View from NERSC

Challenges and opportunities for increasing the impact of DOE libraries and tools in collaboration with the facilities
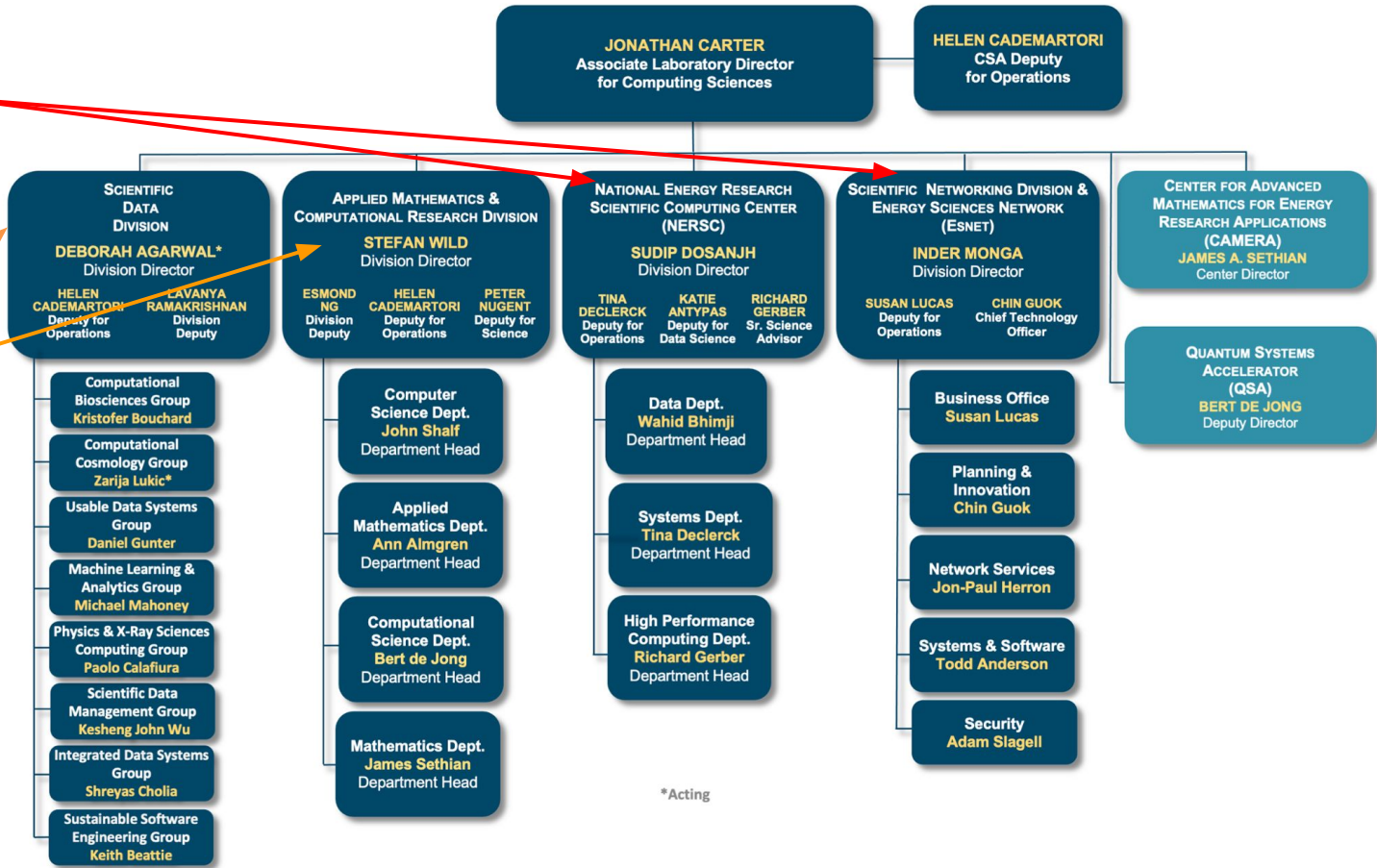
PESO Community Workshop
Argonne National Laboratory

