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Stacks in HPC

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Charliecloud

Unprivileged Containers for User-Defined Software Stacks in HPC

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Los Alamos National Laboratory



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 - Mission: To solve National Security challenges through Scientific Excellence
 - Part of the NNSA “Tri-Lab” partnership with Lawrence Livermore and Sandia Labs
 - We perform a wide variety of classified and open scientific research and development.
-
- Funded primarily by the Department of Energy, we also do extensive work for/with the Departments of Defense and Homeland Security, the Intelligence Community, et al.
 - Our strategy reflects US government priorities including nuclear security, intelligence, defense, emergency response, nonproliferation, counterterrorism, and more.
 - We help to ensure the safety, security, and effectiveness of the US nuclear stockpile.
 - Since 1992, the United States no longer performs full-scale testing of nuclear weapons. This has necessitated continuous, ongoing leadership in large-scale simulation capabilities realized through investment in high-performance computing.

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LANL HPC Division

- LANL's history in high-performance computing is long and storied, dating back to the early '50s.
- Accomplishments include:
 - Helped IBM develop the 1st transistor-based supercomputer, Stretch
 - Our CM-5 was #1 on the inaugural Top500 List
 - The 1st vector computer, Cray-1, deployed here
 - 1st hybrid supercomputer (using IBM POWER and PlayStation Cell processors), Roadrunner, was also 1st to break the PetaFLOP/s barrier
- Led by Gary Grider, creator of Burst Buffer technology
- We support over 2000 unique users across more than 100 different classified/open science projects on 20+ clusters



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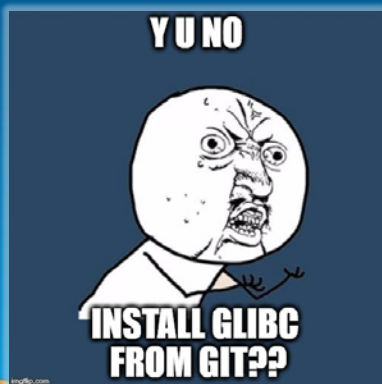
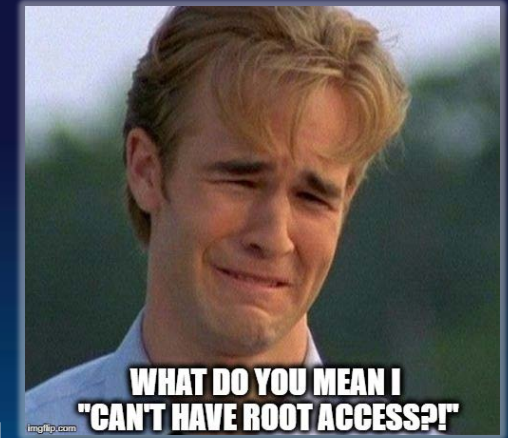
First World Problems in HPC

Problem #1: HPC clusters have narrowly focused software stacks.

- They do serial and parallel-MPI tasks well...but that's it.
- Compute node images are often in RAM/NFS & kept small.
- Managing multiple OSs, and required expertise, is rare & labor intensive.

Problem #2: We're old. And not getting any younger.

- Schools are teaching clusters, "parallel"/scalable/distributed software development...but usually "embarrassingly parallel" (e.g., map/reduce)
- All the "cool kids" are using Ubuntu (or Arch, or Alpine...), not RHEL
- Modern Machine Learning and Data Analytics tool suites are non-trivial



Problem #3: We are finite, as is our time.

- We generally won't install extra software with low user demand.
- Unique or unusual use cases tend to be lower priority.
- The line between "innovator" and "crackpot" is often rather blurry....

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The Solution: UDSS/UDI/BYOE

User-Defined Software Stacks (UDSS) allow users to supply not only their own applications/source to run on HPC systems but also the environment -- up to and including entire OS images -- in which they should run!

Advantages include portability, usability, consistency, time savings...

