GEMC: speed up, docker and singularity

Deployment with Containers
Shifts, Rotations of magnetic fields
Code speed up
Workflow for simulations on the grid (OSG), and offsite farms

New Tag: 4a.2.4
Docker, Singularity Images

M. Ungaro, Hall-B

GEMC Development: clas12Tag 4a.2.4

JLAB_VERSION goes from **2.1** to **2.2**. In practical terms, this mean geant4 upgraded

4.10.02.p03 to **4.10.03.p02**

(improved track navigation, e.m. physics, physics api small but non backward compatible changes)

Other changes:

CLHEP upgraded to 2.3.4.5
Qt upgraded to 5.9.1
ROOT upgraded to 6.12.06

GEMC Development: clas12Tag 4a.2.4

Magnetic Fields

Torus Map upgraded from 2008 version to "April 2018":

Torus Symmetric map

From gemc.jlab.org:

Translating/Rotating a Field

The options **DISPLACE_FIELDMAP** and **ROTATE_FIELDMAP** can be used to shift a field map origin and/or rotate a field map.

Shift example:

```
-DISPLACE_FIELDMAP="srr-solenoid, 3.5*mm, 0*mm, 0*mm"
```

this will shift the map origin from (0, 0, 0)mm to (3.5, 0, 0)mm

Rotation example:

```
-ROTATE_FIELDMAP="srr-solenoid, 15*deg, 0*deg, 0*deg"
```

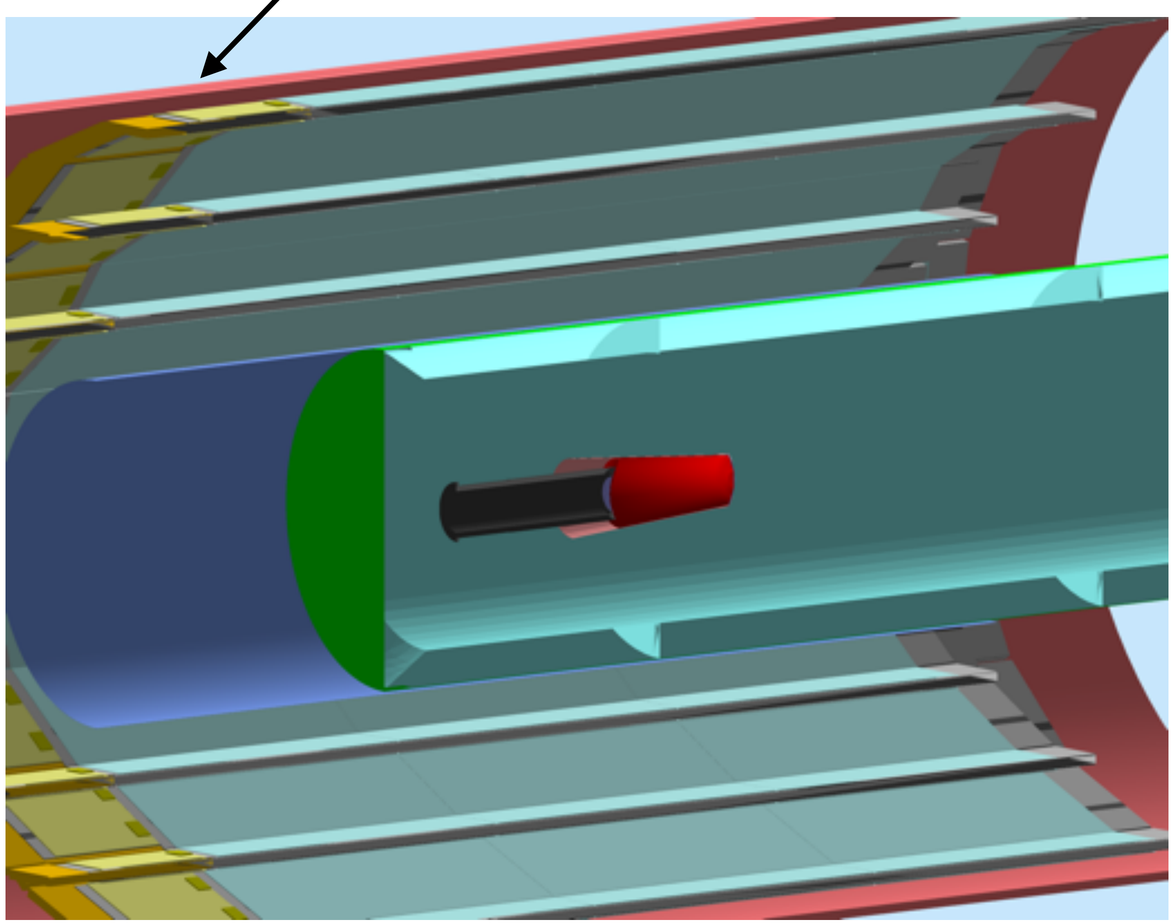
this will rotate the map 15 degrees along the x-axis.

GEMC Development: clas12Tag 4a.2.4

Geometry / Digitization Changes

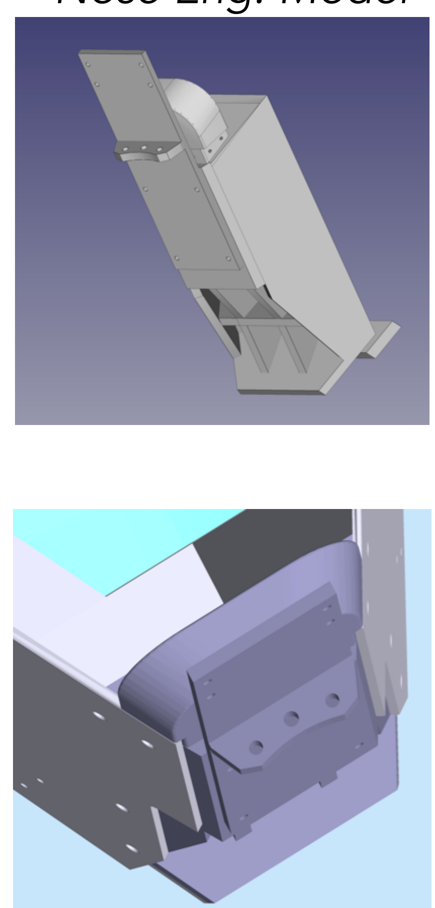
- FMT shift by 8mm
- FMT background hits
- use run number 11 as default in the gcard
- bst tungsten and heat shield
- LTCC Nose CAD model

