Chong Chen
Lead Product Architect, IBM Platform LSF Family
chong@ca.ibm.com

Using Docker in High Performance Computing

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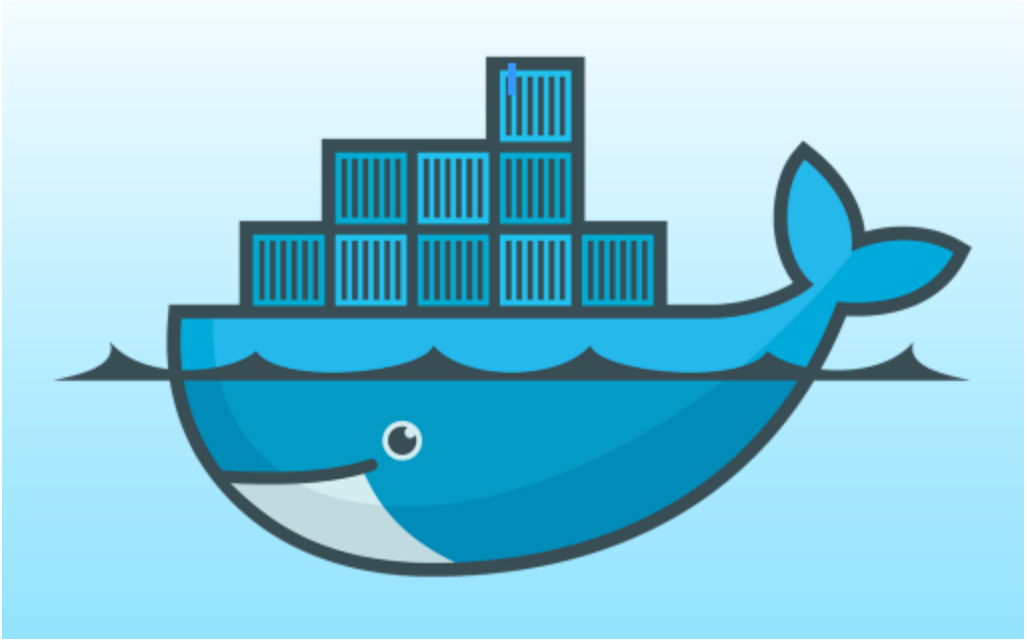
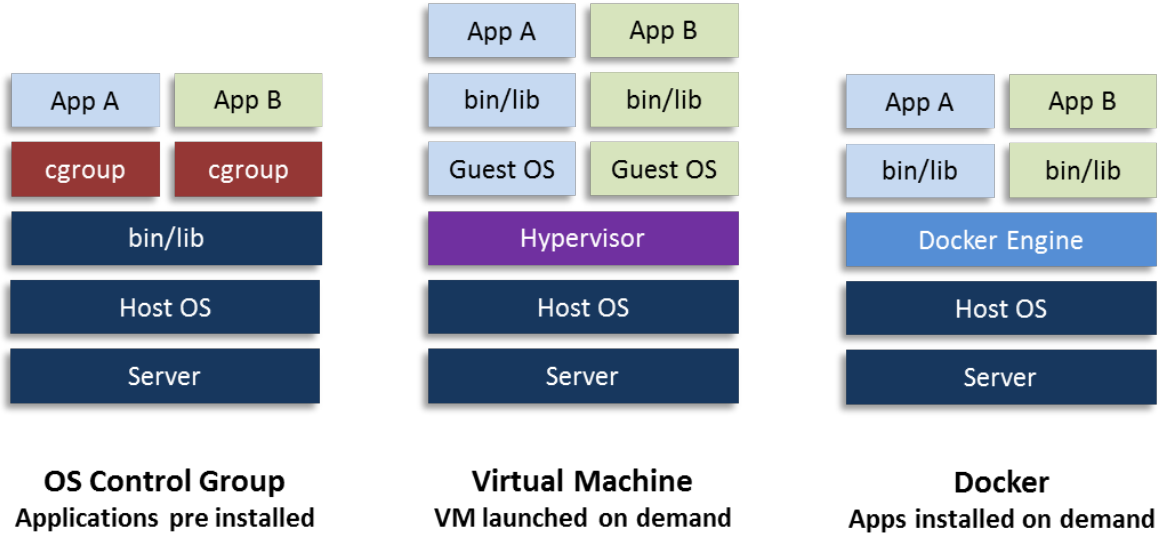
Agenda