Potential disadvantages include missing functionality (HSN, accelerators, filesystems), performance degradation; thus, addressing these should be part of the design of any HPC-focused solution!

In rare, specific cases, certain packages may address this independently by building static binaries or otherwise coupling dependencies with executables

- Works everywhere
- No privileges required
- Requires build-time support
- May or may not be feasible
- For everyone else, our options are...



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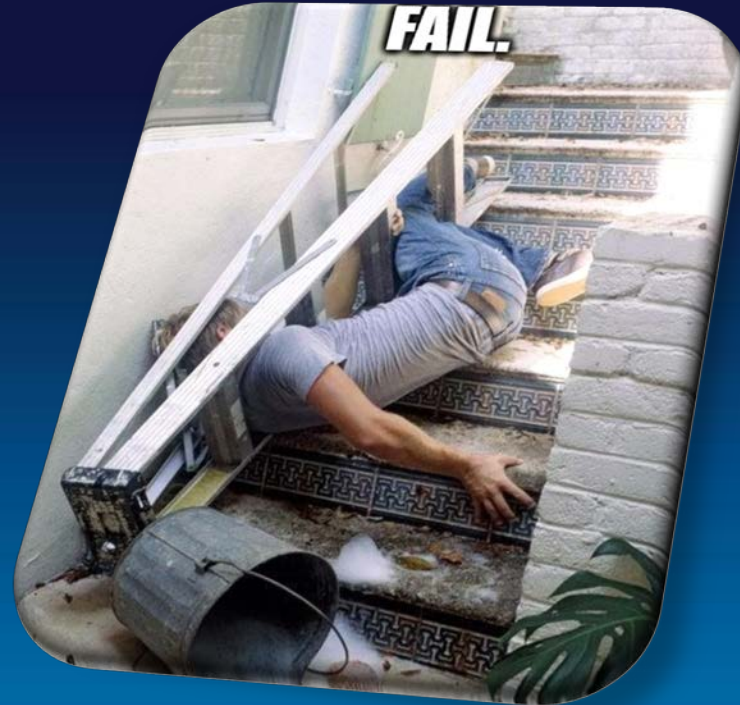
Option #1: Compile It Yourself

Advantages

- Available everywhere immediately
- Requires no privileges
- No additional privacy/security risk
- Direct access to all hardware
- No performance penalty
- Theoretically applies to any open source software library/app/stack

Disadvantages

- ...but it's, like, 2017. And stuff.
- Tedious and time-consuming
- Error-prone
- Hard to update
- No standard workflow
- Provides neither portability nor consistency



Nope.

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Option #2: Environment Manager

Advantages

- Available for most IA32/x64 systems
- Requires no privileges
- No additional privacy/security risk
- Direct access to all hardware
- No performance penalty

Disadvantages

- Frequently still requires building from source (time/space constraints)
- Varying degrees of HPC support
- Varying degrees of reproducibility, portability, consistency, workflow
- Users/consultants bear entire burden

If You Must...

- Good options include EasyBuild, Lmod, Spack
- Also Anaconda, nixOS



*“There’s GOT to be a
BETTER WAY!!”*

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Option #3: Virtualization (VMs)

Advantages

- Ultra-flexible (any kernel/OS/arch)
- Strong-to-complete isolation
- Common use cases perform well

Disadvantages

- Performance suffers for most HPC use cases, often significantly
- Performance/isolation tradeoffs
- Infrastructure can be complex
- Direct/performant access to hardware may require privileges
- Not all “exotic” HPC hardware supported
- Entire OS must be provisioned and booted, separate hostname/IP, etc.



Should HPC become the Cloud?

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Option #4: Containers

Advantages

- Enough flexibility (only share kernel)
- Enough isolation (namespaces, etc.)
- Standard, reproducible workflow
- Bare-metal performance (or close)
- Minimal or no user/consultant burden (presumes correct solution choice)
- Extremely simple and easy-to-use (presumes correct solution choice)

Disadvantages

- Require recent Linux kernel/distro (SLES 12SP2, RHEL 7.4, Ubuntu 16.04, Linux LTS 4.4/4.9) **or** privilege
- Occasional growing pains due to newness (feature-complete in 2013)
- Container expertise in HPC still rare; thus, bad info/myths are pervasive!