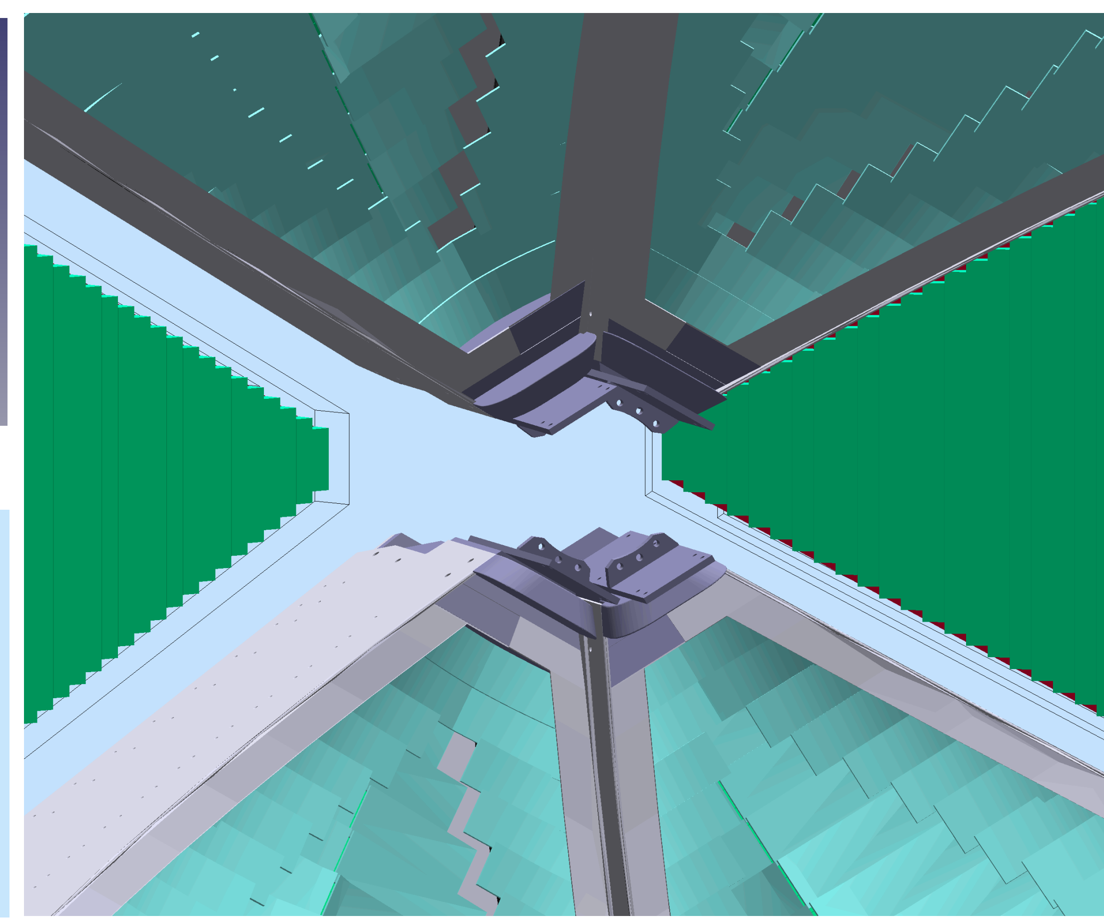
Neoprene 2.7mm



BST Tungsten and Heat Shield

Nose Eng. Model





Nose GEMC implementation

M. Ungaro, Hall-B

GEMC Development: clas12Tag 4a.2.4

env variable "**GEMC_DATA_DIR**" as a base path in the gcard (gcard is now portable to other systems)
to be ported to a command line / gcard option as well

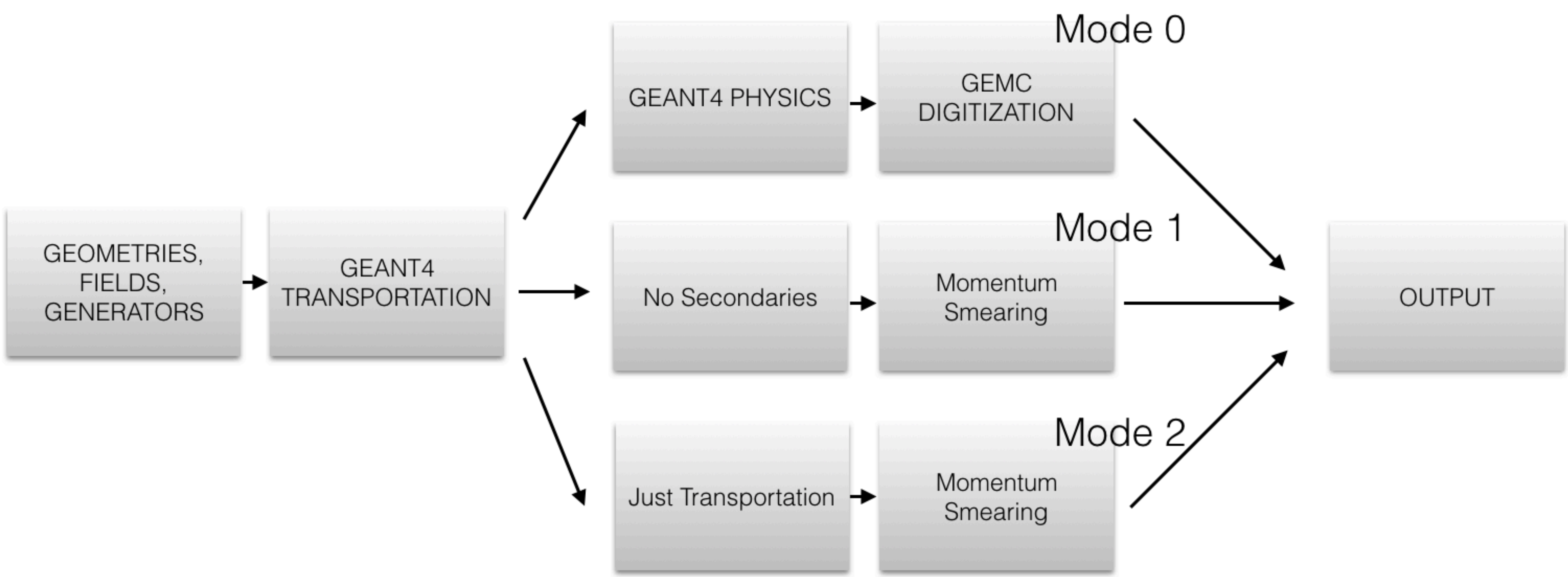
```
<!-- target. Notice variation give the target type. Can be: lH2, lD2, ND3 -->
<detector name="/group/clas12/gemc/4a.2.3/experiments/clas12/targets/cad/"   factory="CAD"/>
<detector name="/group/clas12/gemc/4a.2.3/experiments/clas12/targets/target" factory="TEXT" variation="cad"/>
```

