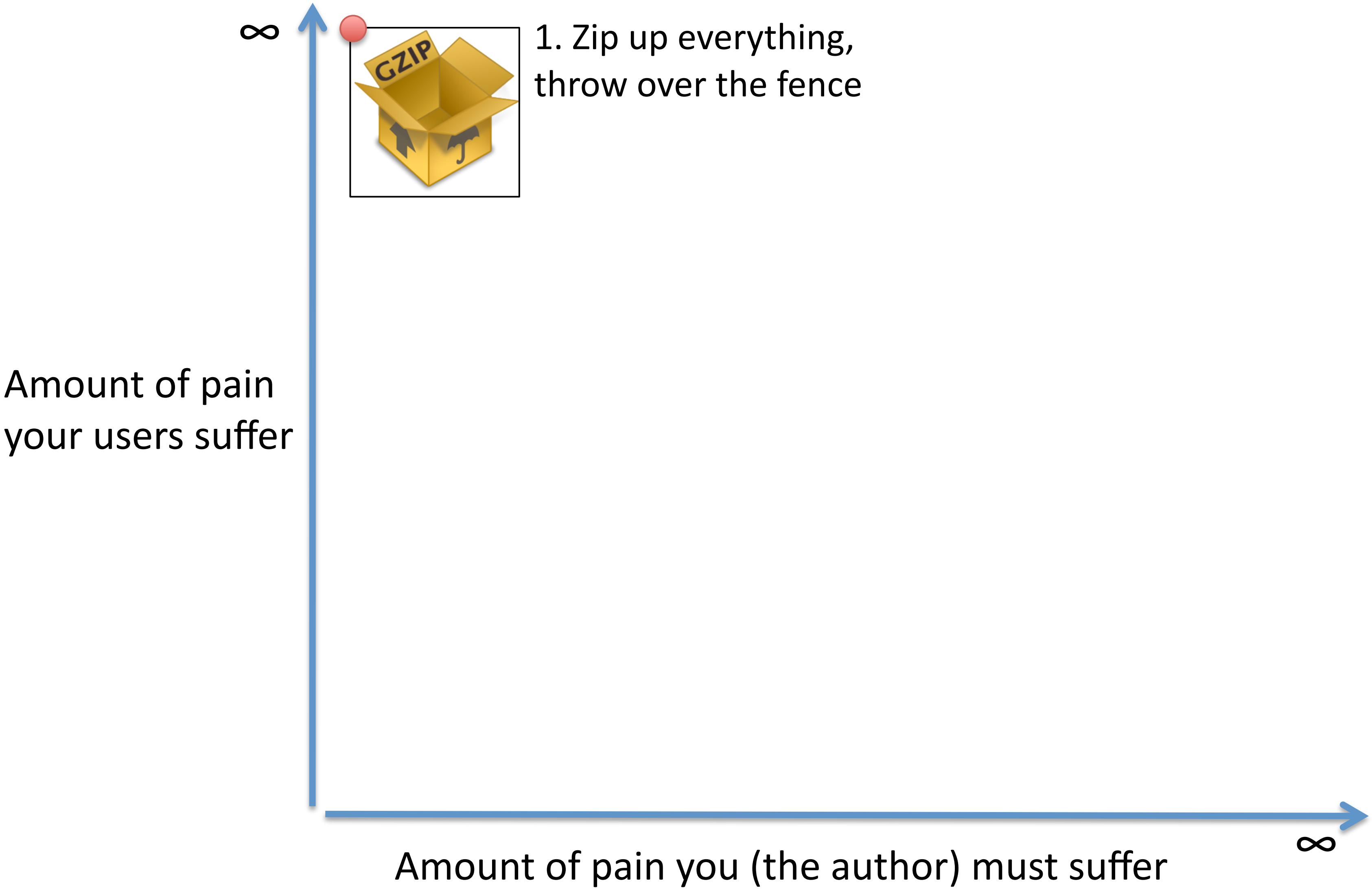
You'll need the following in order to build and use graph-tool:

- GCC, version 4.2 or above (version 4.5 is recommended).
- The boost libraries, version 1.42 or above.
- Python, version 2.5 or above (version 3 is not yet supported).
- The expat library.
- The SciPy python module.
- The Numpy python module.
- The CGAL C++ geometry library, version 5 or above.
- Graphviz for graph drawing, with the python bindings enabled (optional).

graph-tool was tested only on GNU/Linux and MacOS X systems, but should also be usable on other systems where the above requirements are available.

Technical

Current ways to distribute research code



∞

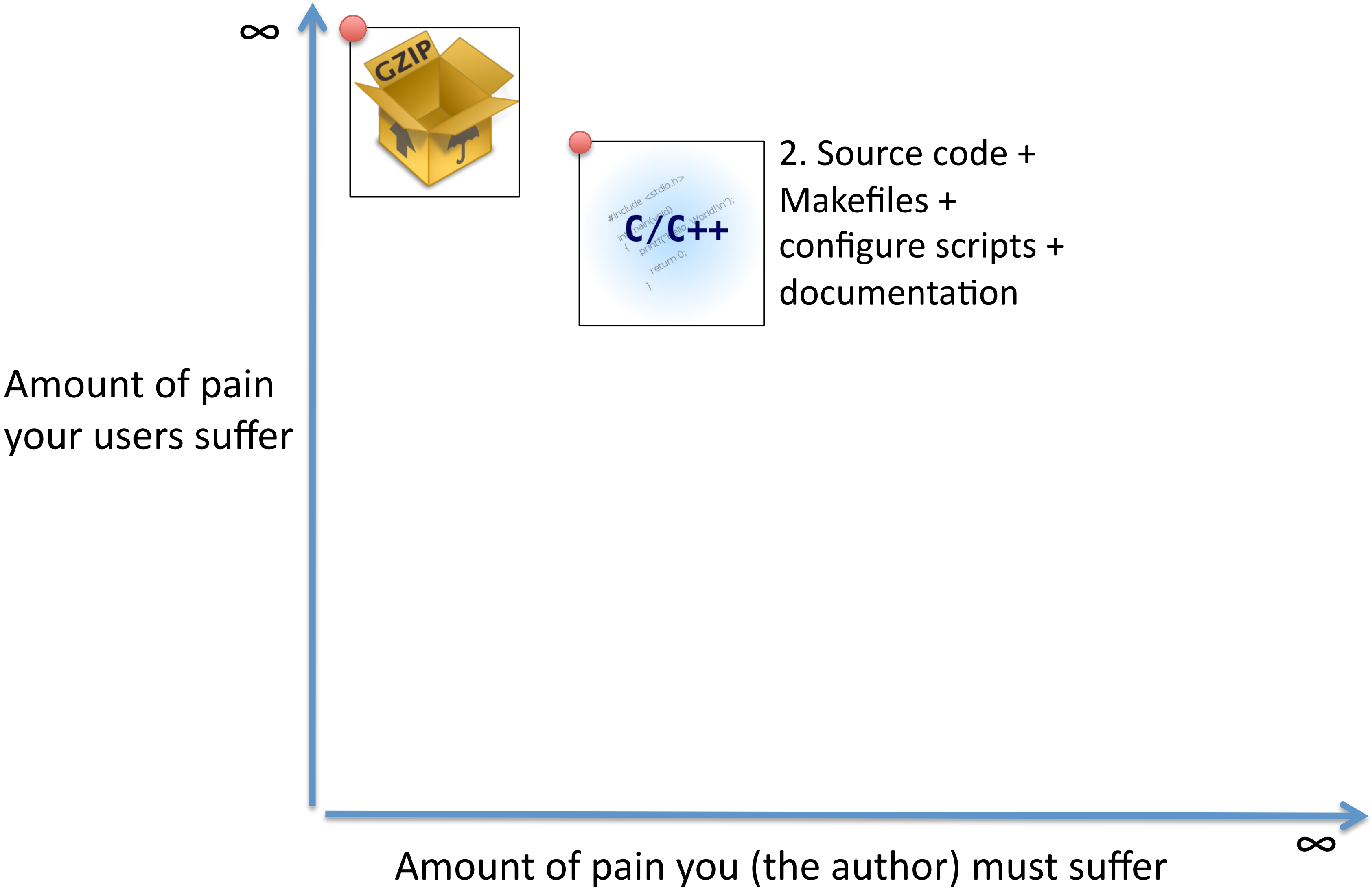
1. Zip up everything,
throw over the fence

