CRAY

ADAC6

Appropriate Use of Containers in HPC

Agenda

- Why HPC containers
- Investigate different container runtimes for HPC
- Integration with batch systems
- Best practices for HPC
- HPC Application performance

Why HPC containers

- **Mobility of computing to both users and HPC centers**
  - Means to capture and distribute software and compute environments
  - Entire workflow can be contained for others to replicate no matter what version of Linux they are running (Kernel ABI compatibility – syscall's)
- **Reproducibility of results – may not mean same performance**
  - MPI-ABI, libraries, host drivers
- **Standard and simplified packaging**
  - Independent Software Vendors (ISV) codes
  - Delivered benchmarks
  - CRI standard and/or propriety formats
- **Legacy workload packaging and execution**

Container Runtime Environments

- **Enterprise, and HPC container environments**
  - opencontainers/runc
    - **236** contributors, 17 release. 3,613 commits
    - Standard image format (Open Container Initiative – OCI)
  - rtk/rtk
    - **197** contributors, 65 releases , 5,539 commits
    - Standard image format (appc Specification – Application Container Image, ACI)
  - NERSC Shifter (github)
    - **11** contributors, 5 releases, 1,712 commits
    - Propriety image format
  - LBL Singularity (syslabs.io)
    - **63** contributors, 19 releases, 4,503 commits
    - Propriety image format

As of 06/18/18

Integration with batch systems

- **Examples of Moab/Torque and Cray ALPS**
  - Application based utilities
  - Limited or no cgroup and kernel namespace support

① $ aprun -n *N* -b **runc** --bundle /tmp/cle.img run $(date +%Y%m%d%H%M)

② $ aprun -n *N* … -b **rkt** run \
    --stage1-name=coreos.com/rkt/stage1-fly:1.21.0 \
    registry-1.docker.io/library/cle:latest --net=host --exec=/bin/hostname

③ $ aprun -n *N* … -b **shifter** --image cle:latest /bin/hostname

④ $ aprun -n *N* … -b **singularity** exec /global/cle.img /bin/hostname

Container Runtime Specifics

- Container runtimes configuration and semantics
- Unique image management
- Runtime arguments are specific

Configuration & Runtime options

- **runc**
  - Embedded in the OCI image definition: `config.json`
- **rkt**
  - /etc/rkt, /usr/lib/rkt, user-defined
    - Repository authentication, data and image locations
    - Command line can override system configurations
- **Shifter**
  - System configuration (/etc/shifter)
    - Authentication, data and image locations
- **Singularity**
  - System configuration $SYSCONFDIR/singularity/singularity.conf
    - Authentication, data and image locations

runc

- **Create a root file system, created via Docker container**

```
$ docker export alpine | tar xvfC - ./rootfs
```

- **Create container configuration file *config.json***

```
$ runc spec
$ vi config.json     # modify the args, see OCI specification
```

- **Run the container**

```
$ runc --log /dev/stdout run $(date +%Y%m%d%H%M)
```

OCI specification: https://github.com/opencontainers/runtime-spec/blob/master/runtime.md

rkt

- **Pull an image locallydocker2aci**

```
$ docker2aci docker://jsparkscraycom/cle:6.0.2
```

- **Run the container**

```
$ qsub –I
salloc: Granted job allocation 88
$ rkt run --no-overlay=true --net=host \
   --stage1-name=coreos.com/rkt/stage1-fly:1.22.0 \
    registry-1.docker.io/jsparkscraycom/cle:6.0.2 \
   ${options} –inherit-env=true \
   --environment=LD_LIBRARY_PATH=$LD_LIBRARY_PATH \
   --exec=/lus/${USER}/a.out -- myargs
```

Shifter

- **Pull an image**

```
$ shifterimg pull jsparkscraycom/test:latest
```

- **Run the container**

```
$ shifter --image jsparkscraycom/test:latest \
/usr/bin/date
```

Singularity

- **Pull an image (if needed)**

```
$ singularity pull docker://jsparkscraycom/test:latest
```

- **Run the container**

```
$ singularity exec \
    docker://jsparkscraycom/test:latest \
    /usr/bin/date
```