↓

```
<!-- target. Notice variation give the target type. Can be: lH2, lD2, ND3 -->
<detector name="experiments/clas12/targets/cad/"   factory="CAD"/>
<detector name="experiments/clas12/targets/target" factory="TEXT" variation="cad"/>
```

GEMC Development: clas12Tag 4a.2.4

FAST MC Mode fixes for: -FASTMCMODE=[10,20]



Mode 0: is the full geant4 simulation.
Mode 1: turns off secondaries.
Mode 2: turns off all physics except transportation.
Mode 10: Same as mode 1 but with process routines enabled.
Mode 20: Same as mode 2 but with process routines enabled.

- Mode 1: ~10x faster.
- Mode 2: ~200x faster.

GEMC Benchmarks

- 7 GeV e- between 15 and 25 degrees in theta, all phis
- 2 GeV gamma between 15 and 25 degrees in theta, phi=0
- 2 GeV proton at 90 degrees in theta

Each cell adds its component plus all the components above.

Adds Solenoid Field →

Adds Torus Field →

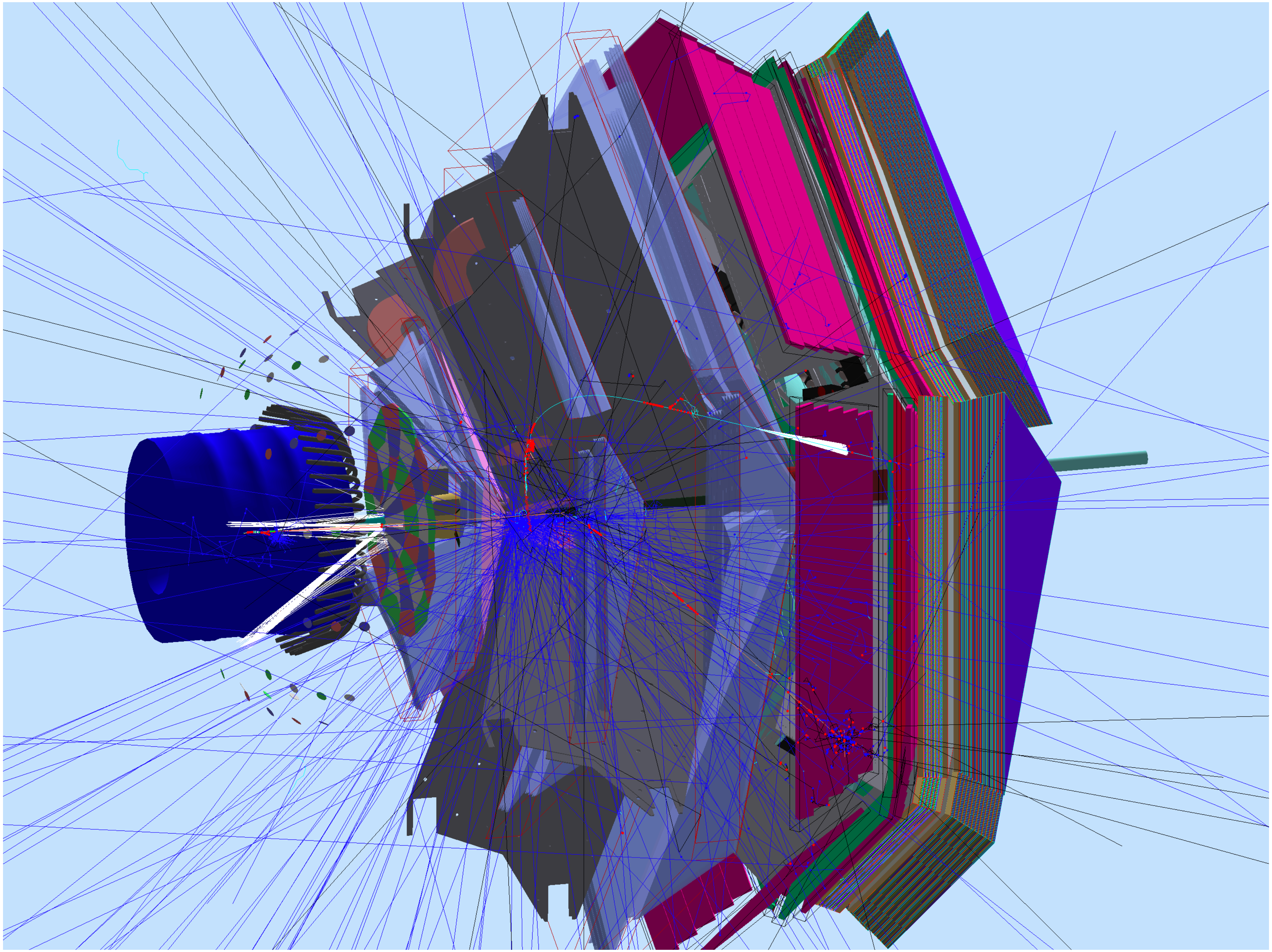
	Production Cut 10 mm		
	time fo 2000 events	Event / seconds	% increase
Target	3.6	555.8	
SVT	5.5	365.9	51.9%
MM	40.9	48.9	648.6%
CTOF	41.1	48.7	0.4%
Solenoid	126.7	15.8	208.4%
HTCC	174.6	11.5	37.9%
FT	179.4	11.2	2.7%
DC	245.8	8.1	37.0%
LTCC	307.1	6.5	24.9%
FTOF	326.3	6.1	6.3%
PCAL	718.8	2.8	120.3%
EC	987.8	2.0	37.4%
Torus	1057.2	1.9	7.0%