Richard Gerber
HPC Department Head
Senior Science Advisor
June 8, 2023

Berkeley Lab Computing Sciences Area

DOE Office of Science National User Facilities
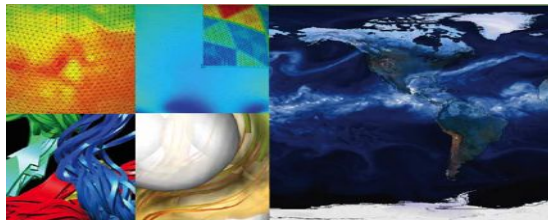
The Computational Research Division (CRD) split

JONATHAN CARTER
Associate Laboratory Director for Computing Sciences

HELEN CADEMARTORI
CSA Deputy for Operations

SCIENTIFIC DATA DIVISION
DEBORAH AGARWAL*
Division Director

HELEN CADEMARTORI
Deputy for Operations

LAVANYA RAMAKRISHNAN
Division Deputy

- Computational Biosciences Group — Kristofer Bouchard
- Computational Cosmology Group — Zarija Lukic*
- Usable Data Systems Group — Daniel Gunter
- Machine Learning & Analytics Group — Michael Mahoney
- Physics & X-Ray Sciences Computing Group — Paolo Calafiura
- Scientific Data Management Group — Kesheng John Wu
- Integrated Data Systems Group — Shreyas Cholia
- Sustainable Software Engineering Group — Keith Beattie

APPLIED MATHEMATICS & COMPUTATIONAL RESEARCH DIVISION
STEFAN WILD
Division Director

ESMOND NG
Division Deputy

HELEN CADEMARTORI
Deputy for Operations

PETER NUGENT
Deputy for Science

- Computer Science Dept. — John Shalf — Department Head
- Applied Mathematics Dept. — Ann Almgren — Department Head
- Computational Science Dept. — Bert de Jong — Department Head
- Mathematics Dept. — James Sethian — Department Head

NATIONAL ENERGY RESEARCH SCIENTIFIC COMPUTING CENTER (NERSC)
SUDIP DOSANJH
Division Director

TINA DECLERCK
Deputy for Operations

KATIE ANTYPAS
Deputy for Data Science

RICHARD GERBER
Sr. Science Advisor

- Data Dept. — Wahid Bhimji — Department Head
- Systems Dept. — Tina Declerck — Department Head
- High Performance Computing Dept. — Richard Gerber — Department Head

SCIENTIFIC NETWORKING DIVISION & ENERGY SCIENCES NETWORK (ESNET)
INDER MONGA
Division Director

SUSAN LUCAS
Deputy for Operations

CHIN GUOK
Chief Technology Officer

- Business Office — Susan Lucas
- Planning & Innovation — Chin Guok
- Network Services — Jon-Paul Herron
- Systems & Software — Todd Anderson
- Security — Adam Slagell

CENTER FOR ADVANCED MATHEMATICS FOR ENERGY RESEARCH APPLICATIONS (CAMERA)
JAMES A. SETHIAN
Center Director

QUANTUM SYSTEMS ACCELERATOR (QSA)
BERT DE JONG
Deputy Director

*Acting

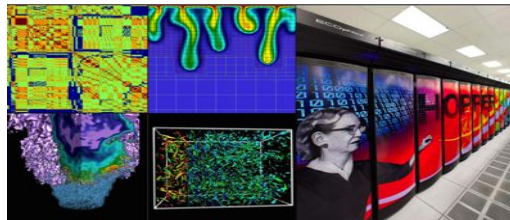# Mission HPC for Office of Science Research

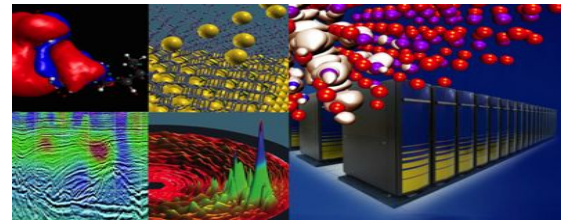**U.S. DEPARTMENT OF ENERGY** | Office of Science