Container Best Practices

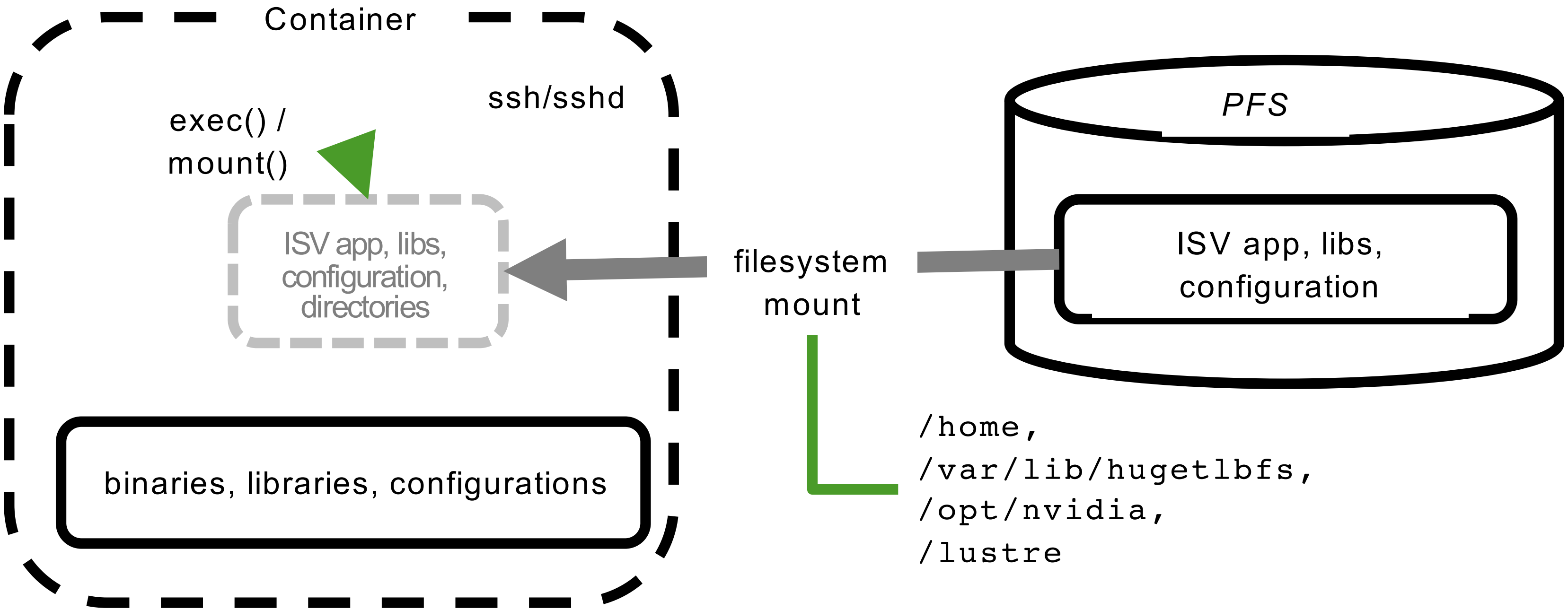
- **Portability**
  - Run anywhere vs. exploit host acceleration
  - Isolated contained environment, aka encapsulation – full vs. partial
- **Image standardization compliance**
  - OCI, ACI and custom (singularity)
- **HPC Optimizations**
  - Override container defaults via mounts and environment variables
    - Libraries and configurations
- **Framework independence**
  - No vendor/runtime lock in
- **Stripped frameworks**
  - opencontainers/runc, Charliecloud, rtk

Containerization Models

- **Enterprise case**
  - Standard runtimes (docker/rkt)
  - Fully encapsulated
    - Everything the application needs is in the container
  - Single application
  - Orchestration software
  - Standard image formats

- **HPC case**
  - HPC runtimes (Shifter/Singularity/...)
  - Partial encapsulation – limited namespaces
    - Access to host resources – networks, storage
    - blurs the line between container and host such that local directories can exist within the container.
  - Multiple applications
  - Batch system integration
  - Image format for scale (pfs)