Amount of pain
your users suffer

∞

Amount of pain you (the author) must suffer

Current ways to distribute research code



∞

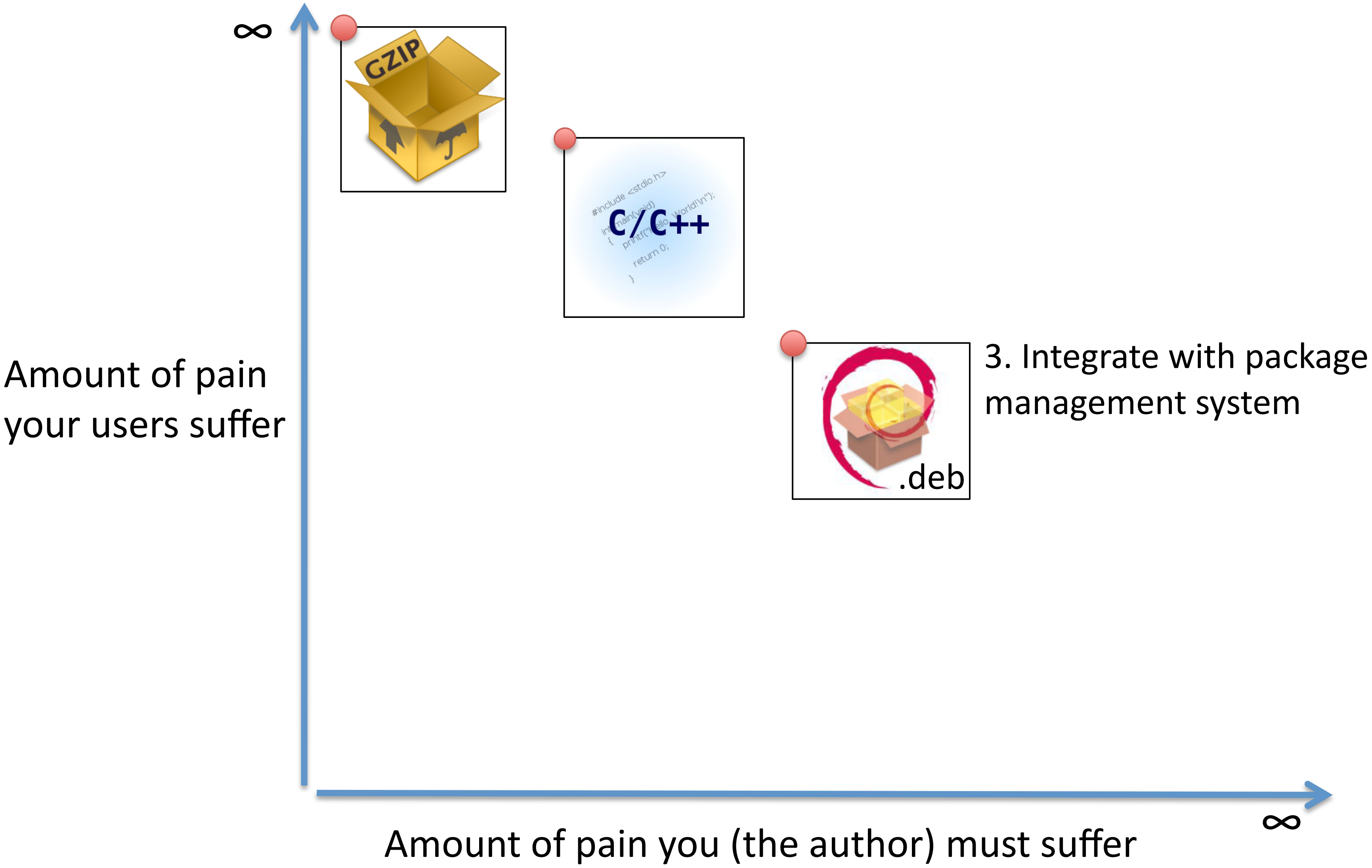
2. Source code +
Makefiles +
configure scripts +
documentation

