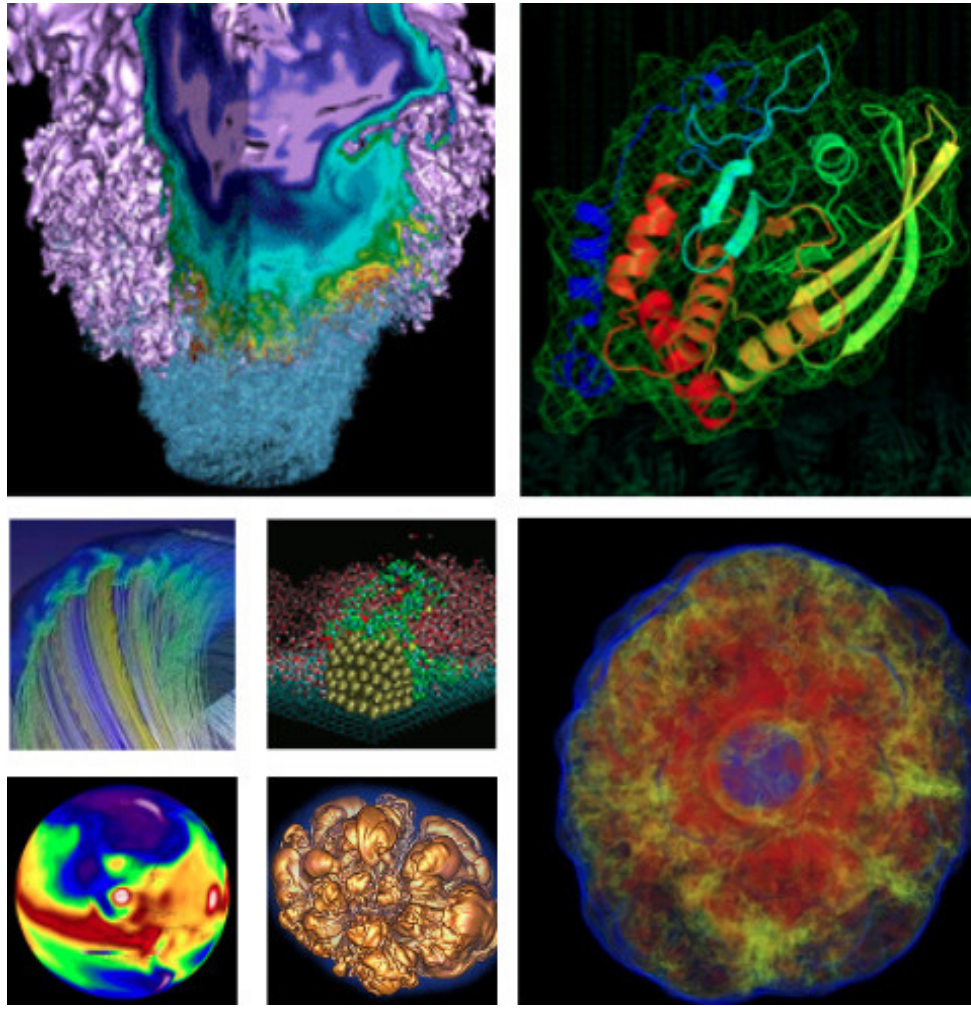
Use of HPC

Short-term developments



National Energy Research Scientific Computing Center

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- Existing supercomputers
  - Cori (32-core/node Haswell @ 2.3 GHz + 68-core/node KNL @ 1.4 GHz)
  - Edison (24-core/node Ivy-Bridge @ 2.4 GHz)
- Upcoming supercomputer
  - NERSC 9 supercomputer (~2019)
    - "accelerators"
    - Not next-gen KNL $\Rightarrow$ no AVX-512 instruction set
- Intel has discontinued development of Knights Landing
  - Intel's homogeneous solution to heterogeneous speed-up with GPGPUs didn't quite work out as planned
    - Claimed as easy to use as Xeon and a significant programming advantage over GPGPUs
  - Next generation (Knights Hill) will be replaced with:

"*a new platform and new micro-architecture specifically designed for exascale*"
- Trish Damkroger (Intel VP)

- Create "official" Geant4 docker repository
  - *e.g.*, https://hub.docker.com/r/geant4
  - Tags for compilers, versions, etc.
  - Use this as standard for per-machine performance comparison
    - No virtualization layer
    - Portable to any HPC/cluster capable of running Docker containers
    - Exact same compiler, configuration, etc. $\Rightarrow$ hardware-vs-hardware
  - Reproducibility
    - (A) associate Dockerfile with Git revision or (B) `docker save ...`
- Performance characterization with respect to:
  - HPC system
    - Cori KNL
    - Cori Haswell
    - Edison
    - Any others?
  - Compiler
    - GNU
    - Intel
    - Clang
    - Any others?
  - OS (*i.e.*, kernel)
    - openSUSE
    - RHEL
    - Any others?

- Created a public CDash dashboard at NERSC: cdash.nersc.gov
  - Built with Docker and deployed in Spin – a containers-as-service (CaaS) platform at NERSC
- Use Geant4 + TiMemory + CDash for performance characterization
  - Nightly and continuous performance testing
  - Separate from our build testing – avoid adding more clutter
  - Longer-term additions:
    - Valgrind reports
    - Code coverage
    - VTune reports (*e.g.*, attach VTune summary as CTest note)

- Docker make it easy to distribute portable pre-built Geant4 packages
  - GUIs are supported
  - Adoption for Geant4 tutorials?

```
# Linux
$ IP=$(ip route ls | tail -n 1 | awk '{print $NF}')

# Darwin
$ IP=$(ipconfig getifaddr $(route get nersc.gov | grep 'interface:' | awk '{print $NF}'))

$ docker run -it -v ${HOME}/.Xauthority:/root/.Xauthority:rw
    -v /tmp/.X11-unix:/tmp/.X11-unix
    -e DISPLAY="${IP}:$(echo $DISPLAY | cut -d ':' -f 2)" ...
```