- **What is Docker?**
- **LSF & Docker**
- **Next step**
- **Q & A**



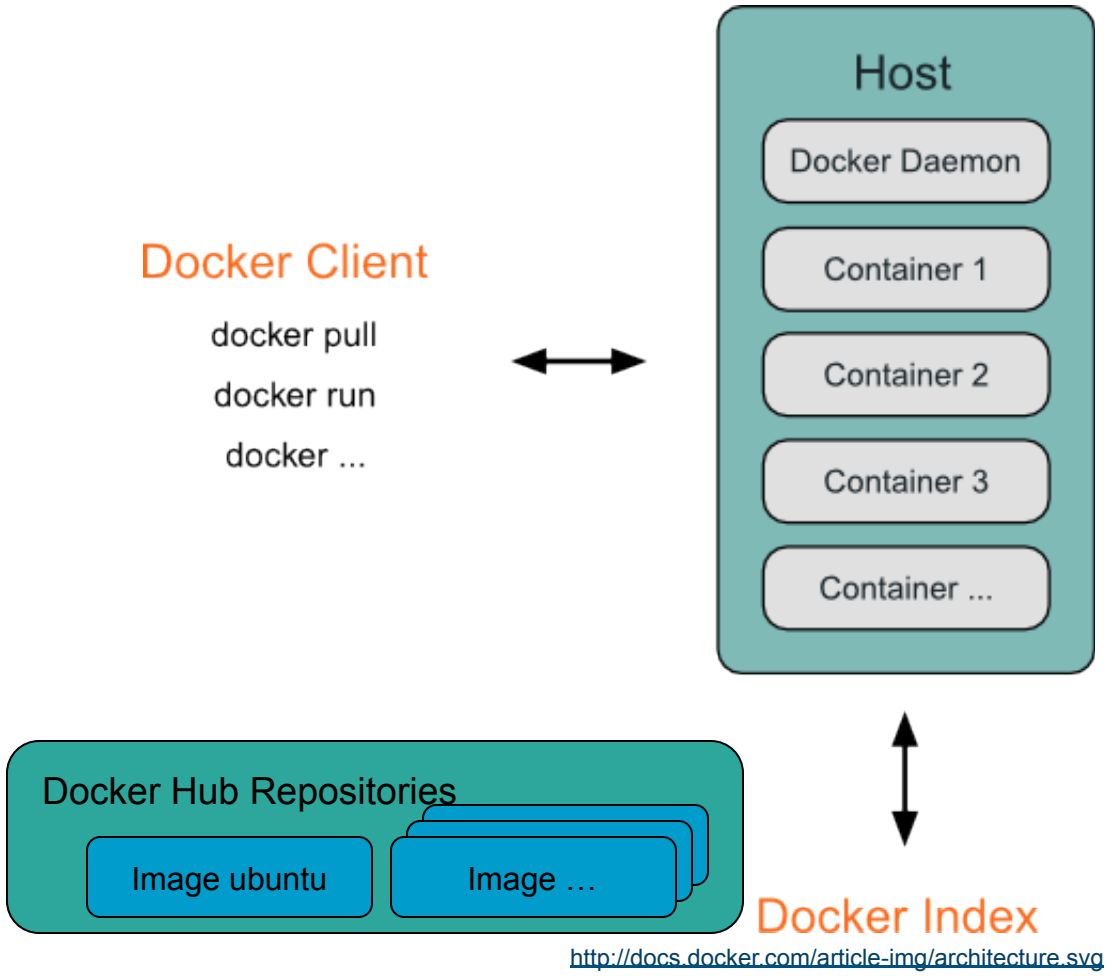
- In short, Docker is a lightweight container technology built on top of linux container, cgroup and AUFS (Another UnionFS)
  - Think of it as “a Virtual Machine, without the overheads or size of a VM, that installs a complete application stack on demand.”



- Hot topic in “cloud & big data” to develop, ship and run applications anywhere and solve “dependency hell” challenges
  - All environment/library/distribution dependencies can be encapsulated within the container, so two applications that would have conflicting libraries requirement can now share the same host.