3 particles in the CLAS12 fiducial volume at ~500 ms / event

GEMC Benchmarks

What happens if the particles are generated **everywhere**?
(typical generator working conditions)

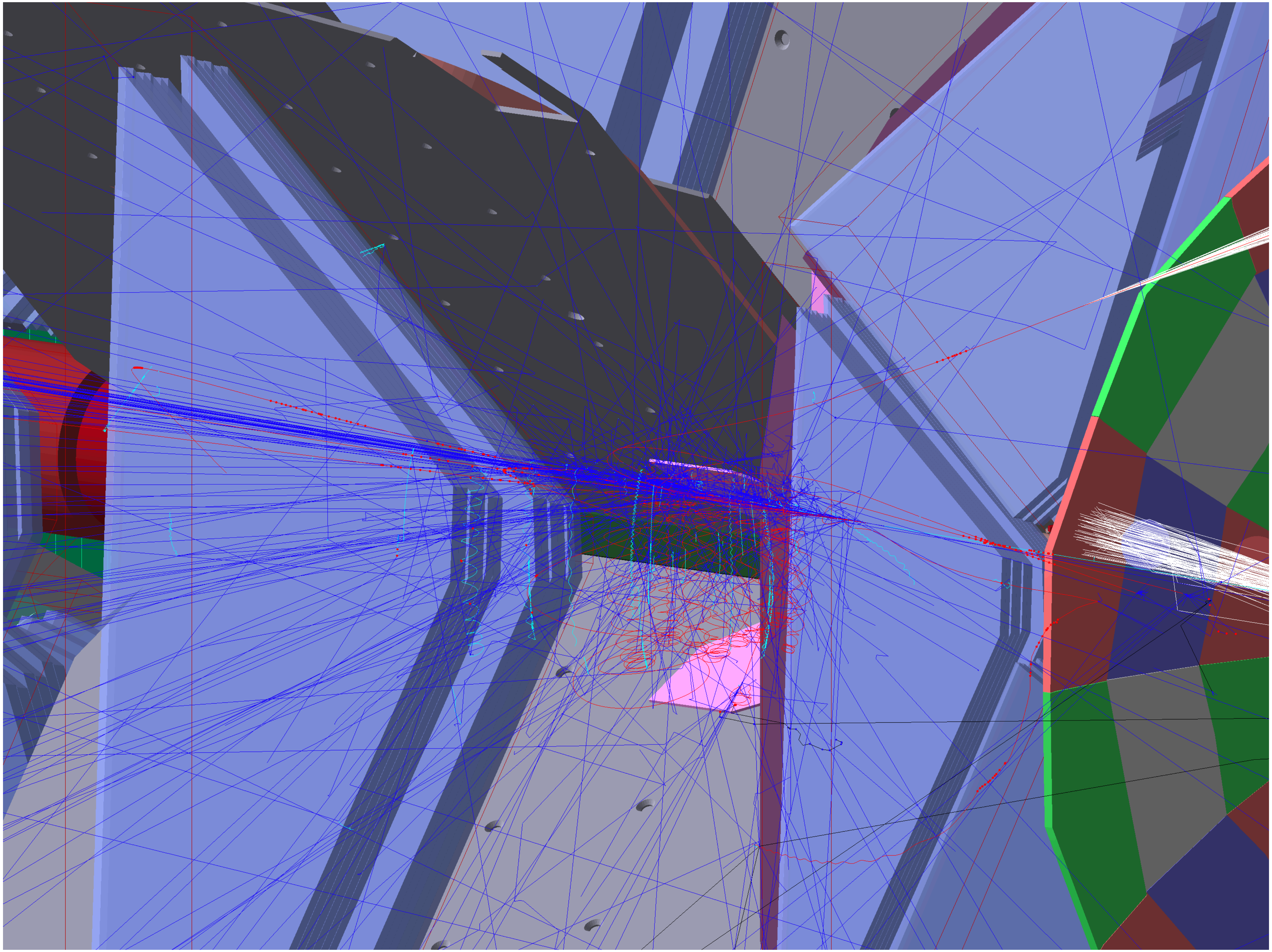
GEMC Benchmarks



electron in torus hardware. Notice: produce secondary electron giving signal in LTCC!

M. Ungaro, Hall-B

GEMC Benchmarks



electron in torus frame. Lots of e+ e- pairs looping in the field.

GEMC Benchmarks

Those (not rare) events came from a rho events generator.
Simulation slow down:

from **500 ms / event** to **1.6 second / event**

- Some of these secondaries produce real hits.
- **Most secondaries** DO NOT, and slow down the simulation unnecessary.

We could eliminate **those secondaries** with the PRODUCTION CUT:

Definition (from geant4, documented @ gemc.jlab.org)

in *geant4* **the production cut is a distance**, not an energy:

- if secondaries can travel more than that distance, they are produced.
- otherwise there is discrete energy loss.