HPC Partial Encapsulation

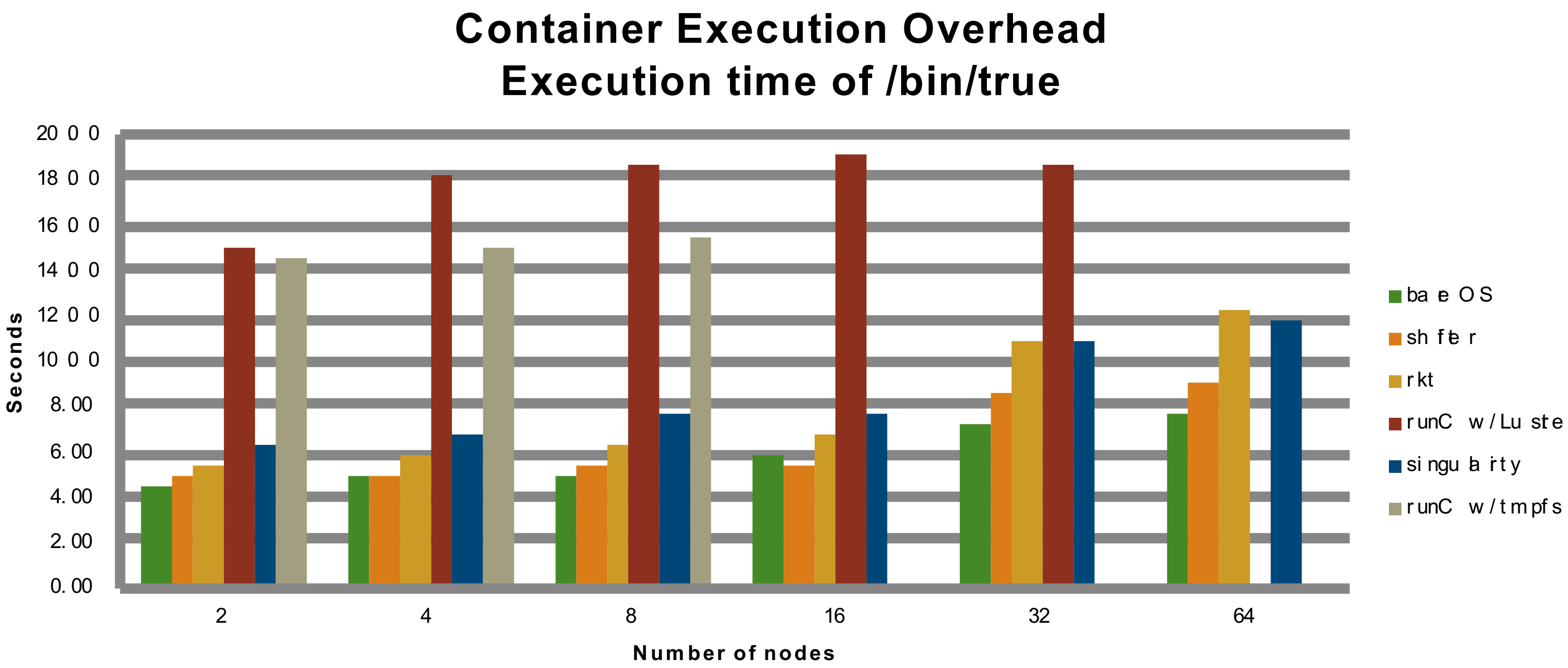


HPC Application performance

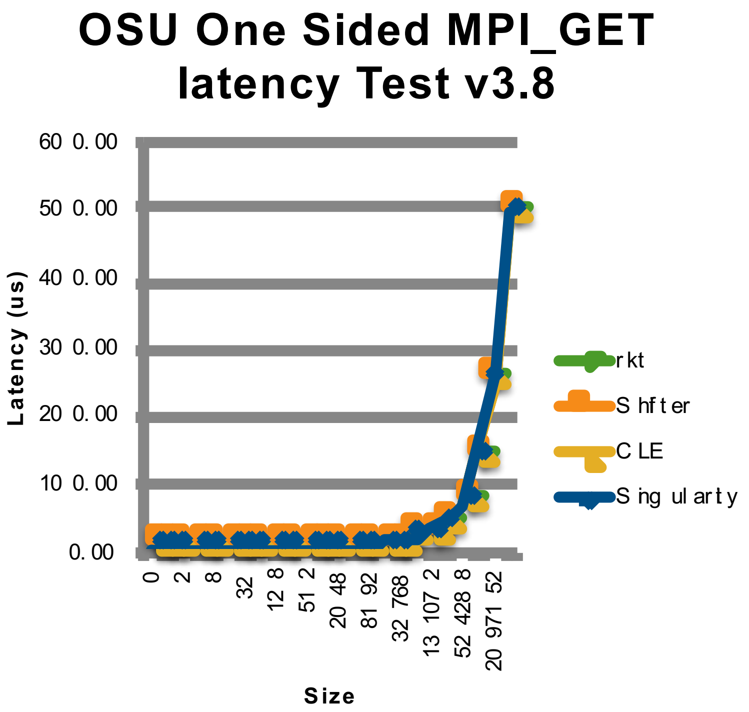
- **Launch times**
  - Time to setup and launch via container runtime
- **Application performance**
  - Hugepage optimization