Amount of pain
your users suffer

∞

Amount of pain you (the author) must suffer

Current ways to distribute research code



∞

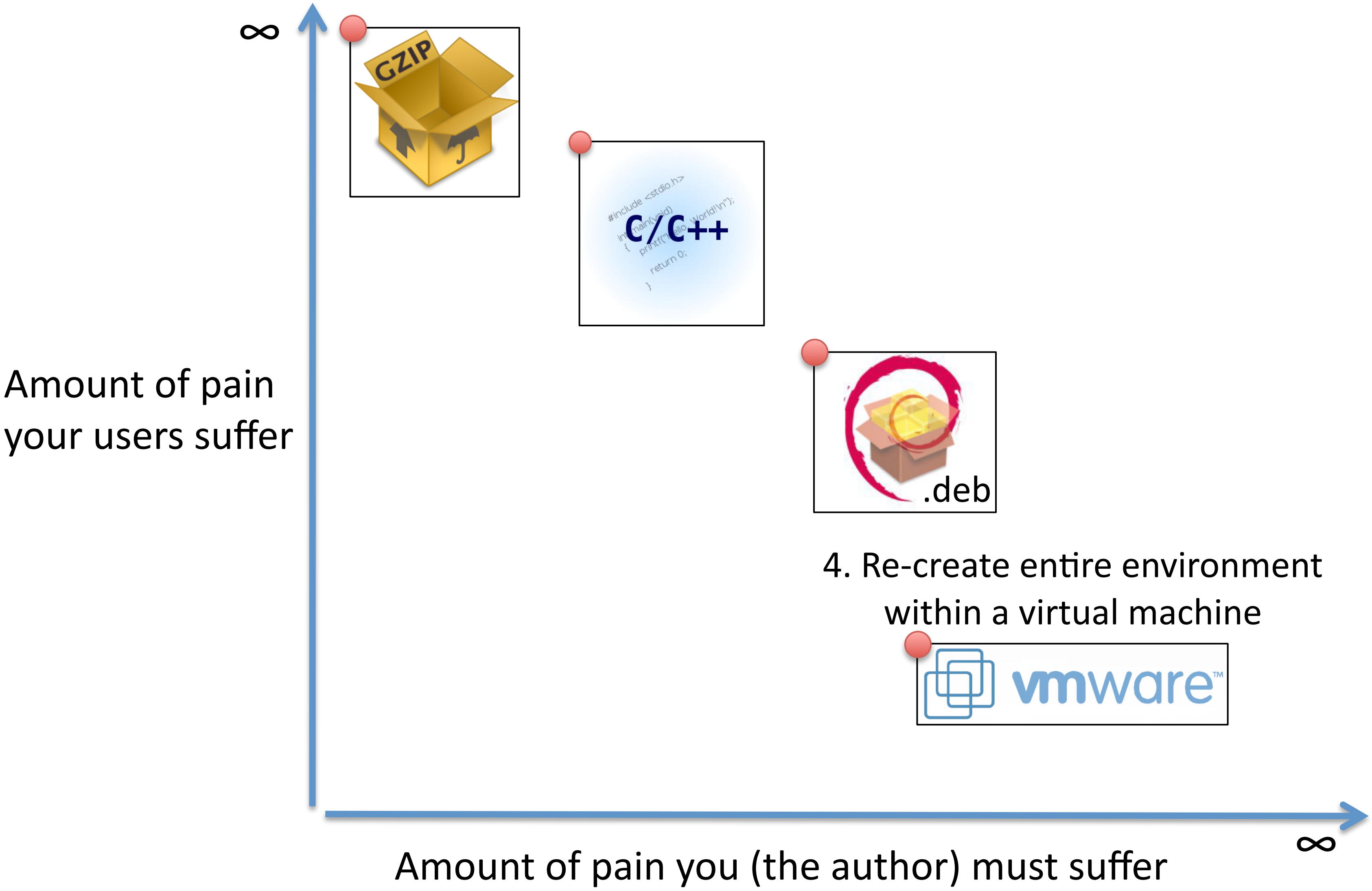
Amount of pain your users suffer

3. Integrate with package management system

∞

Amount of pain you (the author) must suffer

Current ways to distribute research code

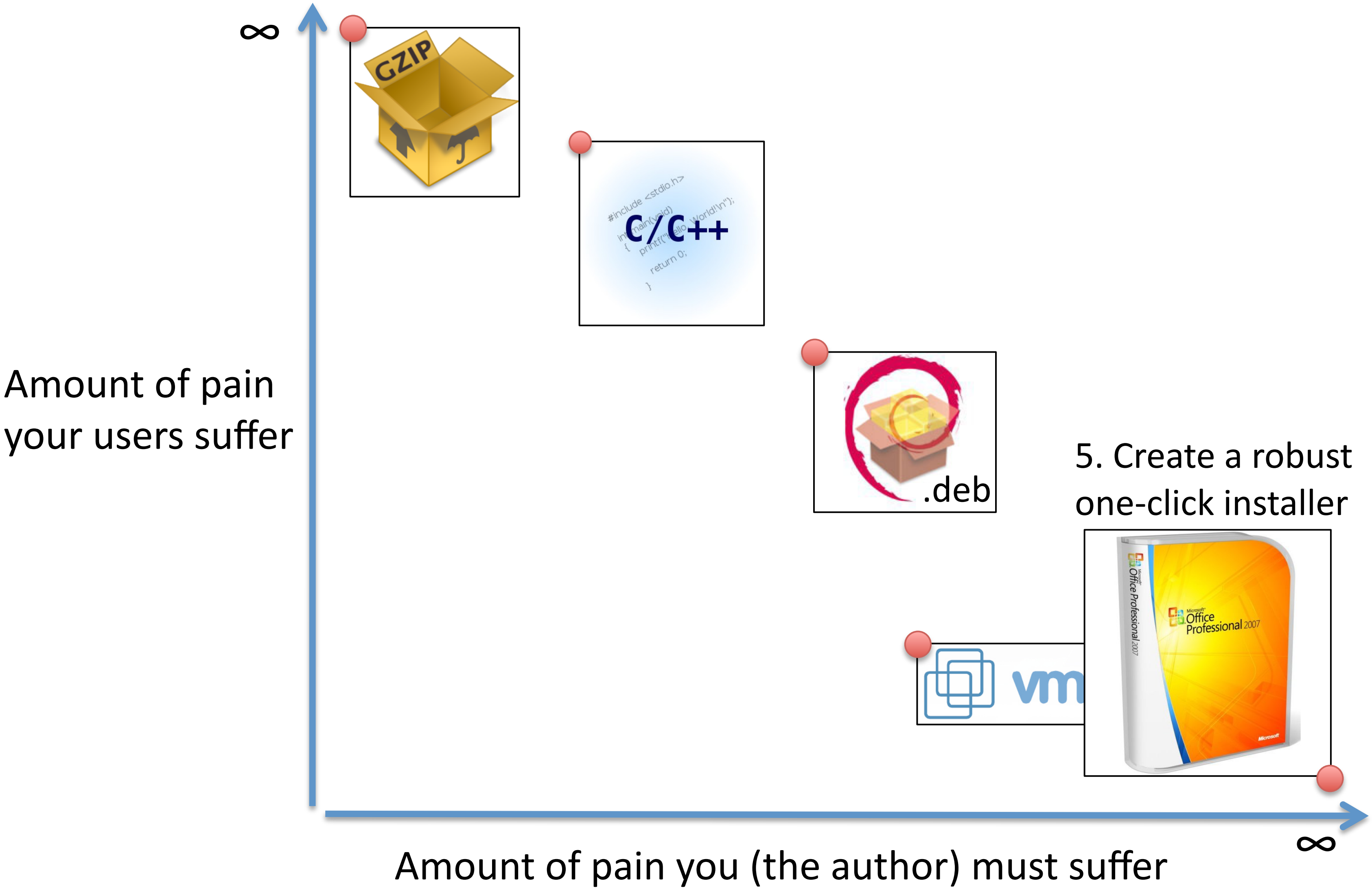


Amount of pain your users suffer

4. Re-create entire environment within a virtual machine

Amount of pain you (the author) must suffer

Current ways to distribute research code

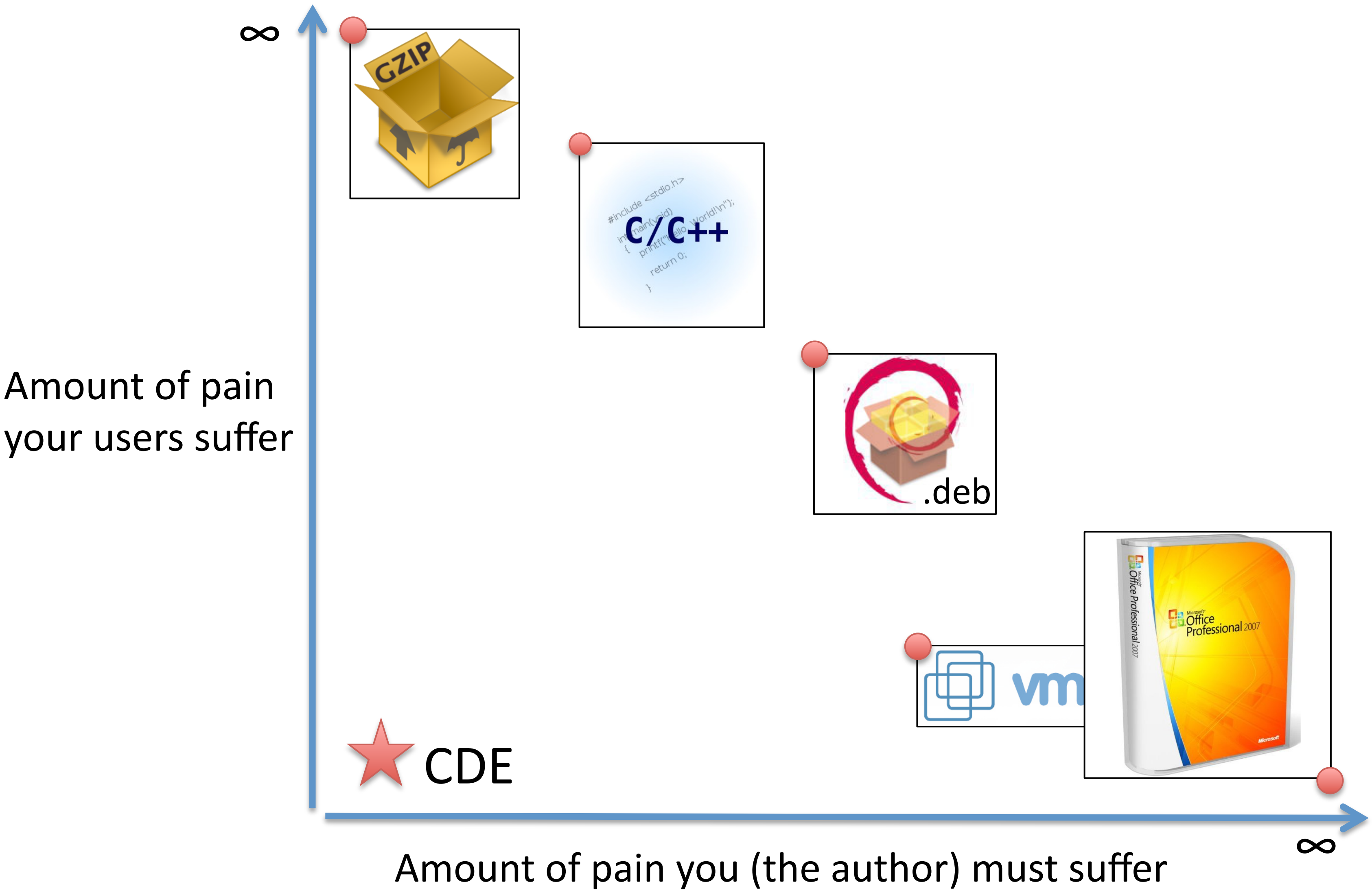


Amount of pain your users suffer

5. Create a robust one-click installer

Amount of pain you (the author) must suffer