Docker Architecture

- The Docker Daemon
- The Docker Client
- Inside Docker
  - Docker Images
  - Docker Repositories
  - Docker Containers



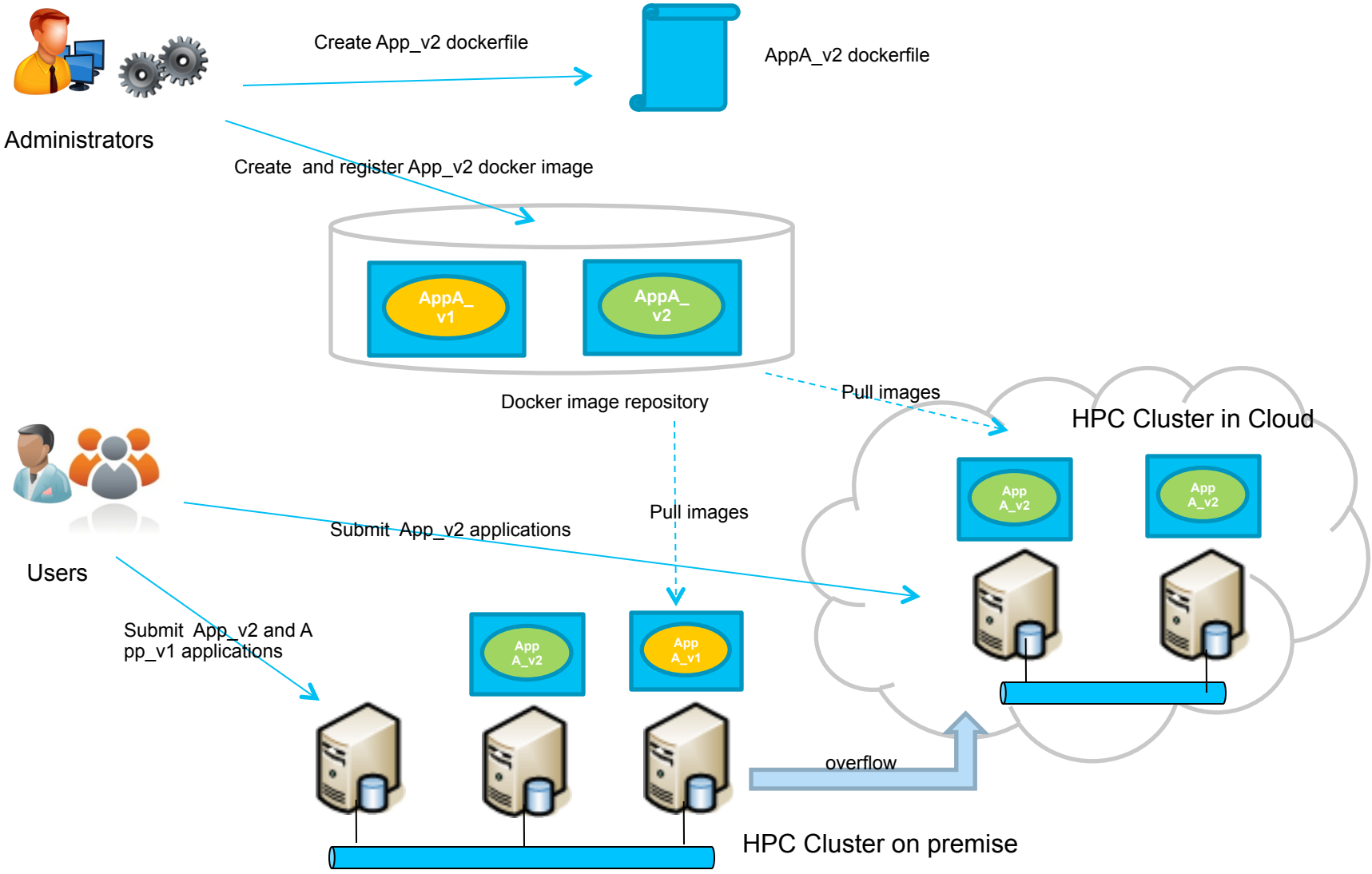
http://docs.docker.com/article-img/architecture.svg

Containers in High Performance Computing

- Not a new idea …
  - Workload resource isolation
  - Process tracking
  - Job controlling
  - Checkpoint/restart, live migration
  - …