Should HPC use containers?

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So...Umm...These Container Things...Like, What Are They?

Good question! Not everyone agrees. Here's our take.

Linux Containers:

- Use one or more kernel **namespaces** to provide isolation for (i.e., “contain”) a process (along with its child processes, if any);
- Envelope/restrict the process(es) such that escape/escalation is “impossible;” and
- Facilitate application security by providing capability constraints, integrity assurance, and content validation via industry-standard formats and workflows.



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Namespaces, You Say?

The Linux Kernel supports 6 namespaces as of version 3.8, 7 as of 4.6.

- 6 Privileged Namespaces (require `CAP_SYS_ADMIN` to create)
 - `mount` – Private filesystem mount points, recursion/propagation controls
 - `pid` – Private view of process IDs and processes, `init` semantics
 - `uts` – Private hostname and domainname values
 - `net` – Private network resources (devices, IPs, routes, ports, etc.)
 - `ipc` – Private IPC resources (SysV IPC objects, POSIX msg queues)
 - `cgroup` – Private control group hierarchy (Linux 4.6+ only)
- 1 Unprivileged Namespace (requires no special capabilities to create)
 - `user` – Private UID and GID mappings
 - Can be combined with other namespaces, even if unprivileged
- System Call API: `unshare(2)`, `clone(2)`, `setns(2)`

Further reading: “Namespaces in Operation” (<https://lwn.net/Articles/531114/>)

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The Container Landscape

Full-featured Container Systems

- Support building, distribution, validation, and execution
- Provide for complete handling of containers throughout lifecycle
- Examples: Docker, Rocket, LXC/LXD
- Most modern container engines now implement Open Container Initiative (OCI) Image and/or Runtime Specification(s)
- Building containers is still a per-system function. OCI does NOT do building!
 - Dockerfiles are the de facto standard; robust, capable DSL
 - CoreOS Rocket supplied acbui ld based around traditional shell-fu

Lightweight Container Systems

- Generally only provide runtime; most leverage Docker ecosystem
- Tend to require existing directory tree (i.e., flattened image) to run in
- Examples: RunC, CCon, NsJail, unshare(1), systemd- nspawn(1)
- ...and of course, Charliecloud!



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Additional Container Elements

The Linux kernel has several additional subsystems that containers use:

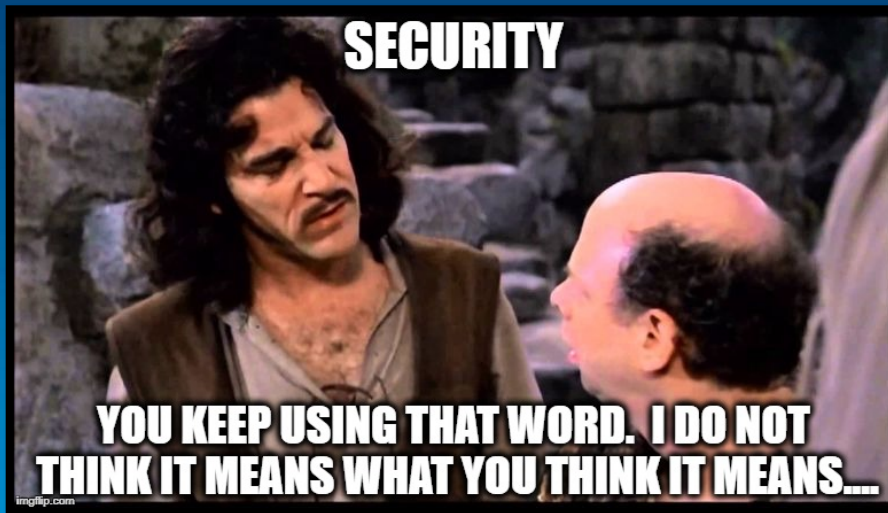
- **cgroups** – Control hierarchical resource management and constraint
 - Latest kernels (4.6+) even have namespaces for this!
 - This is how modern schedulers/RMs track/control job resource usage
- **seccomp- bpf** – Berkeley Packet Filter-based system call filtering
 - Frequently used to prevent containers exceeding their scope
- **prctl (PR_SET_NO_NEW_PRIVS)** – Prevent privilege escalation
 - Permanent, kernel-level flag that prevents `execve()` ever granting privileges
 - Preserved across all calls to `fork()`, `clone()`, and `execve()`
- **SELinux** – Labeling system for filesystems and applications
 - Allows admins precise control over actions, roles of applications
- **AppArmor** – Profile-based MAC system for limiting applications' abilities
 - Similar to SELinux but without filesystem labeling features