Current ways to distribute research code



∞

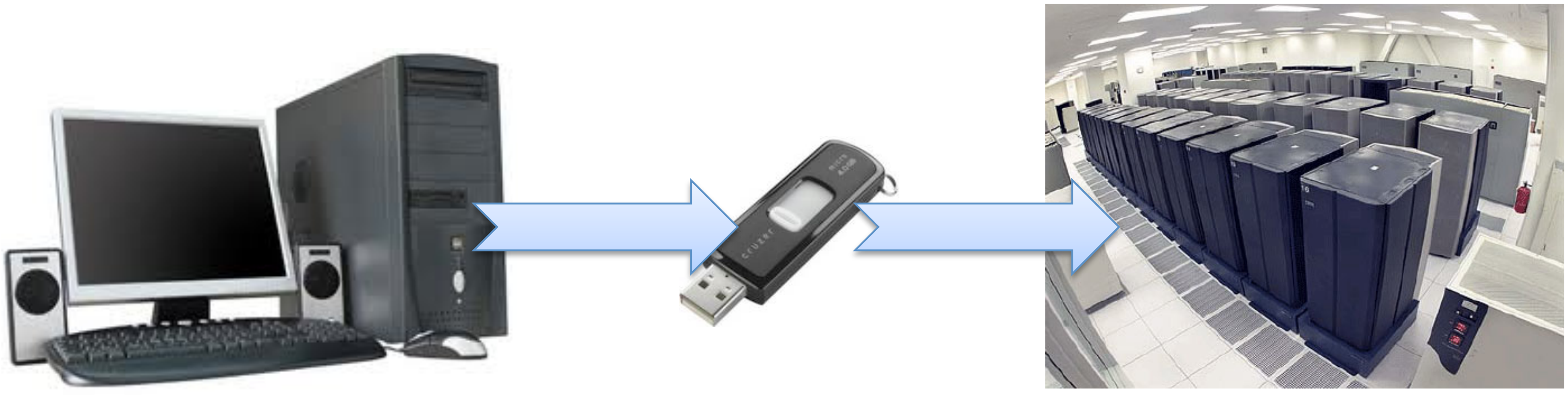
Amount of pain your users suffer

CDE

∞

Amount of pain you (the author) must suffer

CDE: Automatic packaging of **C**ode, **D**ata, and **E**nvironment



1. Create package on your Linux computer

Prepend any set of commands with ‘**cde**’, and CDE runs them and automatically packages up their dependencies

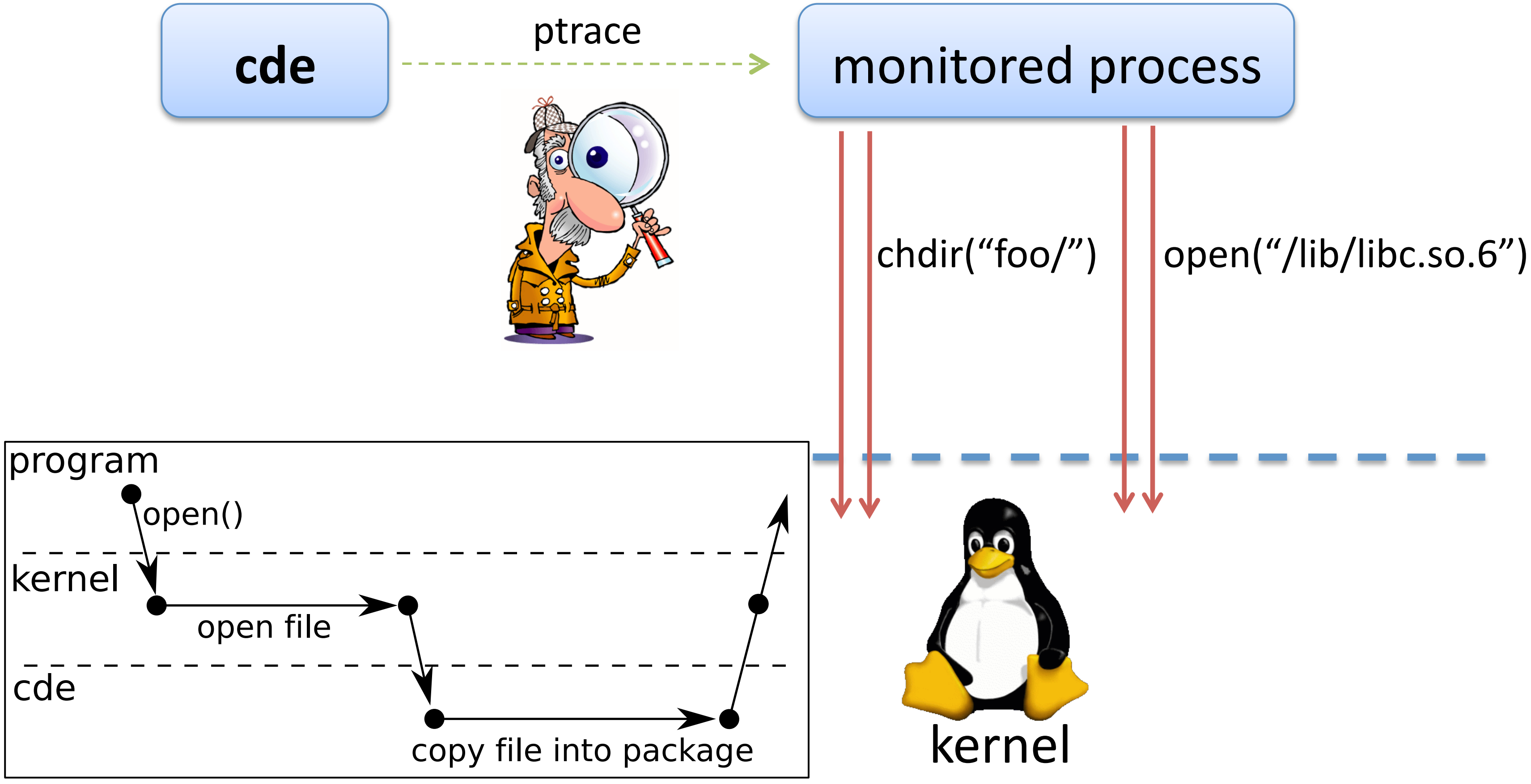
2. Transfer package

A package is simply a directory of files (~10MB – 500MB)

3. Execute software from within package on any modern Linux computer

Prepend those same commands with ‘**cde-exec**’, and CDE runs them natively without any installation