- Examples:
  - IBM AIX WLM
  - Linux control group
  - Virtual machine
  - …

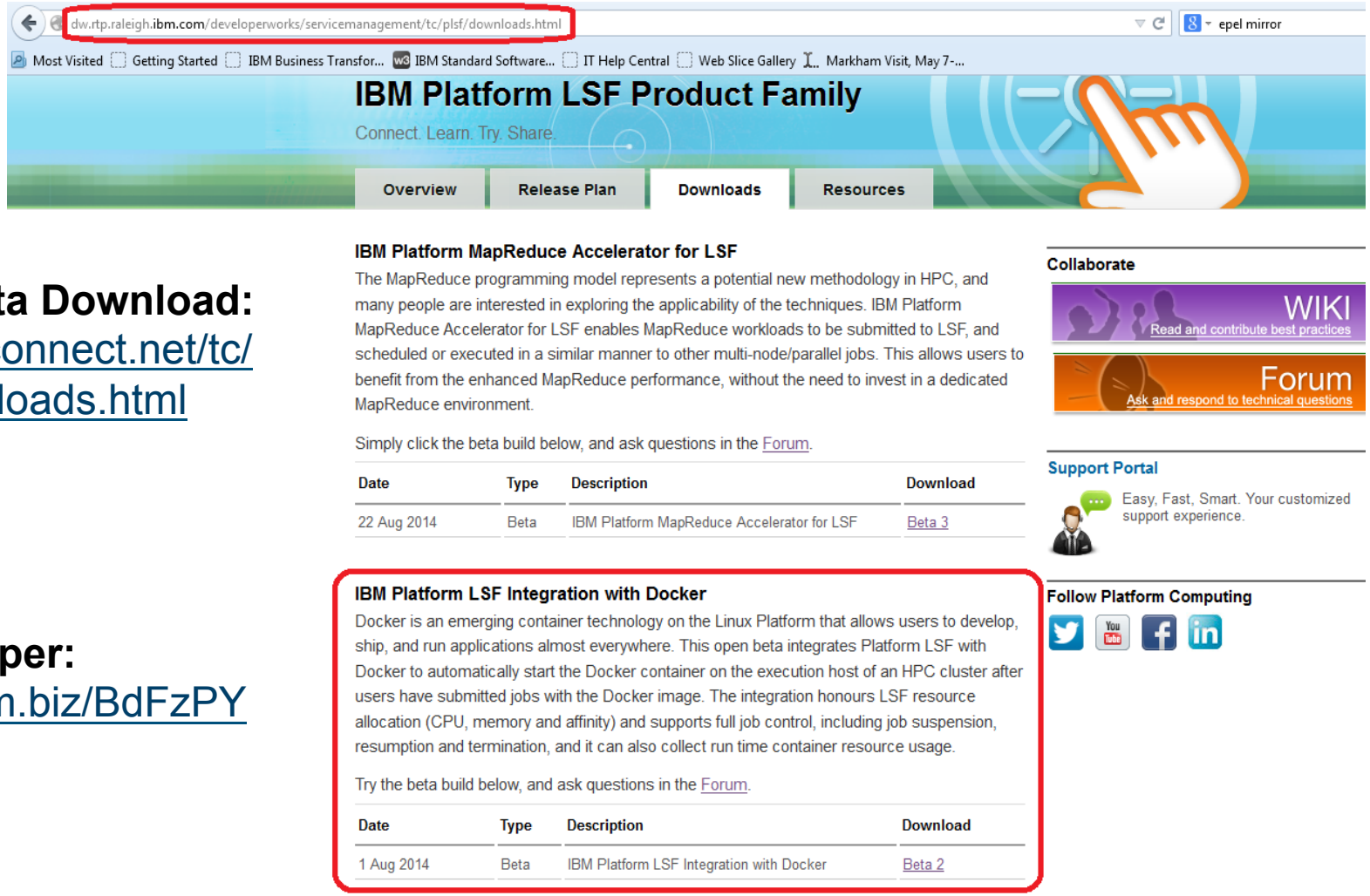
Docker in High Performance Computing



Potential Benefits

- Resource guarantee and performance isolation
  - Docker leverages Linux control group, a nature extension to cgroup
- Application encapsulation and cloud mobility
  - Application typically has lots of dependency on numerous libraries for correct execution. Challenge to move application from one system to another or out on to cloud.
  - Docker makes it easy
- Application lifecycle management
  - Allows different version of applications easily coexisting in the same environment.
- Consistency, repeatability and compliance
  - Docker provides a way to run application in a known pre-defined environment. Each time, application runs in the exactly the same environment
- Lightweight, fast and transparent
  - Docker offers identical application performance on bare metal system and fast management operations.