GEMC Benchmarks

New option in gemc can set a production cut for a list of volumes.
(under the hood, this produce a G4Region in geant4):

PRODUCTIONCUTFORVOLUMES

Tentatively: 10cm for 4a.2.4. Bigger than probably needed. Studies undergoing.
The clas12 lines below do not change the DC occupancy coming from luminosity beam background.

```
<!-- production threshold for passive volumes -->

  <!-- beamline shielding: 10cm-->
  <option name="PRODUCTIONCUTFORVOLUMES" value="innerShieldAndFlange, outerFlange, outerMount, nut1, nut2, nut3, nut4,
  nut5, nut6, nut7, nut8, nut9, taggerInnerShield,  main-cone, main-cone, adjuster1, adjuster2, adjuster3,
  DSShieldFrontLead, DSShieldBackLead, DSShieldInnerAss, DSShieldBackAss, DSShieldFrontAss, DSShieldBackCover,
  DSShieldFrontCover, DSShieldFlangeAttachment, DSShieldFlange,  100" />

  <!-- vacuum line: 10cm-->
  <option name="PRODUCTIONCUTFORVOLUMES" value="connectUpstreamToTorusPipe, connectTorusToDownstreamPipe,
  downstreamPipeFlange,  100" />

  <!-- torus magnet: 10cm-->
  <option name="PRODUCTIONCUTFORVOLUMES" value="BoreShield, CenterTube, DownstreamShieldingPlate, DownstreamVacuumJacket,
  WarmBoreTube, apex, Shield1, Shield2, Shield3, Shield4, Shield5, Shield6, Shield7, shell1a, shell1b, shell2a, shell2b,
  shell3a, shell3b, shell4a, shell4b, shell5a, shell5b, shell6a, shell6b, 100" />
```

This reduces the rho events from 1.6 to 0.7 s / event. More studies needed.
More volumes can be added, cuts optimized.

GEMC Distribution

Software installation instructions (JLAB_VERSION 2.2)

These instructions are verified on:

Linux:

- CentOS 7

Mac:

- Sierra
- High Sierra

These are instructions to install JLAB_VERSION 2.2. You can find supported JLAB_VERSION releases instructions below:

- Development Version
- Version 2.2
- Version 2.1
- Version 2.0

General Requirements:

- csh shell
- cmake >= 3.3 (for geant4. check with *cmake --version*)
- network connection to download the various packages during installation
- wget
- scons version 2 to 2.5.1
- mysql
- git
- recommended: qt

⌘ MAC OS specific requirements

Make sure you have the latest xcode tools with:

```
xcode-select --install
```

You can install the dependencies with homebrew:

List of packages

Ubuntu (Debian-line) specific requirements

You can install the dependencies with apt-get:

List of packages

Fedora (red-hat line) specific requirements

You can install the dependencies with dnf (or yum):

List of packages

Installation:

1. Choose a place (JLAB_ROOT) to install the software

   A good choice for **JLAB_ROOT** is **/opt/jlab_software**:

   ```
   set JLAB_ROOT=/opt/jlab_software
   ```

   Create the working directory:

   ```
   mkdir -p $JLAB_ROOT/2.2
   ```

2. Get the installation scripts:

   ```
   cd $JLAB_ROOT
   wget http://www.jlab.org/12gev_phys/packages/sources/ceInstall/ceInstall_2.2.tar.gz
   tar -zxpf ceInstall_2.2.tar.gz --strip-components 1 -C 2.2
   ```

3. Set the environment variables. You should put these lines in your login script:

   ```
   setenv JLAB_ROOT /opt/jlab_software
   source $JLAB_ROOT/2.2/ce/jlab.csh
   ```

4. Start a new shell. Now you should see a log similar to this

   ```
   > Common Environment Version: <2.2>  (Wed March 18 2018)
   > Running as mauri on 1.800.gemc.cool.org
   > OS Release:    Darwin_macosx10.13-x86_64-clang9.0.0
   > JLAB_ROOT set to:     /opt/jlab_software
   > '/opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0' is not a directory. Creating it.

   !! Attention:  BANKS  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/banks/1.4/bin  not found
   !! Attention:  CCDB  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/ccdb/ccdb-1.06.02/lib  not found
   !! Attention:  CLHEP  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/clhep/2.3.4.5/lib  not found
   !! Attention:  EVIO  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/evio/5.1/bin  not found
   !! Attention:  GEANT4  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/geant4/4.10.03.p02/bin  not found
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   !! Attention:  JANA  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/jana/0.7.7p1/bin/jana  not found
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   !! Attention:  MYSQL  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/mysql/lib  not found
   !! Attention:  QT    installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/qt/5.9.1/5.9.1/clang_64/lib  not found
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   !! Attention:  SCONS  installation check /opt/jlab_software/2.2/scons_bm/1.6/site_tools  not found
   !! Attention:  XERCESC  installation check /opt/jlab_software/2.2/Darwin_macosx10.13-x86_64-clang9.0.0/xercesc/3.2.0/lib  not found
   ```

   If you do, great! The enviroment seems correct and you're ready to run the installation scripts. Every script that you run below will replace the warning log with a successful one. Notice: if you already have some existing environment variables that you want to keep, use the option "keepmine":

   ```
   source $JLAB_ROOT/2.2/ce/jlab.csh keepmine
   ```

5. Choose the packages you wish to install by executing the corresponding script:

   ```
   cd $JLAB_ROOT/2.2/install

   ./go_clhep
   ./go_xercesc
   ```

   If you have a system installation of qt (see instructions on requirements on how to install it):

   ```
   ./go_qt system
   ```

   Otherwise the following command will downlowad the qt installer for you. Follow instructions for the installation:

   ```
   ./go_qt
   ```

   Continue with the rest of the package installation:

   ```
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   ./go_ccdb
   ./go_mlibrary
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After many years, even with many improvements on the installation scripts, the compilation of gemc from scratch remains a **difficult task**.

geant4, qt, cadmesh, various compilers, scons and cmake, etc present challenges with their upgrades and virtually every release of Mac and Linux OSes. And that's ok: we want to use the latest technologies and bug fixes. But it makes the **installation grueling on the users and on system admins for offsite farms.**

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```

GEMC Distribution: Docker images

No requirements on the OS version, or the OS (Mac, Linux, Windows)
No libraries needed other than have the "docker" app installed.
(https://www.docker.com/community-edition)

Installing gemc is now a one liner.

GEMC Distribution: Docker images

```
docker run -it --rm jeffersonlab/clas12tags:4a.2.4 bash
```

GEMC Distribution: Docker images

```
docker run -it --rm jeffersonlab/clas12tags:4a.2.4 bash
```

jefferson lab cloud docker repository

The first time you run this, it will download the image (just a few minutes).
Every subsequent time execution is instantaneous.

GEMC Distribution: Docker images

```
docker run -it --rm jeffersonlab/clas12tags:4a.2.4 bash
```

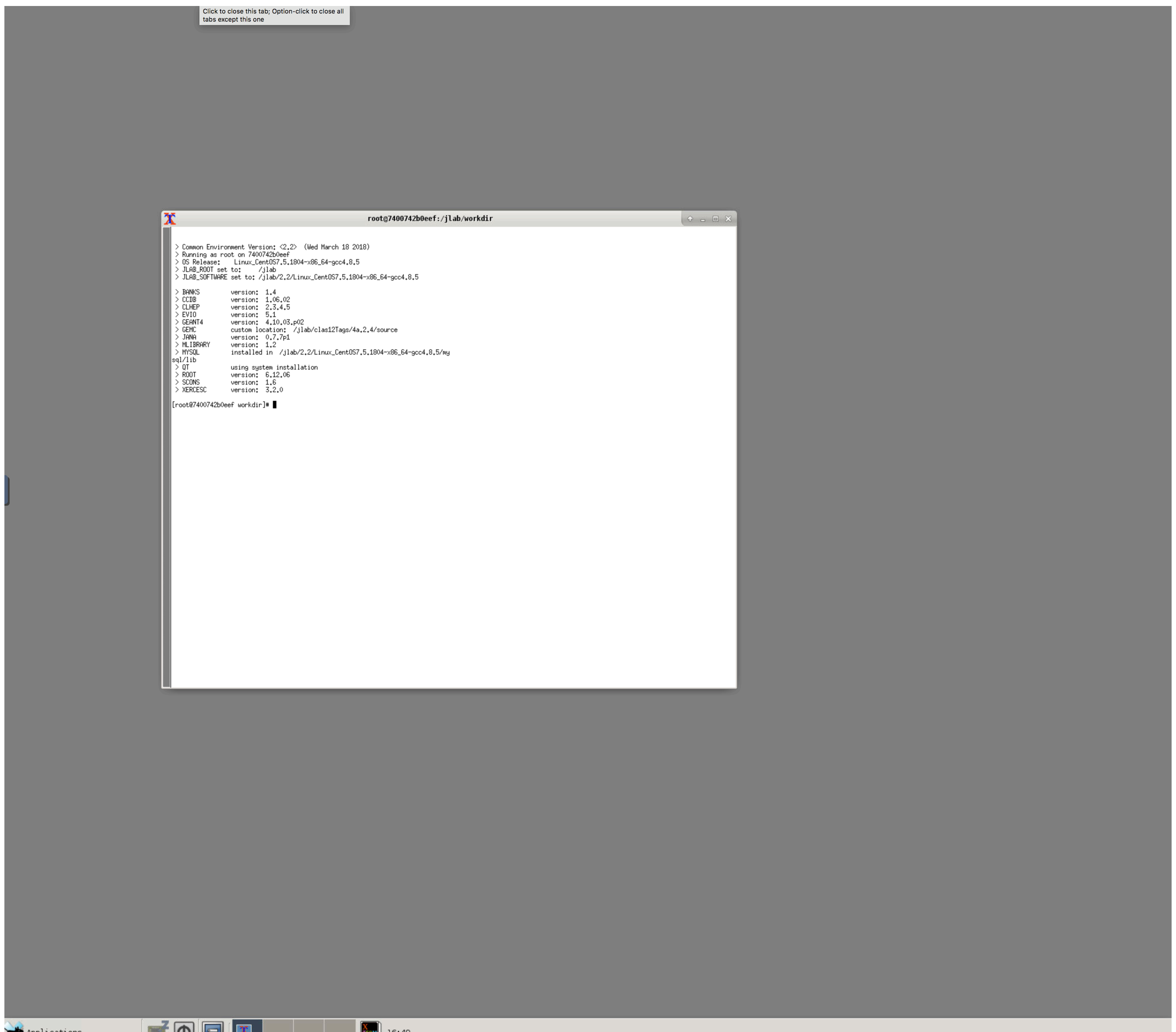
```
%>docker run -it --rm jeffersonlab/clas12tags:4a.2.4 bash


 > Common Environment Version: <2.2>  (Wed March 18 2018)
 > Running as root on d83191ce8cd4
 > OS Release:    Linux_CentOS7.5.1804-x86_64-gcc4.8.5
 > JLAB_ROOT set to:     /jlab
 > JLAB_SOFTWARE set to: /jlab/2.2/Linux_CentOS7.5.1804-x86_64-gcc4.8.5

 > BANKS    version:  1.4
 > CCDB     version:  1.06.02
 > CLHEP    version:  2.3.4.5
 > EVIO     version:  5.1
 > GEANT4   version:  4.10.03.p02
 > GEMC     custom location:  /jlab/clas12Tags/4a.2.4/source
 > JANA     version:  0.7.7p1
 > MLIBRARY    version:  1.2
 > MYSQL    installed in  /jlab/2.2/Linux_CentOS7.5.1804-x86_64-gcc4.8.5/mysql/lib
 > QT       using system installation
 > ROOT     version:  6.12.06
 > SCONS    version:  1.6
 > XERCESC     version:  3.2.0

