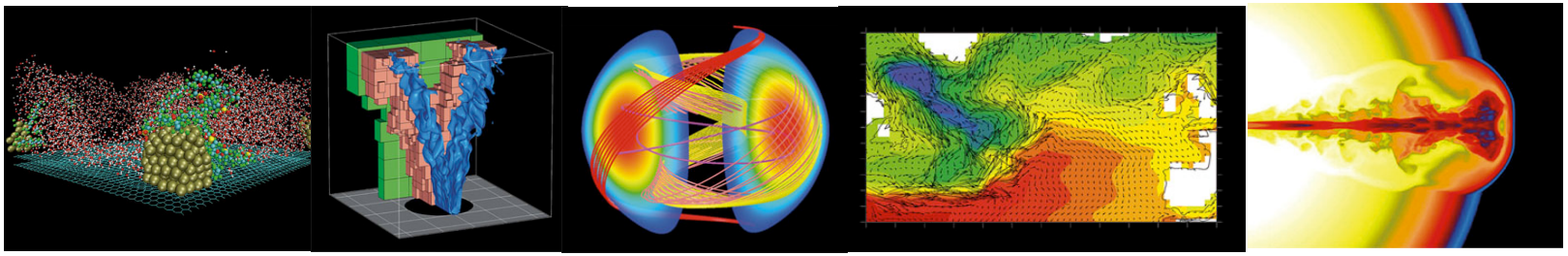


# NERSC Workload Analysis

John Shalf
SDSA Team Leader
jshalf@lbl.gov

## NERSC User Group Meeting
September 17, 2007

Berkeley Lab

NERSC

Office of Science
U.S. Department of Energy

# Workload Analysis

- Purpose
  - Understand NERSC User Requirements
  - Prioritize software library and tool optimization and deployment
  - Inform NERSC Sustained System Performance (SSP) Benchmark Selection
    - "Benchmarks are only useful insofar as they model the intended computational workload." Ingrid Bucher & Joanne Martin, LANL, 1982
    - Effective performance on SSP to reflect effective performance on NERSC workload

# Balancing Requirements

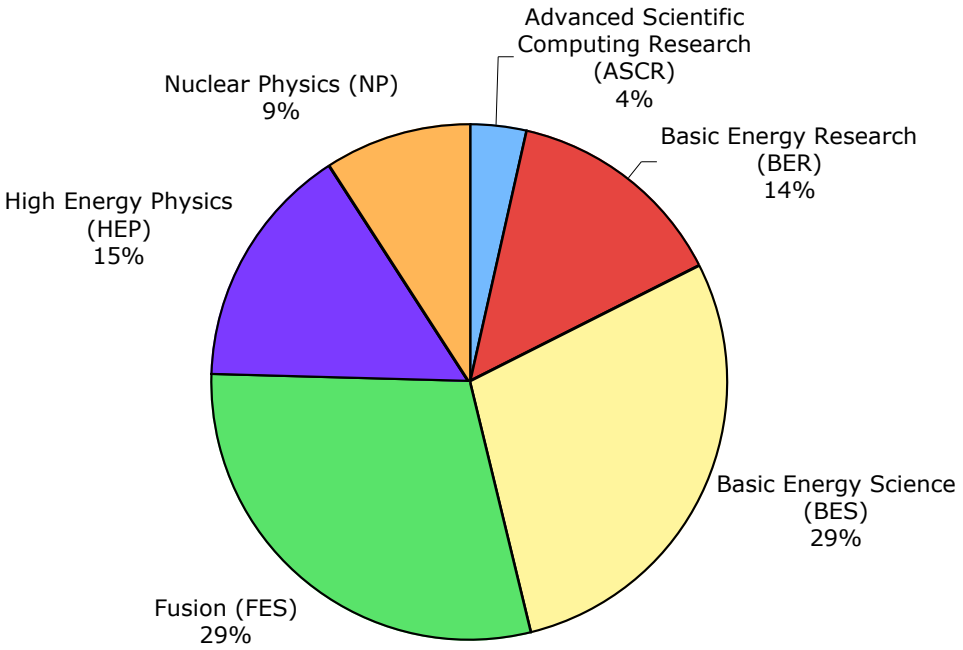
- NERSC Workload overview
  - ~3000 users
  - ~300 projects respresenting a broad range of science
  - ~700 codes (>2 codes per project on average!)
  - 15 science areas for 6 Office of Science divisions
- Select a subset (<10) codes to represent the requirements of the workload
  - Weight based on code's contribution workload? (workload coverage)
  - Weight equally for each area of science? (algorithm/science-area coverage)
- Attempt to cover both dimensions
  - Still daunting
  - Search for islands of coherence in the codes or algorithm selection by different scientific disciplines