Using Docker with IBM Platform LSF



Open Beta Download:
http://smconnect.net/tc/plsf/downloads.html

White paper:
https://ibm.biz/BdFzPY

How to use it

```
# [lsfadmin@gecko1]$ lshosts
HOST_NAME      type    model  cpuf ncpus maxmem maxswp server RESOURCES
gecko1       X86_64 Intel_EM  60.0    16  63.9G   1.9G    Yes (mg docker)
gecko2       X86_64 Intel_EM  60.0    16  63.9G   1.9G    Yes (mg docker)
gecko3       X86_64 Intel_EM  60.0    16  63.9G   1.9G    Yes (mg docker)
```

Docker image name

```
[lsfadmin@gecko1]$ bsub -Is -a "docker(panxun/bwa)" /bin/sh
Job <402> is submitted to default queue <interactive>.
<<Waiting for dispatch ...>>
<<Starting on gecko2>>
$ echo $LSB_JOBID
$ 402
$ hostname
Docker_SL-402
$ cat /etc/lsb-release
DISTRIB_ID=Ubuntu
DISTRIB_RELEASE=14.04
DISTRIB_CODENAME=trusty
DISTRIB_DESCRIPTION="Ubuntu 14.04 LTS"
```

Cluster name and LSF JobID

```
[lsfadmin@gecko1]$lsrun -m gecko2 docker ps
CONTAINER ID   IMAGE              COMMAND       CREATED          STATUS          PORTS          NAMES
df3840bf1ab1  panxun/bwa:latest /bin/sh       8 minutes ago    Up 8 minutes                   Docker_SL-402
```

A real example

