

Sustainability and Reproducibility via Containerized Computing

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Computational Science & Engineering Software Sustainability and Productivity Challenges (CSESSP Challenges)

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Typical Email About Build Problems

```
From: Xyzzy User
Date: Sun, Oct 11, 2015 at 6:55 PM
Subject: need help with python/IPython setup at NERSC
To: Xyzzy Developer
```

Hi,

```
I updated xyzzy, xyzzy_init_tools, and xyzzy_viewer
I recompiled/installed all three on Edison.
```

```
Using your example script
```

```
.../xyzzy-initialization-tools/example_script/xyzzy_script.py
(and setting use_beam=1)
```

```
I find that Xyzzy runs and a beam appear to be generated.
```

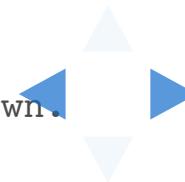
```
I've never gotten xyzzy_viewer to work on NERSC.
Neither the python script nor the IPython Notebook.
```

```
So, I wrote some simple python code to read the HDF5 files.
However, it appears their structure has changed significantly.
So, I thought I should try harder to use the xyzzy_viewer code.
```

```
I used pip to successfully install the latest version of IPython
locally on Edison.
```

```
However, there's something wrong with my environment
or my Python installation and I can't seem to fix it on my own.
```

```
I use the bash shell
```





Build Once

```
$ git clone -q https://github.com/radiasoft/containers
$ cd containers
$ bin/build docker radiasoft/beamsim
[...snip...]
$ docker push radiasoft/beamsim
$ bin/build vagrant radiasoft/beamsim
```



Install Anywhere

On your Mac:

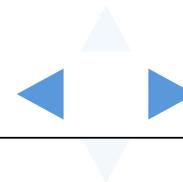
```
$ curl radiasoft.download | bash -s beamsim
Installing with vagrant ...
```

On Linux:

```
$ curl radiasoft.download | bash -s beamsim
Installing with docker ...
```

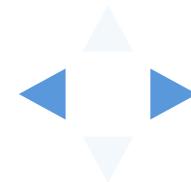
On your PC:

```
> vagrant init radiasoft/beamsim
> vagrant up
[...snip...]
> vagrant ssh
```





Versioned Containers
=> Reproducibility





Source Code and Future

- Just scripts - Containerization simplifies CM
- Fork me - <http://github.com/radiasoft>
- /containers - build scripts to create images
- /download - install scripts to start containers
- rsl.link/srcc - article and bibliography
- TODO - dockerless Linux (AVFS?), simulation repo, auto-updating, package inventory, Windows installer

THANK YOU!

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