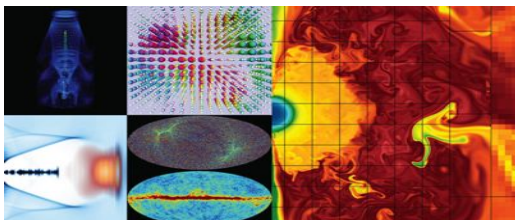Largest funder of physical science research in the U.S.
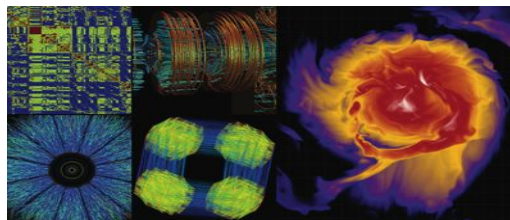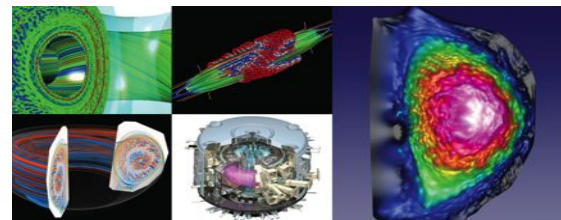

Bio Energy, Environment

Computing

Materials, Chemistry, Geophysics

Particle Physics, Astrophysics

Nuclear Physics

Fusion Energy, Plasma Physics
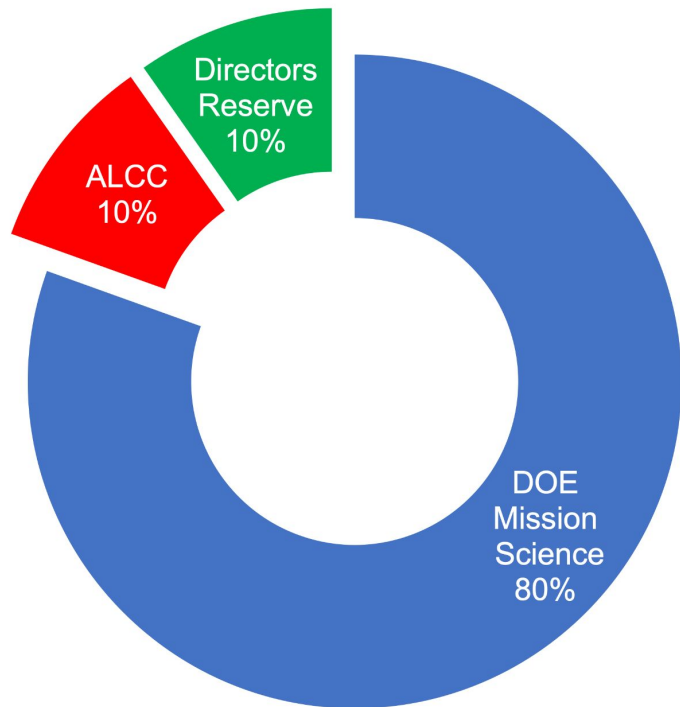
9K users, 1K projects, 50 states, 40 countries, universities & national labs

BERKELEY LAB — Bringing Science Solutions to the World

U.S. DEPARTMENT OF ENERGY | Office of Science

Allocation Programs

Directors Reserve 10%

ALCC 10%

DOE Mission Science 80%

Distributed by DOE Office of Science program managers

Competitive awards run by DOE Advanced Scientific Computing Research Office
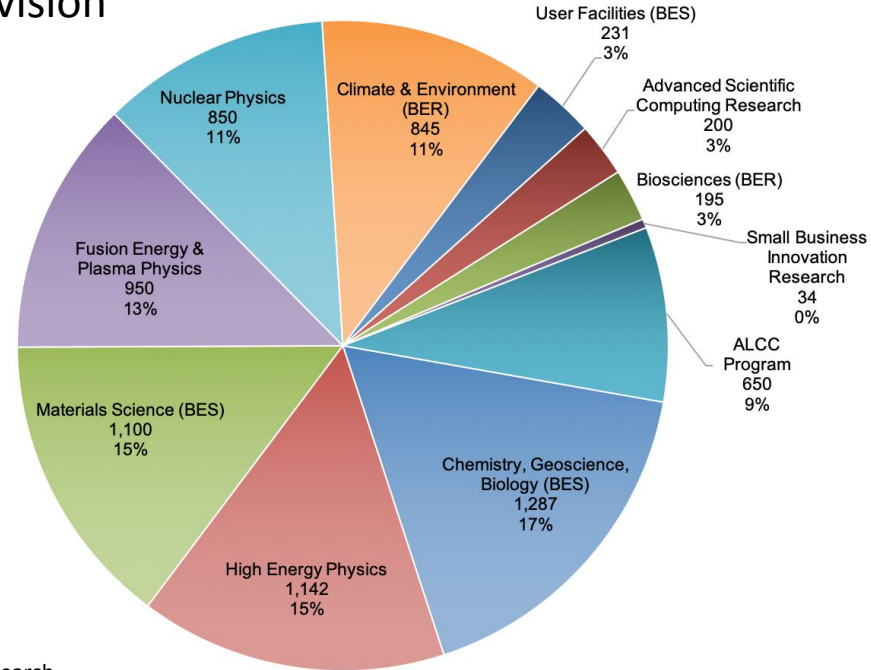
Strategic awards from NERSC