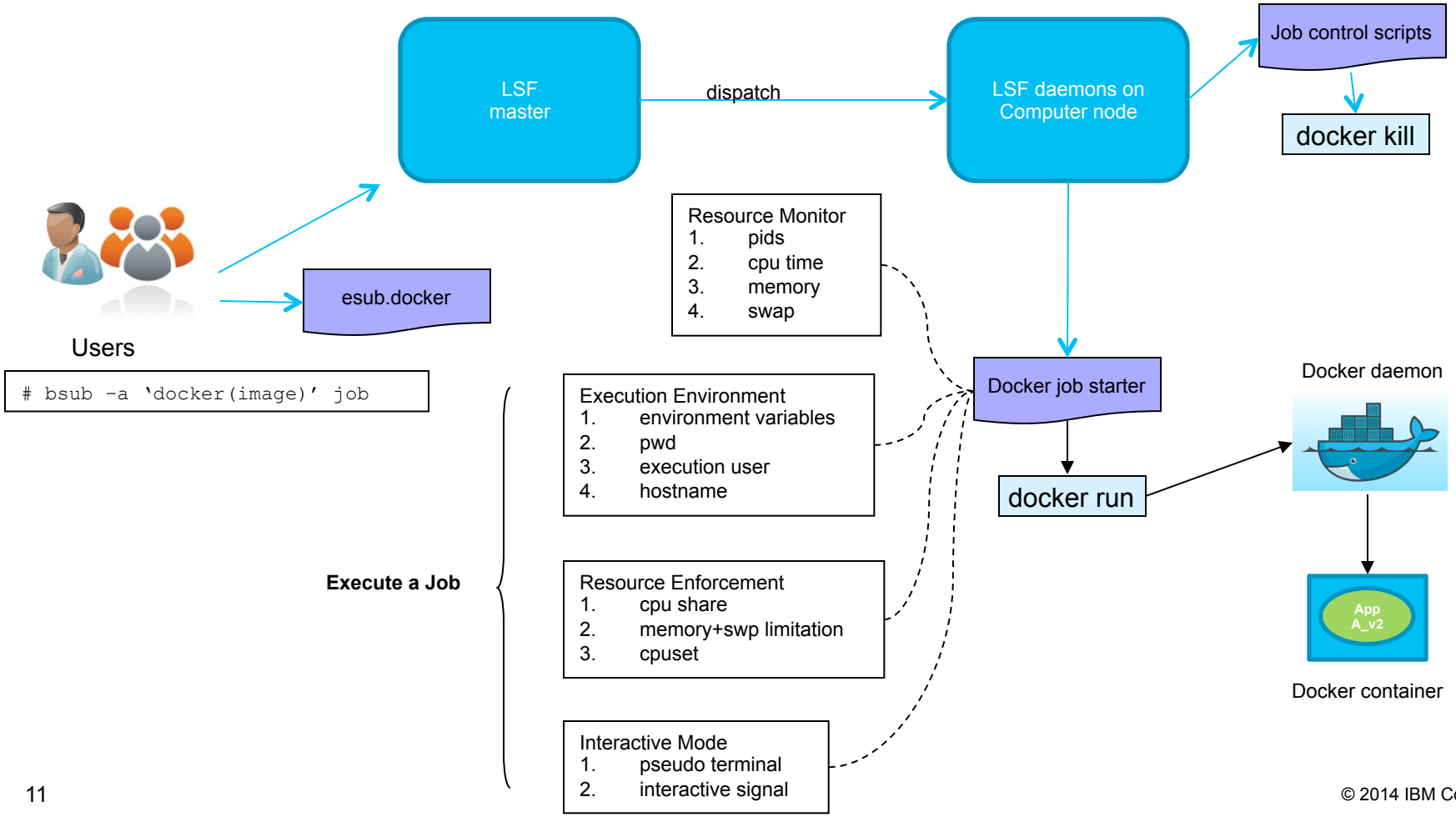
Docker image name

```
[lsfadmin@gecko1]$ bsub -n 4 -cwd "/gpfs/fpo/scratch/%J_%I" -a "docker(panxun/bwa)"
"bwaaln -t 4 -l 40 -n 3 -k 2 /gpfs/fpo/bwadata/UCSC_HG19/ucsc.hg19.fasta /gpfs/fpo/
bwadata/GZIP_FASTQ_3PAIR/SRR034939_1.fastq.gz > SRR034939_1.sai"
Job <404> is submitted to default queue <normal>.

[lsfadmin@gecko1]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME    SUBMIT_TIME
404     lsfadmi RUN   normal     gecko1      gecko2      *939_1.sai Jul 22 23:59

[lsfadmin@gecko1]$ bpeek 404
<<output from stdout>>
Unable to find image 'panxun/bwa' locally
Pulling repository panxun/bwa

[bwa_aln_core] calculate SA coordinate... 75.86 sec
[bwa_aln_core] write to the disk... 0.04 sec
[bwa_aln_core] 262144 sequences have been processed.
[bwa_aln_core] calculate SA coordinate... 74.39 sec
[bwa_aln_core] write to the disk... 0.04 sec
[bwa_aln_core] 524288 sequences have been processed.
[bwa_aln_core] calculate SA coordinate... 73.04 sec
...

[lsfadmin@gecko1 tmp]$ ls -l /gpfs/fpo/scratch/404_0/SRR034939_1.sai
-rw-rw-r-- 1 lsfadminlsfadmin 67334144 Jul 23 00:05 /gpfs/fpo/scratch/404_0/
SRR034939_1.sai
```