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Let's Talk Security

As with all aspects of Cybersecurity, true security isn't merely the absence of access but rather the presence of protection!

- Container security relies entirely on the separation of authorities which exists inside the Linux kernel. If the kernel fails, the container fails.
- Container security relies, among other things, on a wide variety of content assurance methodologies (e.g., non-repudiation, CAS) along with aforementioned protections.
- Lightweight container solutions have the advantage of leaving much of that to others.



Question: Is Docker "Insecure?"

Short Answer: Nope.

Longer Answer: Absolutely, positively, without a doubt...nope. Not any more. Ignore the FUD.

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Why Charliecloud?

- Docker has a great security story (now) but not a great performance story!
 - OverlayFS is sloooooooooow due to layering
 - File removal is done literally by “whiting out”
 - Subtle nuances with, e.g., Yum/RPMD
 - Charliecloud leverages OCI-like “flattened” directory structure
- HPC users don’t need flexibility/overhead of `config.json`
 - Inside user namespace, other namespaces can be created/joined using `unshare(1)`, `nsenter(1)`
 - Additional security hardening coming soon
- A simple API should result in small, simple code
 - Charliecloud weighs in at fewer than 1000 LoC
 - Compare to NSJail (4,000), Shifter (19,000), Singularity (14,000), and Docker (133,000)!