Creating a package with cde



cde

ptrace

monitored process

chdir(“foo/”)

open(“/lib/libc.so.6”)

kernel

program

open()

kernel

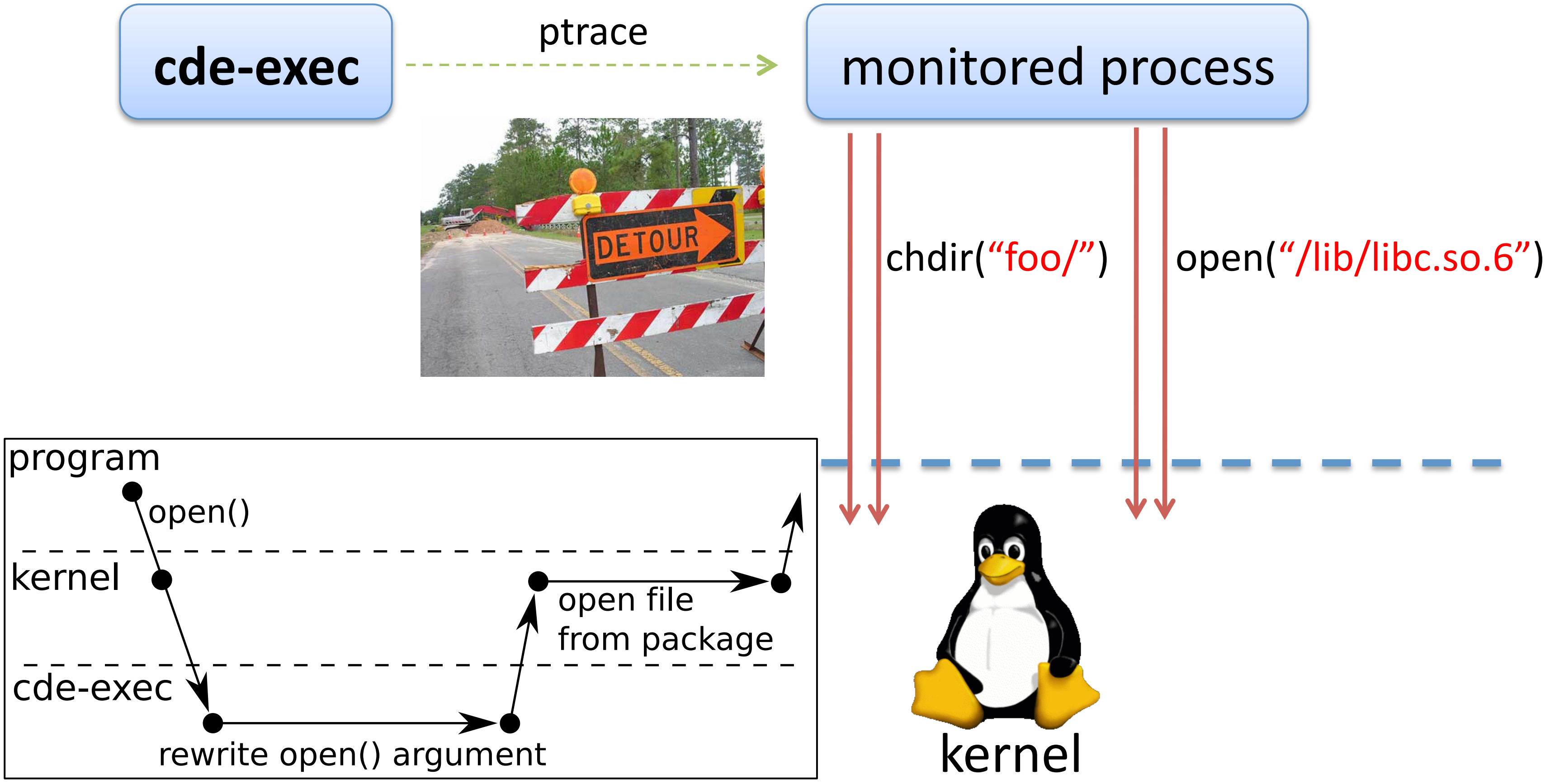
open file

cde

copy file into package

Timeline

Executing a package with cde-exec



cde-exec

ptrace

monitored process

chdir(“foo/”)

open(“/lib/libc.so.6”)

kernel

program

open()

kernel

open file
from package

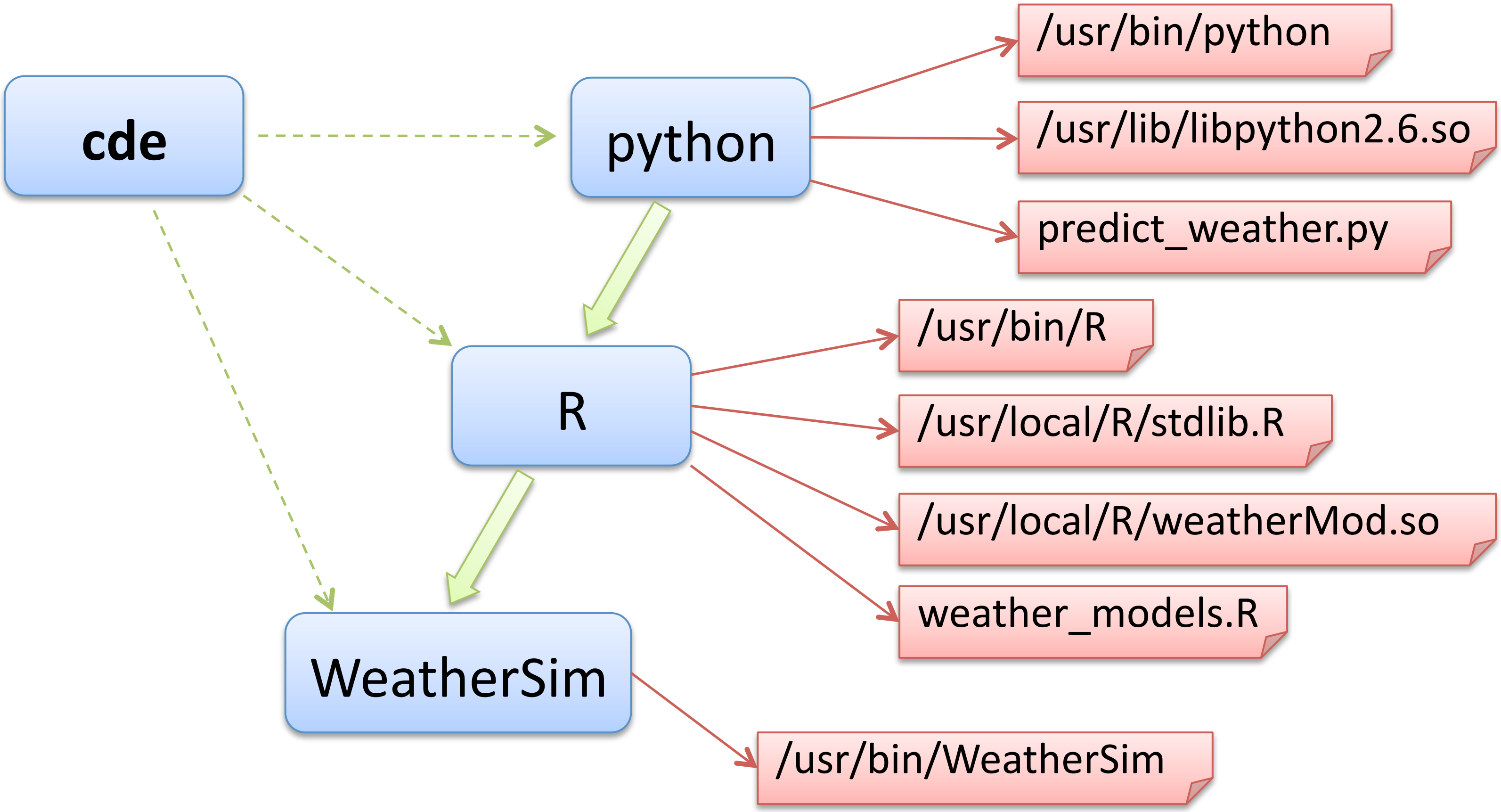
cde-exec

rewrite open() argument

Timeline

Creating a package with cde

```
cd /home/pg/expt/
cde python predict_weather.py
```