Downloading and installing image

How it works

- Leverage existing IBM Platform LSF plugins mechanism (esub, job starter, job control etc)



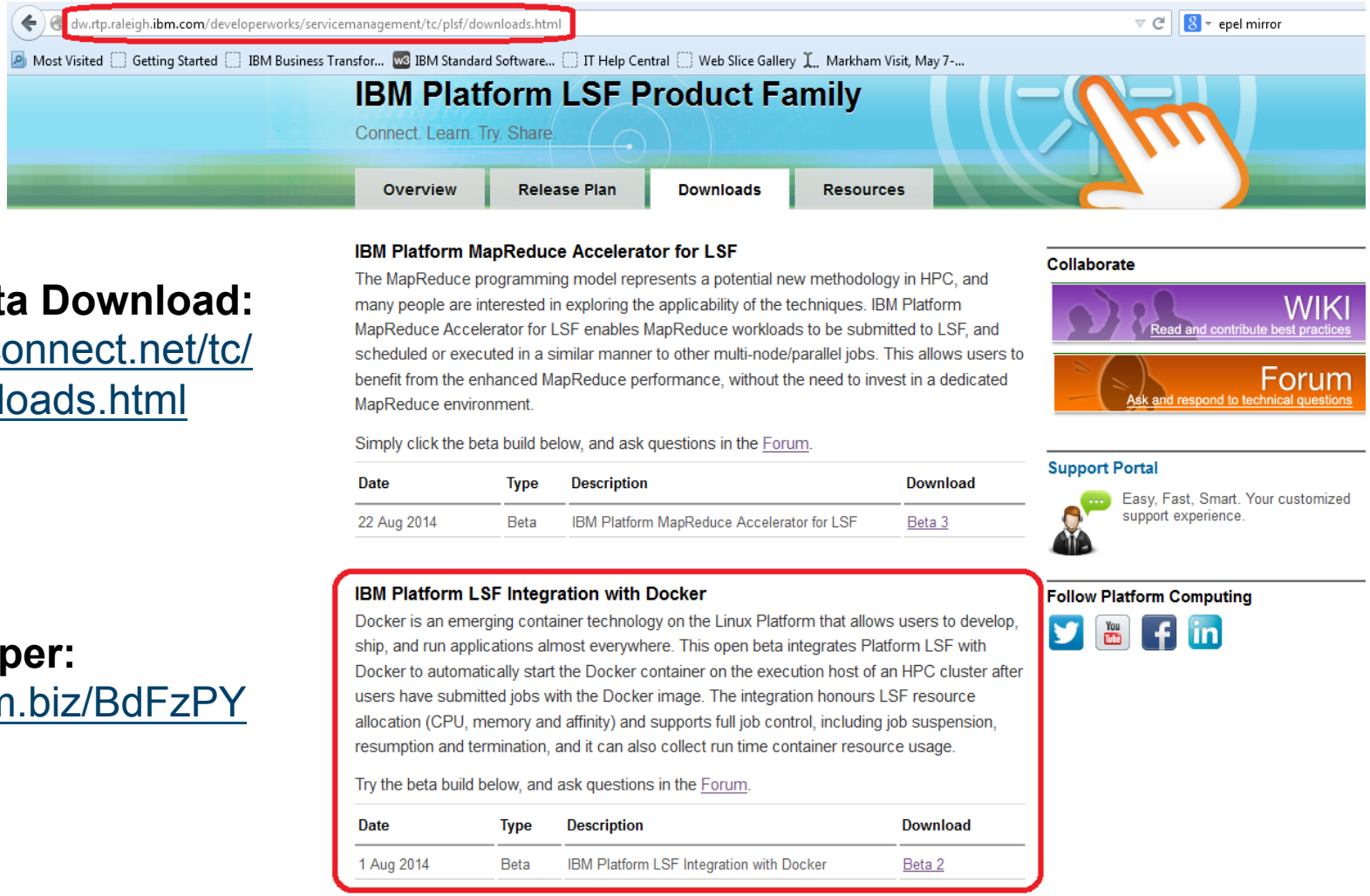
Resource Requirement and Enforcement

- CPU Shares
  - Translate IBM Platform LSF total number of slots to relative cpu share on docker.
    bsub –n <num> -> docker run –c <num>
- Memory Fencing
  - Enable IBM Platform LSF cgroup feature and translate –M/-v to docker memory option
    bsub –M/-v -> docker run –m
- Affinity & NUMA aware scheduling
  - IBM Platform LSF selects which hosts and which cores/sockets and pass information to docker to enforce it.
    -n 4 R "span[hosts=1] affinity[core]" -> docker run -cpuset

Next Step and Interest Areas

- Tighter integration with IBM Platform LSF job resource collection framework
  - Leverage built-in runtime IBM Platform LSF resource collection and reporting mechanism instead of using bpost
- Docker image aware scheduling
  - Docker image can be big and it takes time to download and install it.
  - Prefer to go to hosts with image pre-installed
- Local image management
  - Image should be cleaned up periodically when not required to save disk space

Please download and try it out



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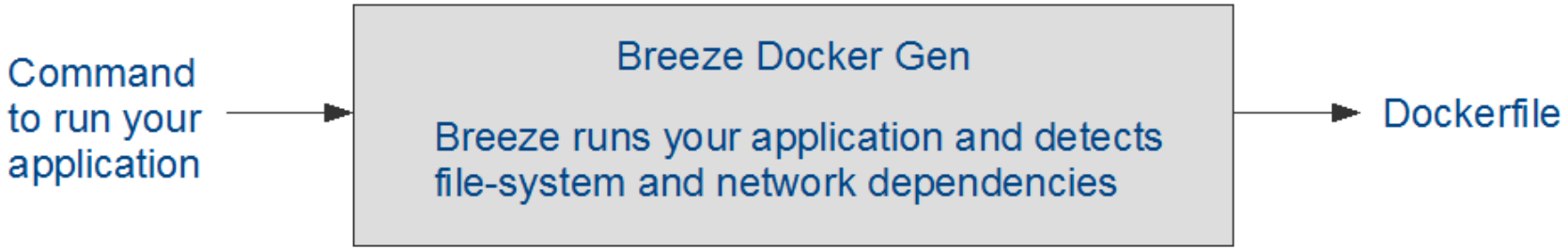
Appendix

Dockerize application

Ellexus make tools to help you solve the problems that arise when deploying and tuning complex Linux applications

Ellexus have a new product: Breeze-Docker-Gen, a tool for automatically generating docker files



Breeze-Docker-Gen uses run-time dependencies and system settings to generate the install layers, addition files and network settings needed by your application so you include only the files you need.