[root@d83191ce8cd4 workdir]#
```

You can now run gemc (batch mode).

GEMC Distribution: Docker images

```
docker run -it --rm -p 6080:6080 jeffersonlab/clas12tags:4a.2.4
```

http://localhost:6080



You can now run gemc (interactive mode).

GEMC Distribution: Docker images

Advantages of Docker over virtual machines

- Virtual machines needs to be booted every time.
- They are slow.
- They are resources hogs.
- Running intensive openGL apps (like GEMC) can be problematic.
- If I change a small thing in gemc, the whole image needs to be reinstalled. Unless users do it by hand (then we're back to square 1).

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- No booting: execution is immediate.
- Docker is fast.
- It's an app running on a shell. Can be seen with a browser or a vnc client.
- Containers are layered up. A small fix in gemc means re-downloading a small container only.
- Local disk can be made available to docker, so one can get gemc from repo and recompile. No libraries needed.
- Image storage in the cloud, tagged.
- Base for singularity.

GEMC Distribution: Docker images

How fast is it?

Test on 4a.2.4, full clas12 geometry, all fields on.

```
gemc clas12.gcard -USE_GUI=0 -N=100 -BEAM_P="e-, 4*GeV, 20*deg, 10*deg"
```

```
Total gemc time: 128.21 seconds.
Events only time: 32.5758 seconds.
```

```
Total gemc time: 92.46 seconds.
Events only time: 22.1616 seconds.
```

```
Total gemc time: 117.02 seconds.
Events only time: 22.6159 seconds.
```

GEMC Distribution: Docker images

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ifarm1401

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my imac

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```
Total gemc time: 128.21 seconds.
Events only time: 32.5758 seconds.
```

ifarm1401

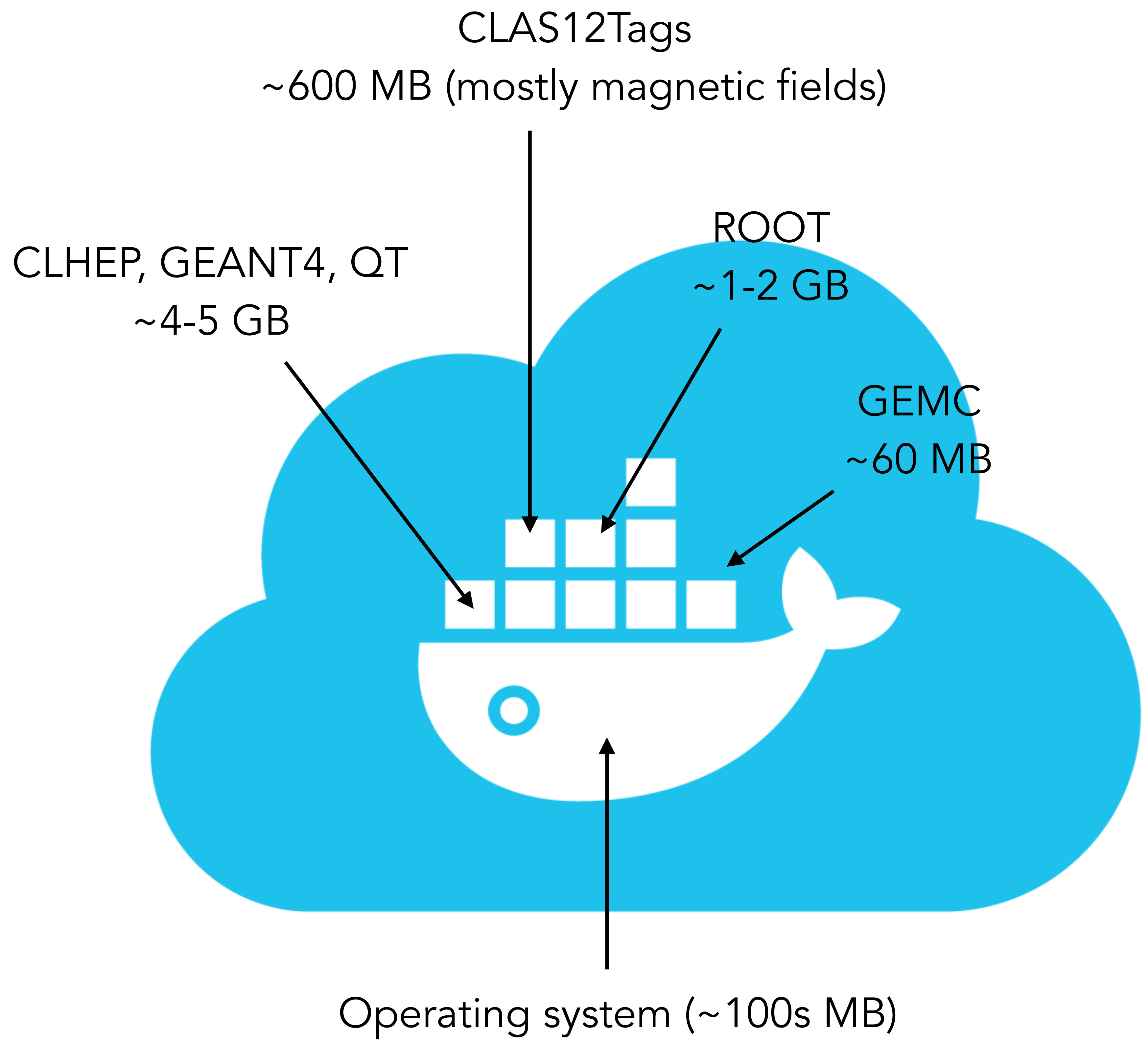
```
Total gemc time: 92.46 seconds.
Events only time: 22.1616 seconds.
```

docker

```
Total gemc time: 117.02 seconds.
Events only time: 22.6159 seconds.
```

my imac

GEMC Distribution: Docker images



Docker and Singularity

Singularity is "the" secure mode to deploy jobs based on docker images on farms.
Singularity is installed on the JLab farm.