  - Environment pass-through

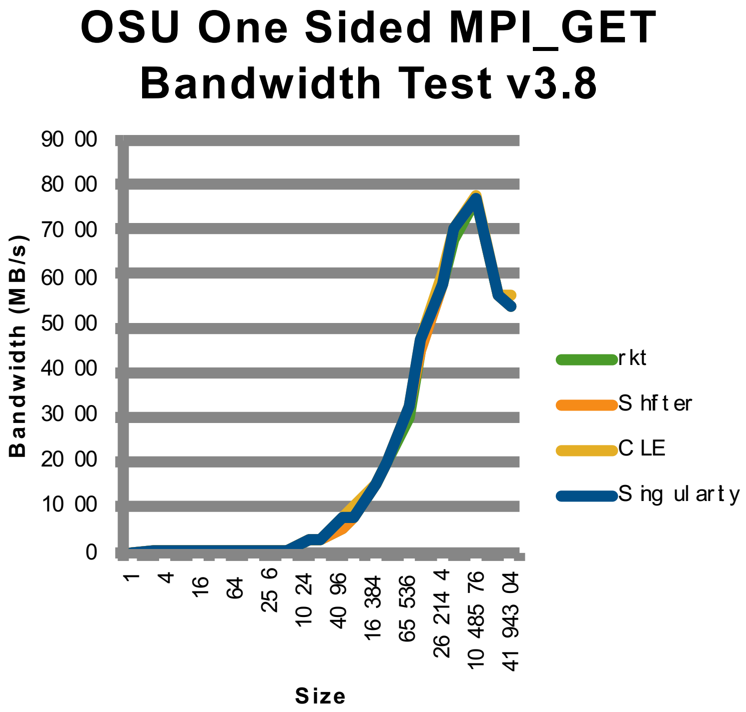
An Updated Performance Comparison of Virtual Machines and Linux Containers
Ref: http://domino.research.ibm.com/library/cyberdig.nsf/papers/0929052195DD819C85257D2300681E7B/$File/rc25482.pdf