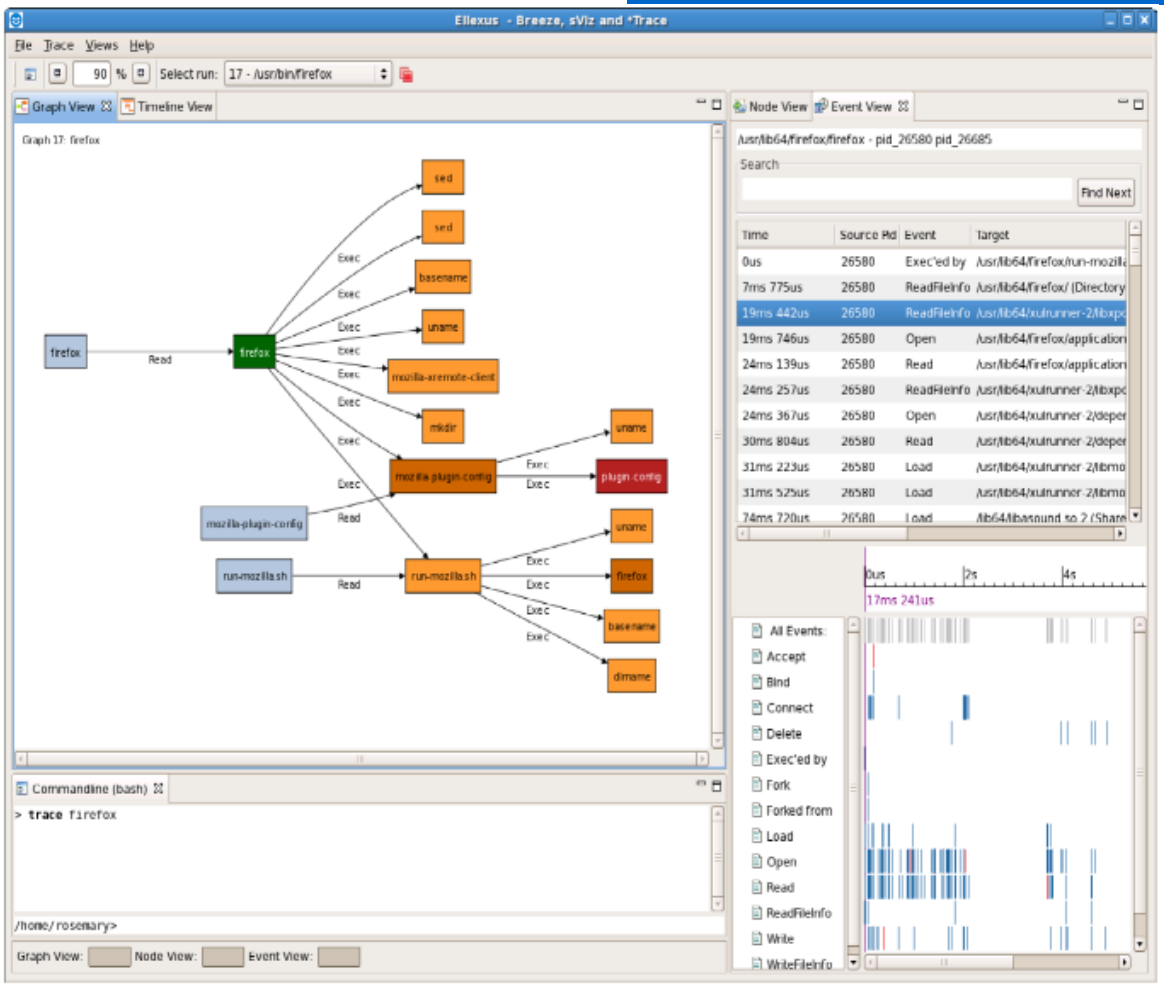
Breeze-Docker-Gen is designed to save time when packaging third party tools or complex applications with unknown dependencies.

Dockerize application

Breeze-Docker-Gen uses the Ellexus Breeze tracing technology to monitor your application as it runs. Breeze sees every program call, every file open and every network access.

It can then generate a list of dependencies and the Docker file from this information.

The screen shot (right) shows the Firefox start up and config sequence in Breeze.



Thank You For Your Time