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Singularity is used at the Open Science Grid (OSG).
Singularity is used at the National Energy Research Scientific Computing Center (NERSC)

How does it work on the grid?
A singularity container is **built from a docker container** and
automagically distributed over ALL the OSG nodes (all the offsite farms).

Docker and Singularity

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Singularity is used at the Open Science Grid (OSG).
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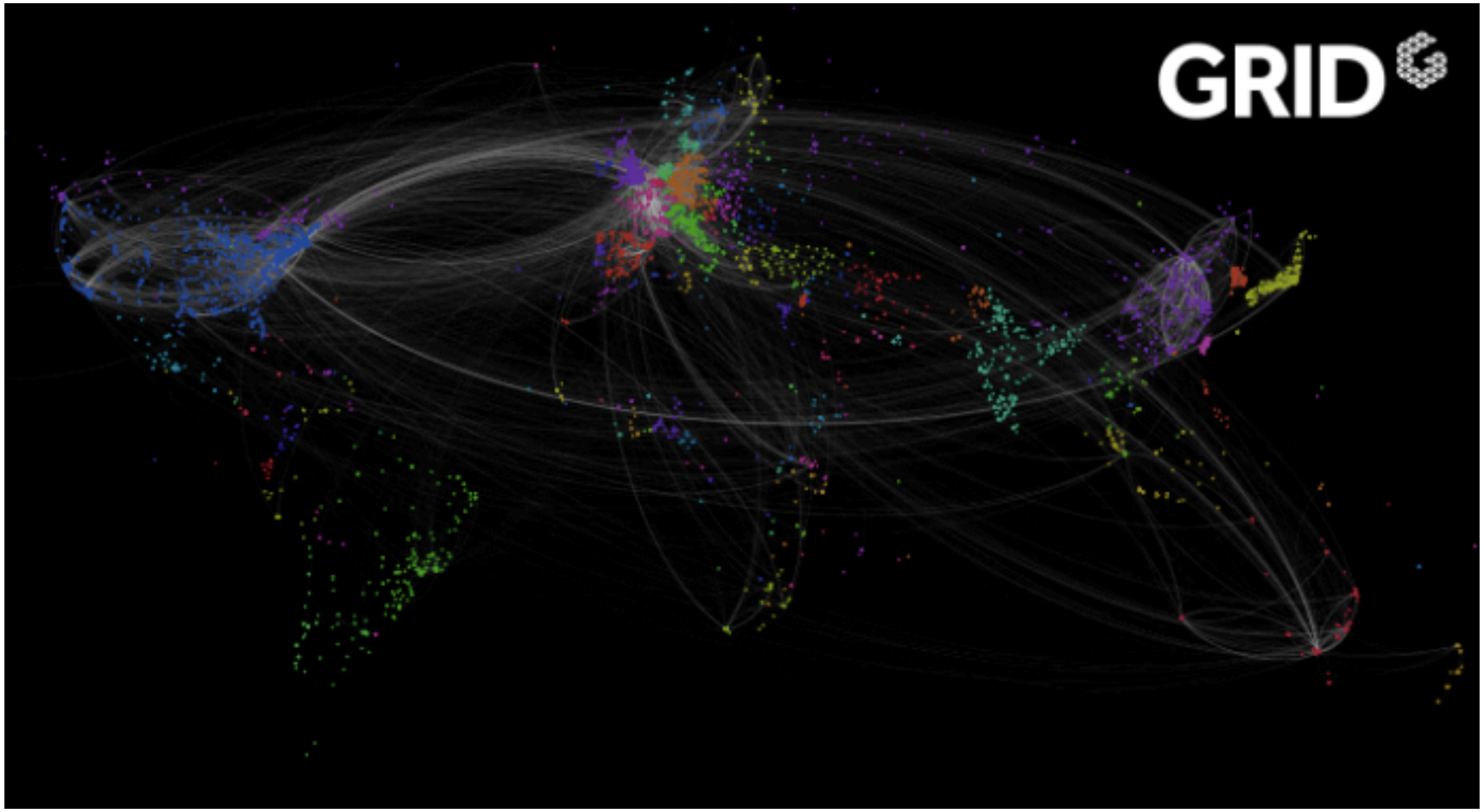
Singularity is in PRODUCTION by GLUEX for their simulation/reconstruction on the farm.
Last month: 100% simulation on OSG, 2B events.

JLab CC is working on Swift 2:
Seamless submission of jobs to OSG NERSC

CLAS12 Simulations, Docker and Singularity

- CLAS12 can now request to be a formal member of OSG (new applications were closed)
- MIT may hire post-doc to help CC in the Swift 2 / Grid effort.
- Universities, Offsite farms can use CLAS12 accounts to add their farm to the grid

JLAB USER
JSUB
Command



Output File

Currently: 10 GB / s connection.
FY2020: should be 100 GB connection.

Summary, Outlook

- 4a.2.4: Same as 4a.2.3 but uses JLAB_VERSION 2.2. In addition:
    - Use new torus field map
    - FMT shift by 8mm
    - use run number 11 as default in the gcard
    - FMT background hits
    - production cut set for individual volumes in the options
    - new geant4 version
    - env variable "GEMC_DATA_DIR" as a base path in the gcard (gcard is now portable to other systems)
    - bst tungsten and heat shield
    - LTCC Nose CAD model
    - magnetic field map displacements and rotations with command line options
    - FAST MC mode 10, 20 output fixed

- Geometry additions
- Shifts, Rotations of magnetic fields
- Code speed up: 2x improvements, can it be 3x? More studies needed.
- Deployment with Containers: Docker is operational: CLAS12 Tags 4a.2.4. Please try.
- Exciting prospects for CLAS12 simulations on OSG