NERSC doesn't pick its users, so we have to meet them where they are and try to guide them towards increased productivity
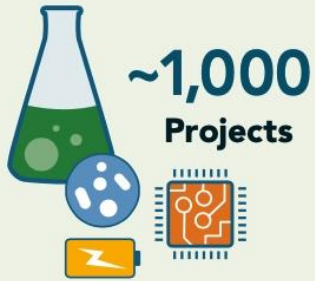
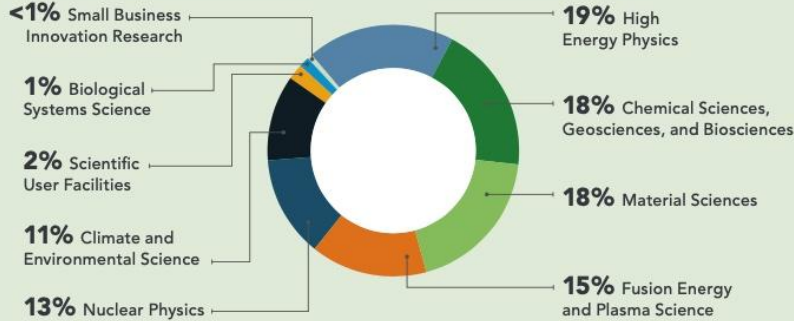# NERSC Workload