Launch Times

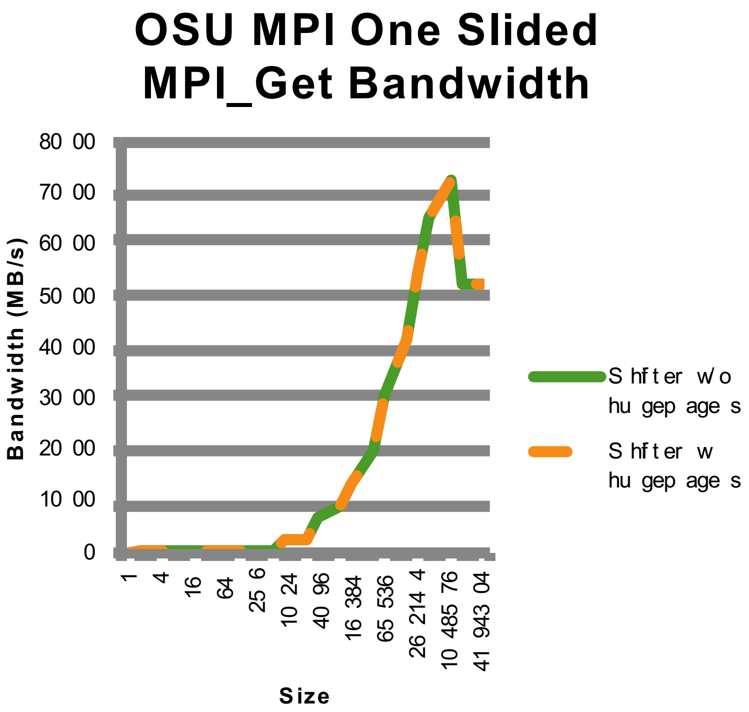


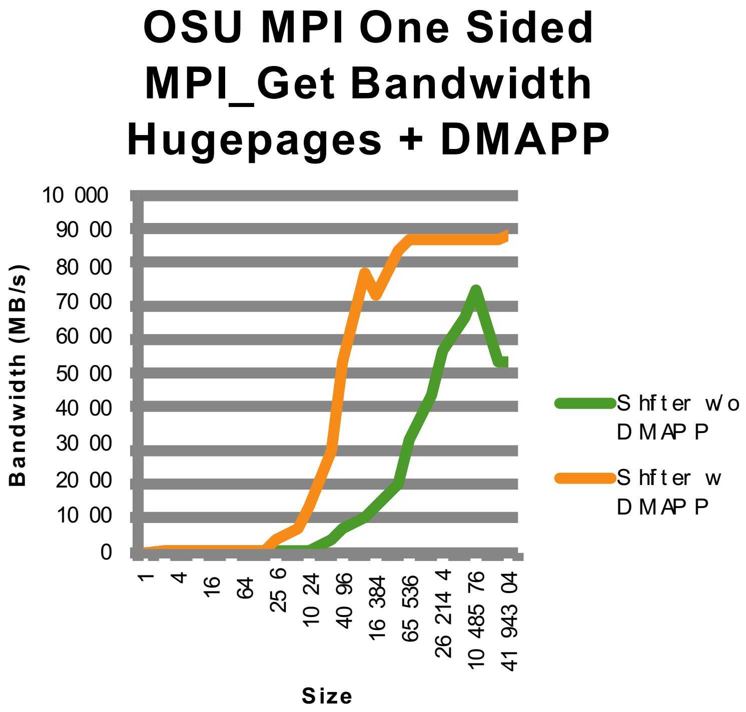
OSU Benchmarks



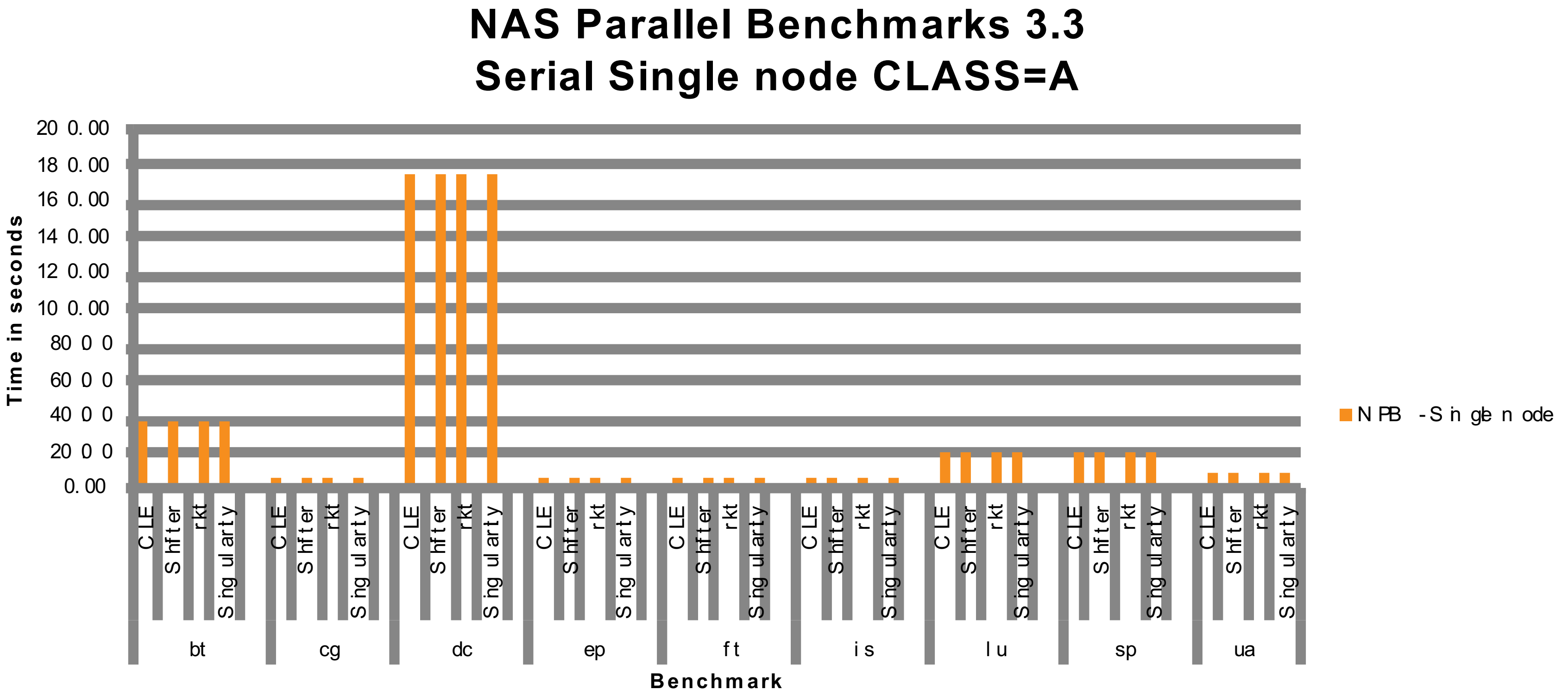


Hugepage / DMAPP

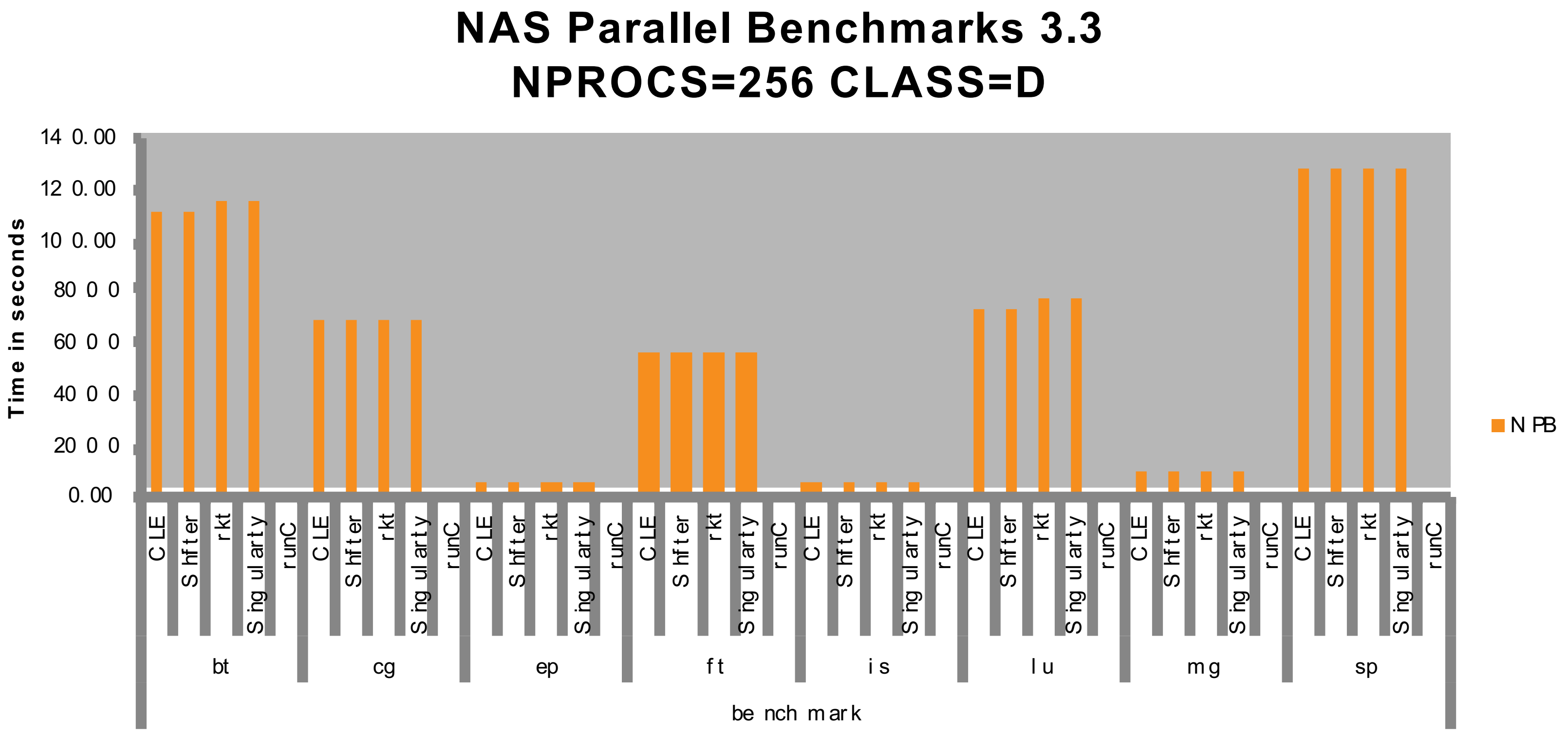




NPB Single node

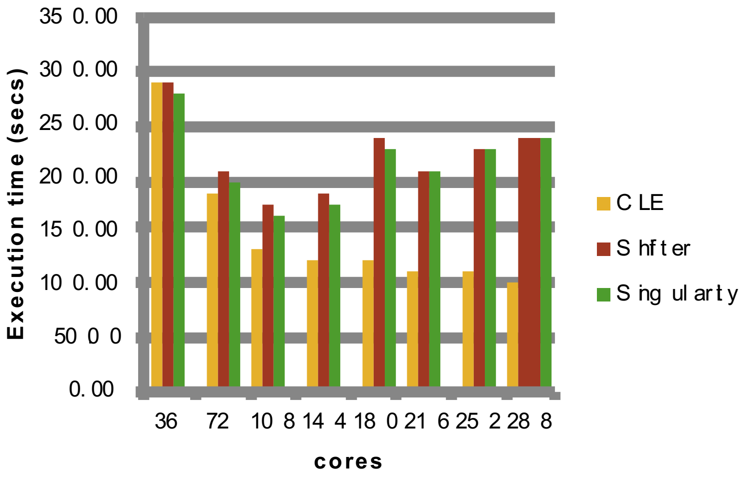


NPB Multi-node

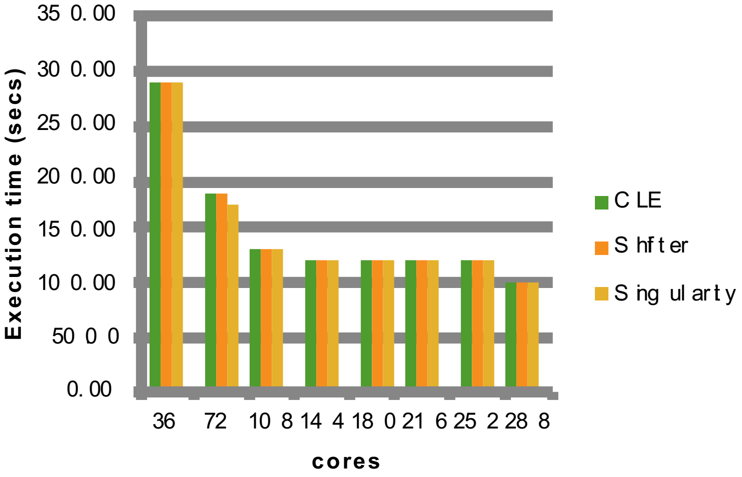