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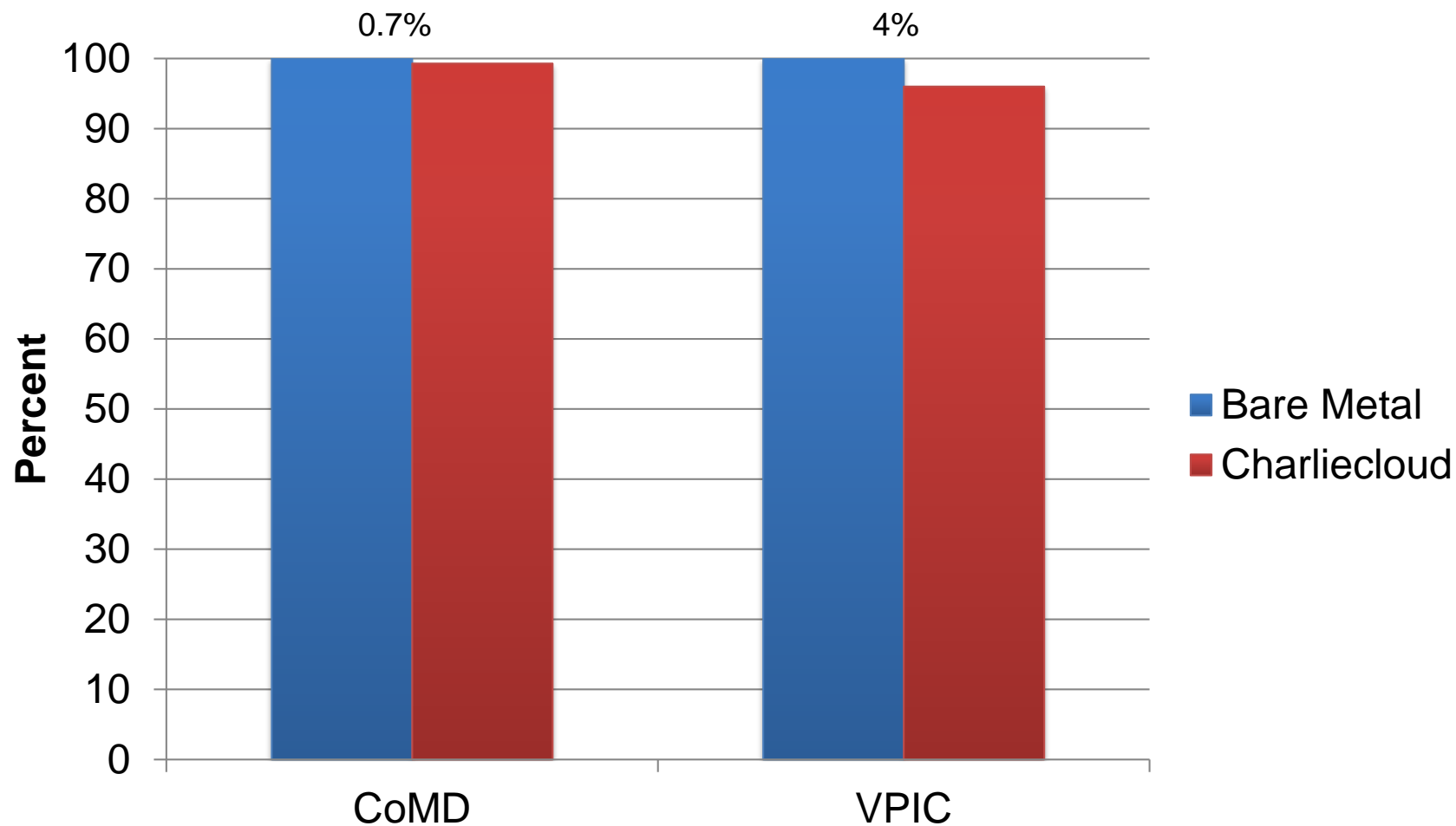
Charliecloud Demo/Walkthrough

```
$ cd ~/charliecloud/examples/serial/hello
$ ls
Dockerfile  hello.sh  README  test.bats
$ ch-build -t hello ~/charliecloud
Sending build context to Docker daemon 15.19 MB
[...]
Successfully built 30662b3f94f3
$ ch-docker2tar hello /var/tmp
57M /var/tmp/hello.tar.gz
```

```
$ ch-tar2dir /var/tmp/hello.tar.gz /var/tmp/hello
creating new image /var/tmp/hello
/var/tmp/hello unpacked ok
$ ch-run /var/tmp/hello -- cat /etc/debian_version
8.9
```

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Charliecloud MPI Performance



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Charliecloud Resources

- Supercomputing 2017 Paper
by Reid Priedhorsky and Tim Randles
 - “Charliecloud: Unprivileged Containers for UDSS in HPC”
 - Los Alamos Tech Report LA-UR-16-22730
 - <http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-16-22370>
- ;login: Article “Linux Containers for Fun & Profit in HPC”
by Reid Priedhorsky
 - <https://www.usenix.org/publications/login/fall2017/priedhorsky>
- Documentation: <https://hpc.github.io/charliecloud> (includes tutorials!)
- Source Code: <https://github.com/hpc/charliecloud>
- Mailing List: charliecloud@groups.io || <https://groups.io/charliecloud>
- Contact Reid (reidpr@lanl.gov), Tim (trandles@lanl.gov),
or Michael (mej@lanl.gov, [@mej0](https://twitter.com/mej0) on Twitter)



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Questions/Comments?

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THANK YOU!

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