Creating a package with cde

```
cd /home/pg/expt/
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```
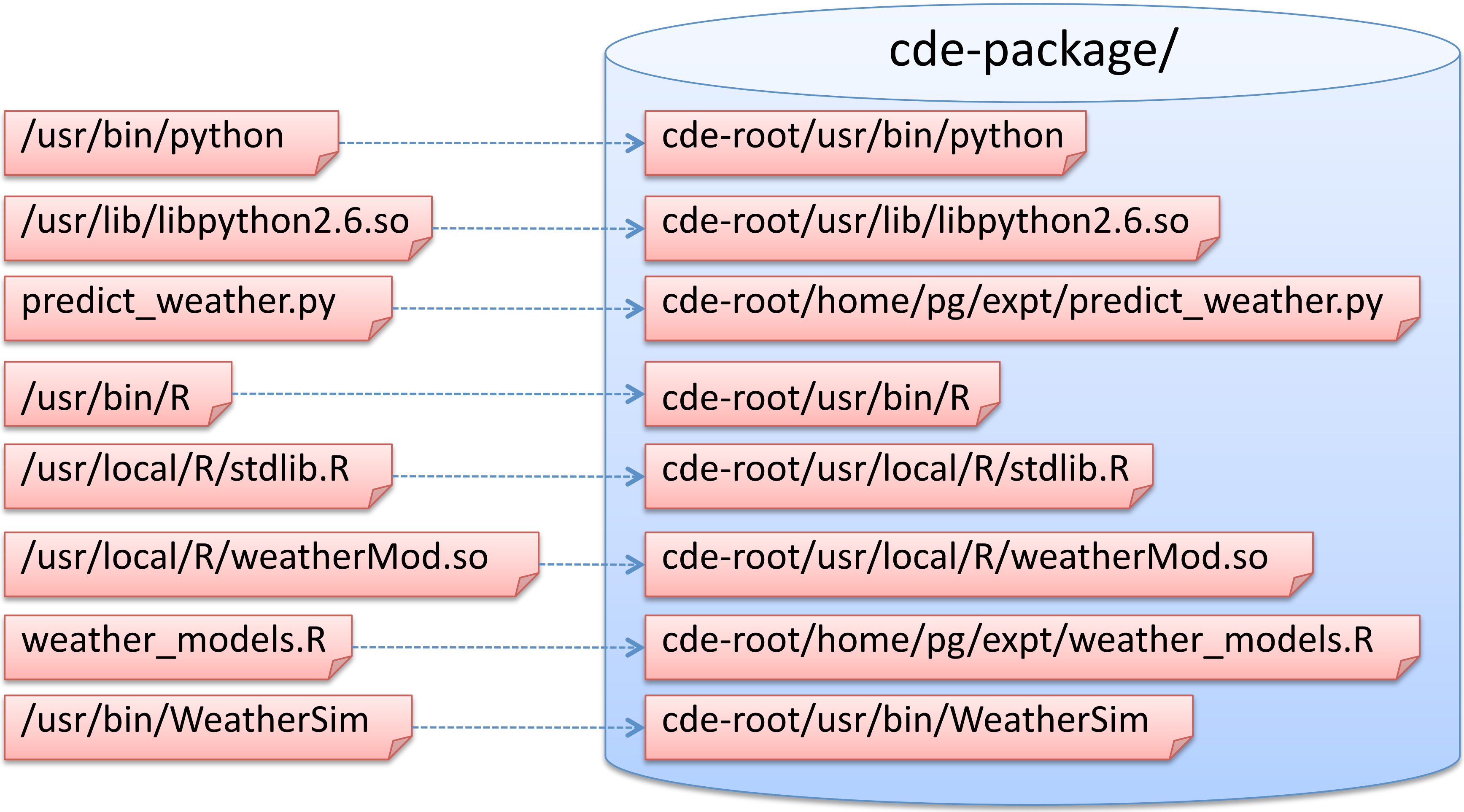



cde-package/

/usr/bin/python → cde-root/usr/bin/python

/usr/lib/libpython2.6.so → cde-root/usr/lib/libpython2.6.so

predict_weather.py → cde-root/home/pg/expt/predict_weather.py

/usr/bin/R → cde-root/usr/bin/R

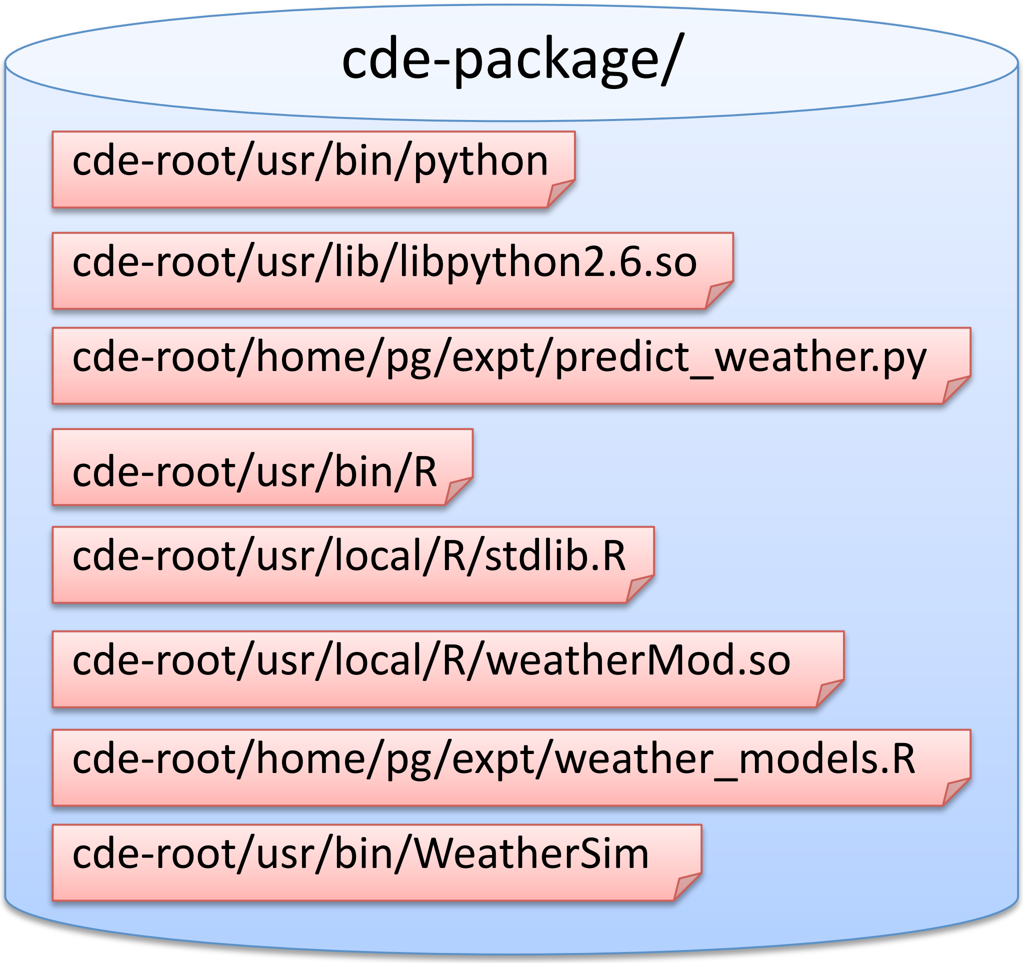
/usr/local/R/stdlib.R → cde-root/usr/local/R/stdlib.R

/usr/local/R/weatherMod.so → cde-root/usr/local/R/weatherMod.so

weather_models.R → cde-root/home/pg/expt/weather_models.R

/usr/bin/WeatherSim → cde-root/usr/bin/WeatherSim

Transfer package to target machine



cde-package/

cde-root/usr/bin/python

cde-root/usr/lib/libpython2.6.so

cde-root/home/pg/expt/predict_weather.py

cde-root/usr/bin/R

cde-root/usr/local/R/stdlib.R

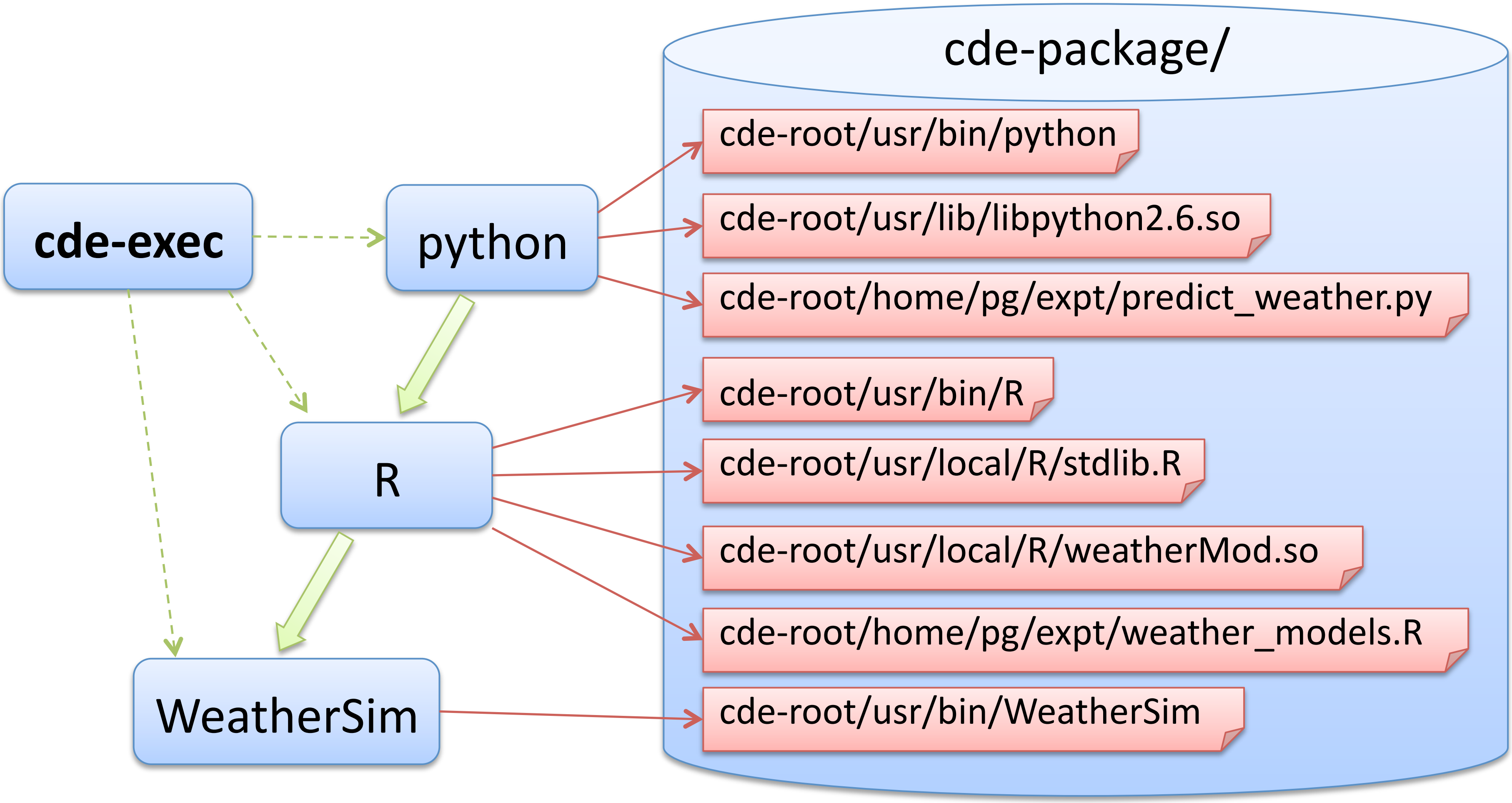
cde-root/usr/local/R/weatherMod.so

cde-root/home/pg/expt/weather_models.R

cde-root/usr/bin/WeatherSim