Quantum ESPRESSO – optimization

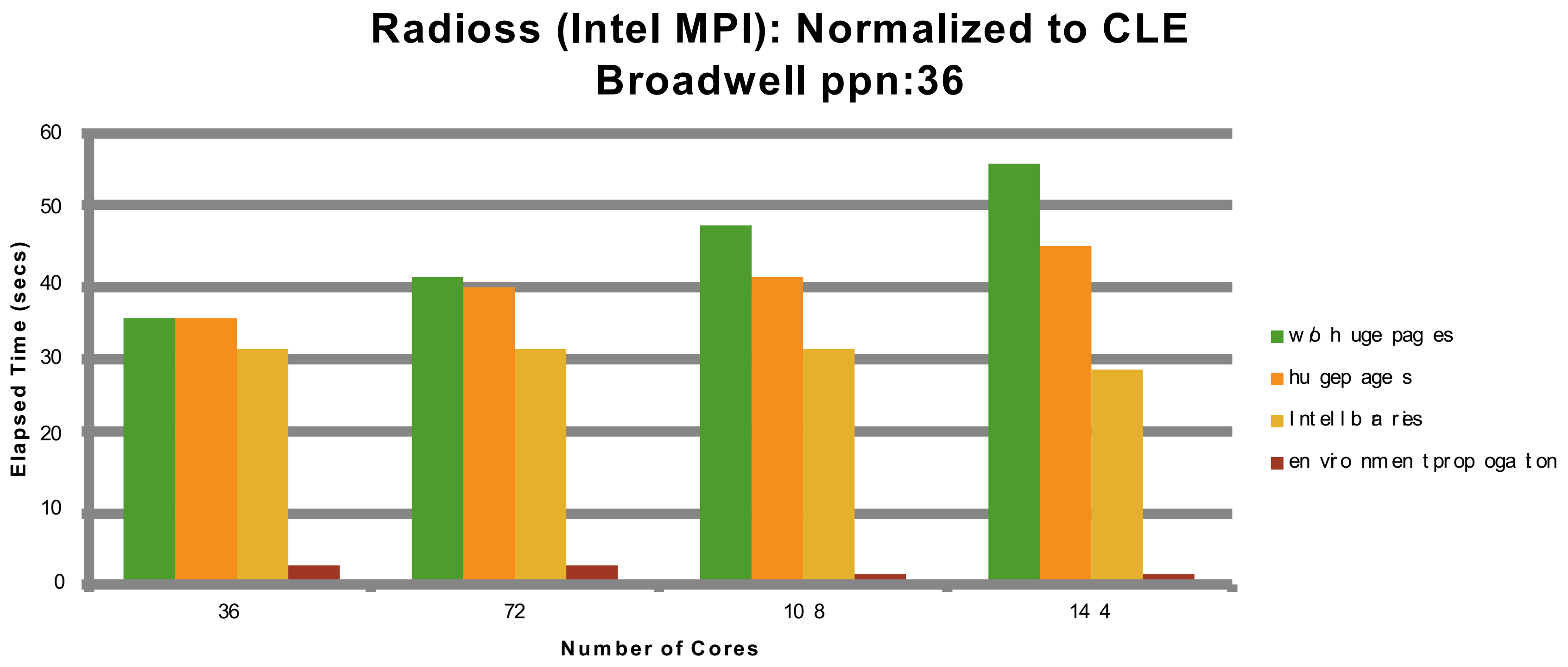
Execution time of QUANTUM ESPRESSO 6.0 / Broadwell none-hugepage



Execution time of QUANTUM ESPRESSO 6.0 / Broadwell hugepage



Radioss – optimization



Conclusions and Future Work

- **Deployment**
  - Enterprise frameworks required per-node image caches
  - Enterprise frameworks, as expected offer more runtime options
  - HPC frameworks enforce strict user security
- **Performance**
  - Native application performance can be achieved, requires host-level access to resources (network, file system)
  - Host environment pass-through
  - Launch time dependent on container infrastructure and image size
- **Future work**
  - Scaling investigation of open container frameworks
    - Shared image storage – faster startup times
  - Abstraction layer standardizing on applications packaging, deployed and run in isolation – OCI.

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