By Program
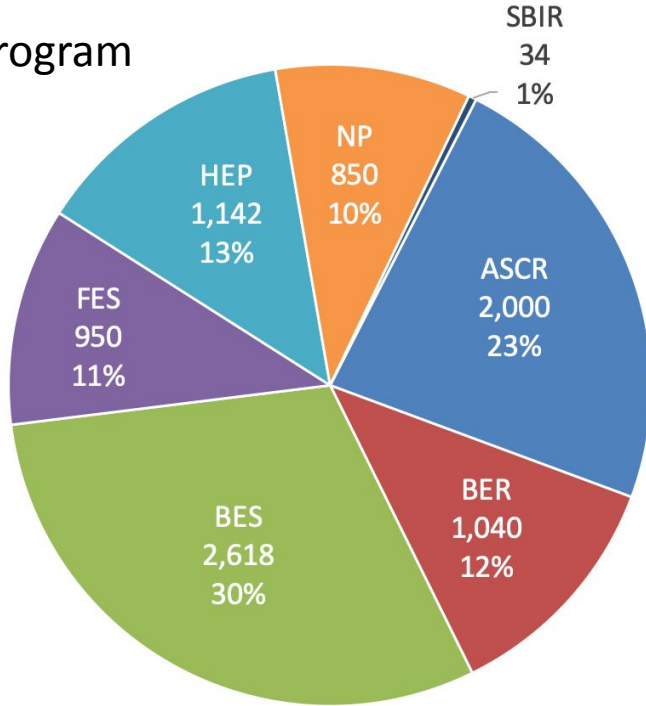
By Division

ASCR - Advanced Scientific Computing Research
BER - Biological and Environmental Research
BES - Basic Energy Sciences (Chemistry, Materials, Geophysics)
FES - Fusion Energy Sciences (including Plasma Physics)
HEP - High Energy Physics
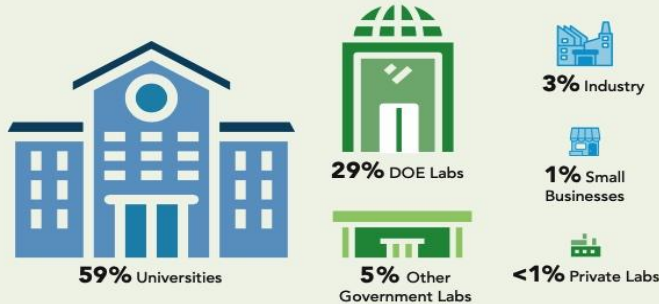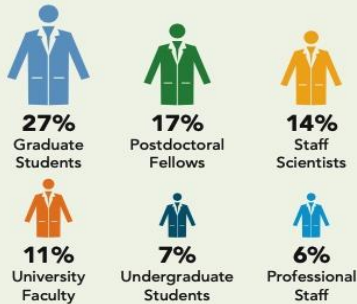NP -Nuclear Physics
SBIR - Small Business Innovation Research

A Diverse Scientific Community of Users

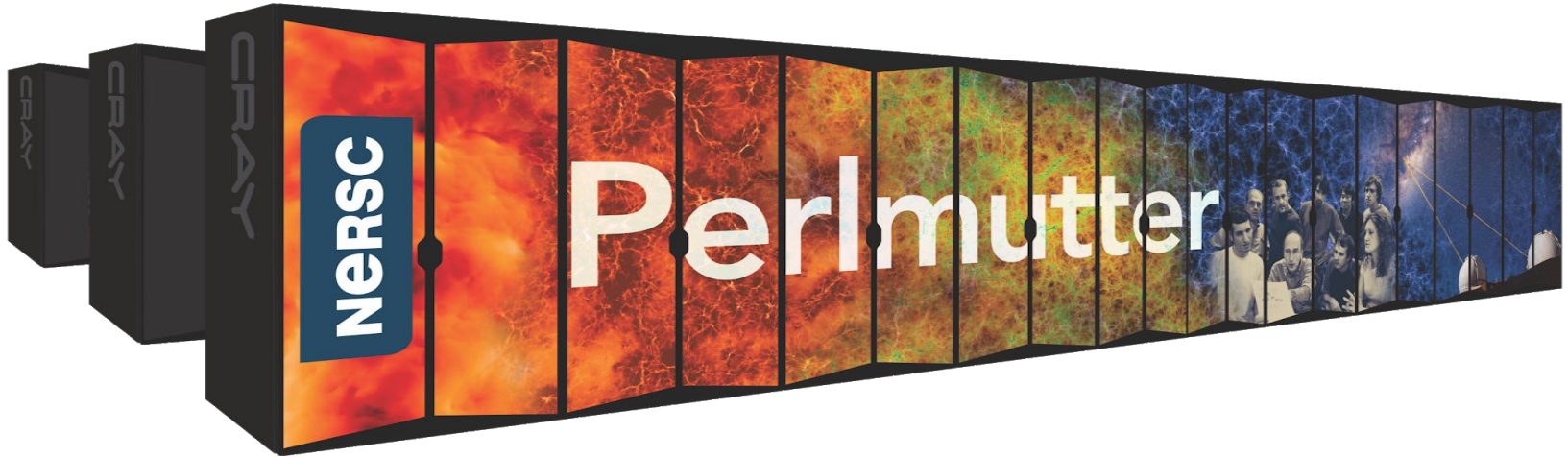**Breakdown of Compute Used by DOE Program**

~1,000 Projects

- <1% Small Business Innovation Research
- 1% Biological Systems Science
- 2% Scientific User Facilities
- 11% Climate and Environmental Science
- 13% Nuclear Physics
- 19% High Energy Physics
- 18% Chemical Sciences, Geosciences, and Biosciences
- 18% Material Sciences
- 15% Fusion Energy and Plasma Science

~9,000 ANNUAL USERS FROM ~800 Institutions + National Labs

- 27% Graduate Students
- 17% Postdoctoral Fellows
- 14% Staff Scientists
- 11% University Faculty
- 7% Undergraduate Students
- 6% Professional Staff