Executing a package with cde-exec

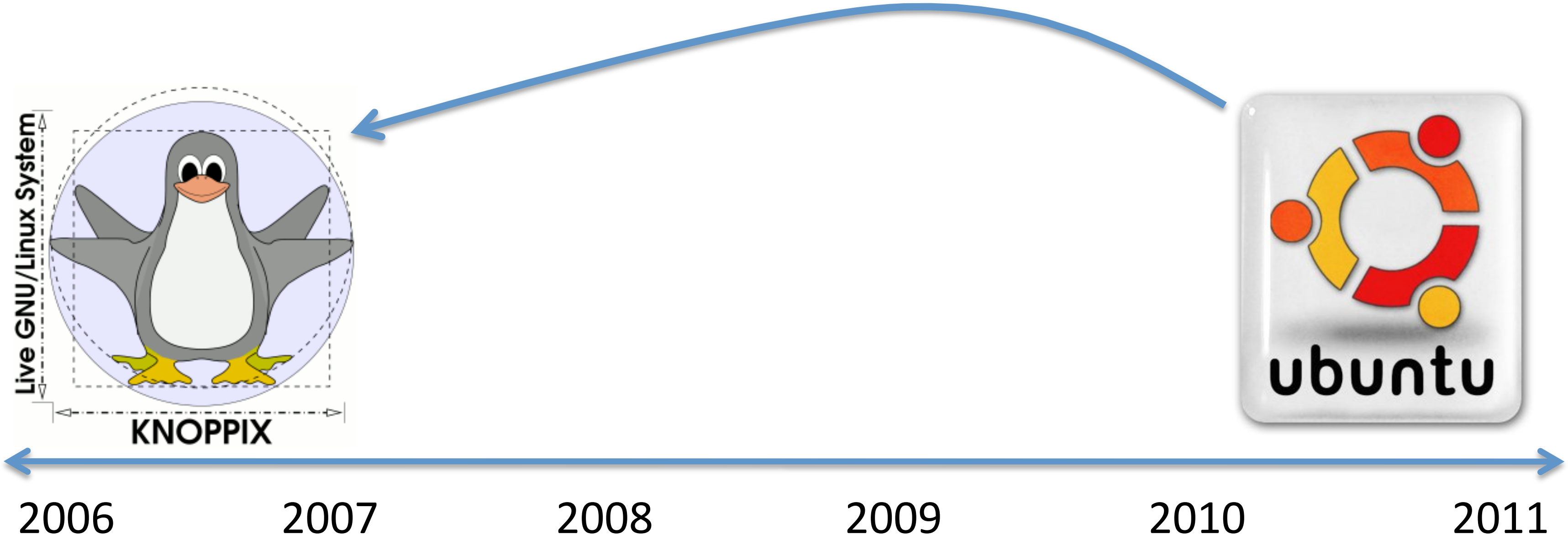
```
cd cde-package/cde-root/home/pg/expt/
cde-exec python predict_weather.py
```



cde-package/
cde-exec
python
R
WeatherSim
cde-root/usr/bin/python
cde-root/usr/lib/libpython2.6.so
cde-root/home/pg/expt/predict_weather.py
cde-root/usr/bin/R
cde-root/usr/local/R/stdlib.R
cde-root/usr/local/R/weatherMod.so
cde-root/home/pg/expt/weather_models.R
cde-root/usr/bin/WeatherSim

“Live” demo

[To watch the demo video, visit: http://vimeo.com/20256490]



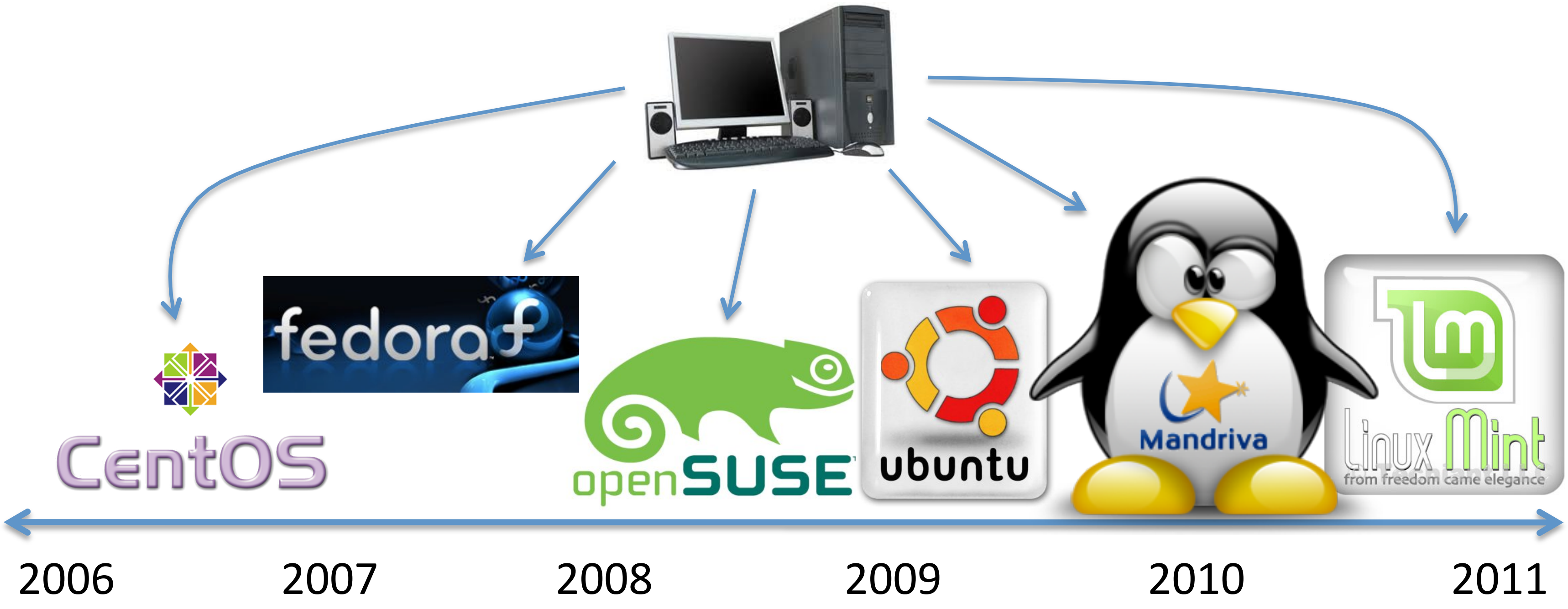
2006 2007 2008 2009 2010 2011

Knoppix 5.0.1
Linux 2.6.17
(black terminal)

Ubuntu 10.10
Linux 2.6.35
(purple terminal)

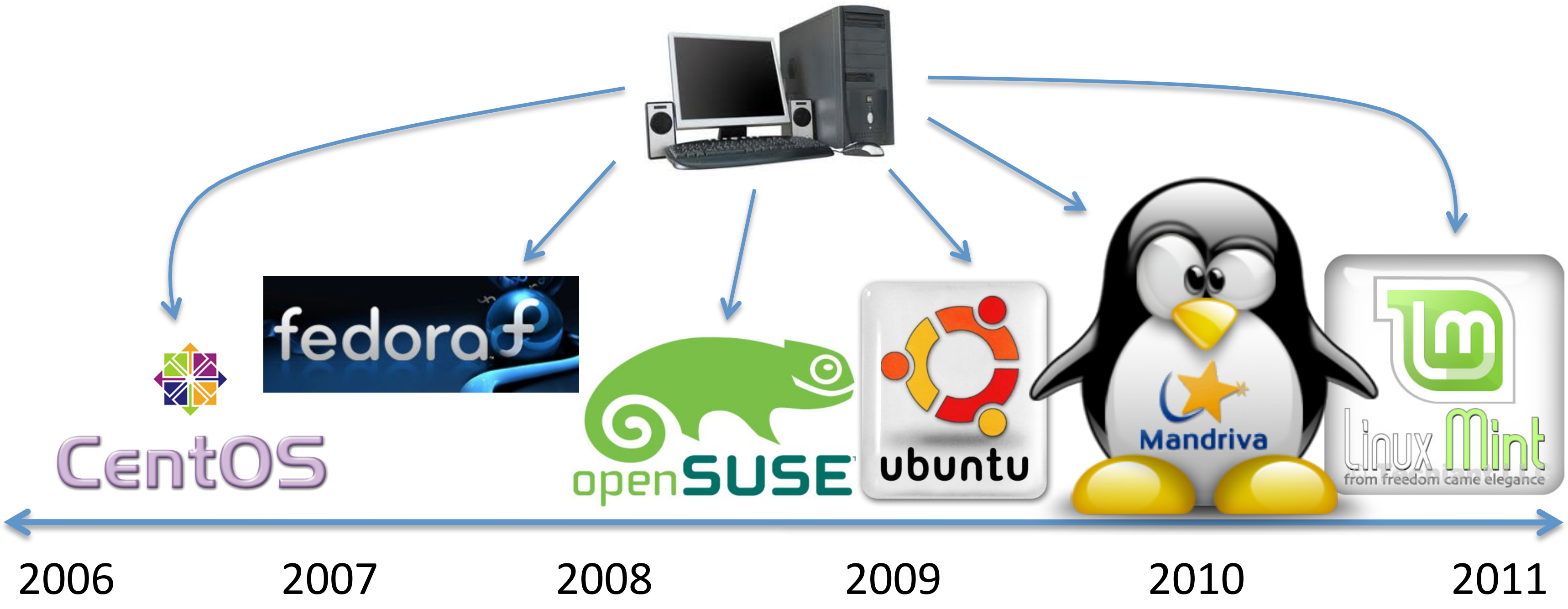
Benefits

1. Creating a CDE package is as easy as running your original experiment
2. Works with existing languages and tools
3. Executing a CDE package requires no installation, setup, or root permissions



Limitations

1. Packages might be incomplete
2. Execution is slower (2% - 30%)
3. Cannot emulate custom hardware
4. Only x86→x86, Linux 2.6→Linux 2.6



Integrating with other tools

CDE + VM: Greater portability than CDE alone, enables longer-term archiving of experiments

CDE + EC2: Instant cloud deployment, enables reviewers to ssh/VNC into a public URL and re-run your experiments

CDE + Git: Easily collaborate with executable experiment repositories

CDE + <*your tool*>: Let's seriously talk!

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Technical

Summary / sales pitch for CDE

Simple promise: If you can run a set of commands on your Linux machine, then CDE allows anyone to easily re-run those same commands on their Linux machine.

Legacy-friendly: Scientists can work in their favorite programming languages or GUI tools.

Battle-hardened: Thousands of downloads, hundreds of subtle bug fixes enable it to work “out-of-the-box”.

Integration-ready: Can serve as a layer below other more sophisticated tools. Let’s discuss integration!