- 59% Universities
- 29% DOE Labs
- 5% Other Government Labs
- 3% Industry
- 1% Small Businesses
- <1% Private Labs

>2,000 Scientific Journal Articles per Year

NeRSC

BERKELEY LAB
Bringing Science Solutions to the World

U.S. DEPARTMENT OF ENERGY | Office of Science

Perlmutter

- 1,792 GPU Accelerated Nodes
  - 4 NVIDIA A100 per node
  - 7,168 GPUs
  - 1 AMD "Milan" per node
- 35 PB FLASH scratch filesystem

- 3,072 CPU only nodes
  - 2 AMD "Milan" per node
  - 512 GB memory per node
  - 393K cores
- HPE Cray "Slingshot 11" network

Levels of Support and Usage Models

- **Our users**
  - Develop and use their own codes / Use community codes
  - Small / Medium / Large teams
  - Independent / Need support
  - Low / Medium / High levels of sophistication
- **We want to support the full workload**
  - But, limited staff
  - Have to consider strategic importance and impact
  - But we also want to help projects and users develop capabilities

Many users run community applications, but we have a very large, long tail that wants to leverage a software infrastructure (2021 data)
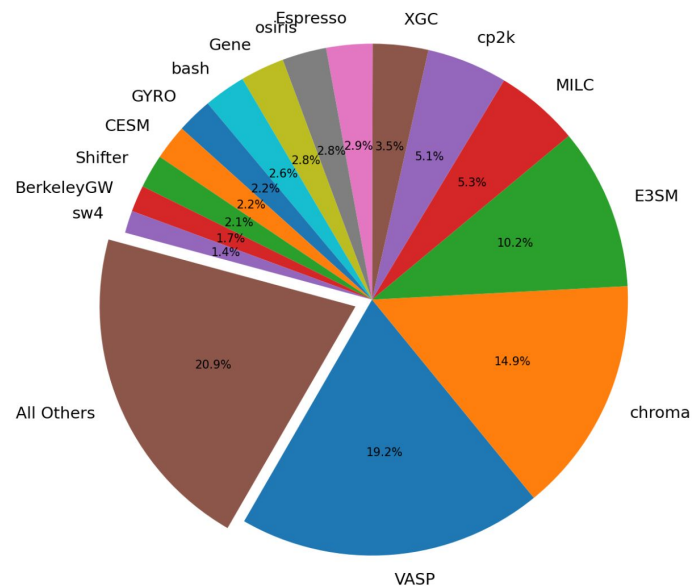
NERSC Current User Software Support

- NERSC has a small team that installs and supports a limited number of applications

- Same for software libraries and tools
  - We try to fill the holes left by vendors for oft-requested libraries and tools
  - Have had a lot of success getting vendor support through procurements; future is less promising

- The E4S suite is installed and is being used (Shahzeb!)

- A sustainable and curated software collection has the potential to bring great value to both users and staff
  - Any coordinated effort should also seize the opportunity to create a way to enable a quantitative measure of usage and impact for each package

- We're happy to entertain other enablement models!

We'd be happy to have vendors optimize, install, and support software

Provides clear support model

Reduces staff effort

Vendors have optimization experts for their architecture

But … may not be agile or as responsive as desired. Versions usually lag.

What Software Do Users Want or Need?

- They evaluate and use what works for them given their optimization targets
  - Cost? Time to get a research result? Capability? Volume of computation? Effort consistent with available personnel resources? Raw performance?
- When choosing software, users' considerations include
  - Functionality and correctness
  - Ease of use
  - Performance
  - Portability and sustainability
  - Documentation and support through software developers or community
  - Ease of Integration into code base/workflow
- Except for the rather obvious packages, it is difficult for facilities to say what users "need" or even "want"
- Many users are open to using new software and methods if they offer advantages
- Would a "standard" HPC user software environment become widely adopted?

What NERSC Considers When Deciding to Support SW

- Level of impact - key enabler of priority science or broad enabler across the board
- Ease of integration
- Forward looking
- Performance - optimization for architecture
- Support model and level of support we have to provide
- Cost
- Impact on system and other jobs
- Security
- Export control and user agreements
- Licenses

Vision of User Support Documentation

https://docs.nersc.gov/applications/berkeleygw/