# Workload Overview

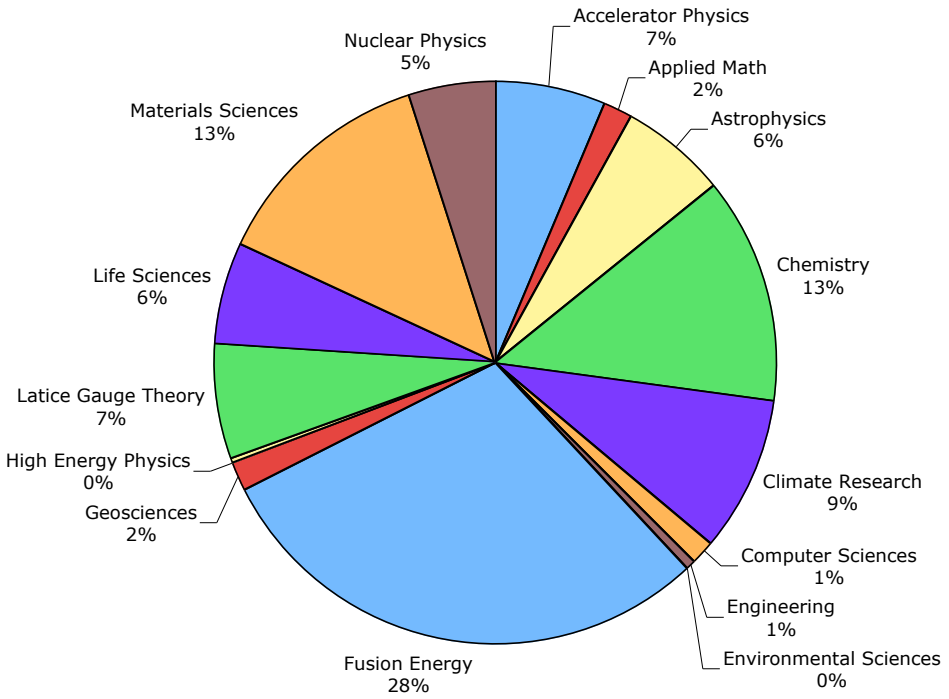
| | | DOE Ofice | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Science Area | Data | ASCR | BER | BES | FES | HEP | NP | Grand Total |
| Accelerator Physics | Normalized Sum of MPP Request | | | 10200000 | | 9768000 | 7580009 | 11546000 |
| | MPP Request Count | | | 3 | | 32 | | 44 |
| Applied Math | Normalized Sum of MPP Request | 10107000 | | 10000 | | | | 10117000 |
| | MPP Request Count | 23 | | 1 | | | | 24 |
| Astrophysics | Normalized Sum of MPP Request | | | | | 9888000 | 2602000 | 12490000 |
| | MPP Request Count | | | | | 42 | 6 | 48 |
| Chemistry | Normalized Sum of MPP Request | 20000 | | 22534000 | | | | 22554000 |
| | MPP Request Count | 1 | | 106 | | | | 107 |
| Climate Research | Normalized Sum of MPP Request | 400000 | 15066000 | | | | | 15466000 |
| | MPP Request Count | 1 | 44 | | | | | 45 |
| Computer Sciences | Normalized Sum of MPP Request | 1400000 | | | | | | 1400000 |
| | MPP Request Count | 41 | | | | | | 41 |
| Engineering | Normalized Sum of MPP Request | 20000 | | 1910000 | | | | 1930000 |
| | MPP Request Count | 2 | | 7 | | | | 9 |
| Environmental Sciences | Normalized Sum of MPP Request | | 170000 | | | | | 170000 |
| | MPP Request Count | | 3 | | | | | 3 |
| Fusion Energy | Normalized Sum of MPP Request | 350000 | | | 40200990 | | | 40550990 |
| | MPP Request Count | 2 | | | 135 | | | 137 |
| Geosciences | Normalized Sum of MPP Request | | | 2704000 | | | | 2704000 |
| | MPP Request Count | | | 15 | | | | 15 |
| High Energy Physics | Normalized Sum of MPP Request | | | | | 500000 | | 500000 |
| | MPP Request Count | | | | | 1 | | 1 |
| Lattice Gauge Theory | Normalized Sum of MPP Request | | | | | 16910000 | 17463000 | 34373000 |
| | MPP Request Count | | | | | 9 | 5 | 14 |
| Life Sciences | Normalized Sum of MPP Request | 50000 | 11019000 | 40000 | | | | 11109000 |
| | MPP Request Count | 1 | 27 | 1 | | | | 29 |
| Materials Sciences | Normalized Sum of MPP Request | 570000 | | 22640750 | | | | 23210750 |
| | MPP Request Count | 3 | | 131 | | | | 134 |
| Nuclear Physics | Normalized Sum of MPP Request | 50000 | | | | | 12696000 | 12746000 |
| | MPP Request Count | 1 | | | | | 31 | 32 |
| Total Normalized Sum of MPP Request | | 12967000 | 26255000 | 50858750 | 40200990 | 37066000 | 33519000 | 200866740 |
| Total MPP Request Count | | 75 | 74 | 264 | 135 | 84 | 51 | 683 |

# ERCAP Allocations 2007 By Office and Science Area

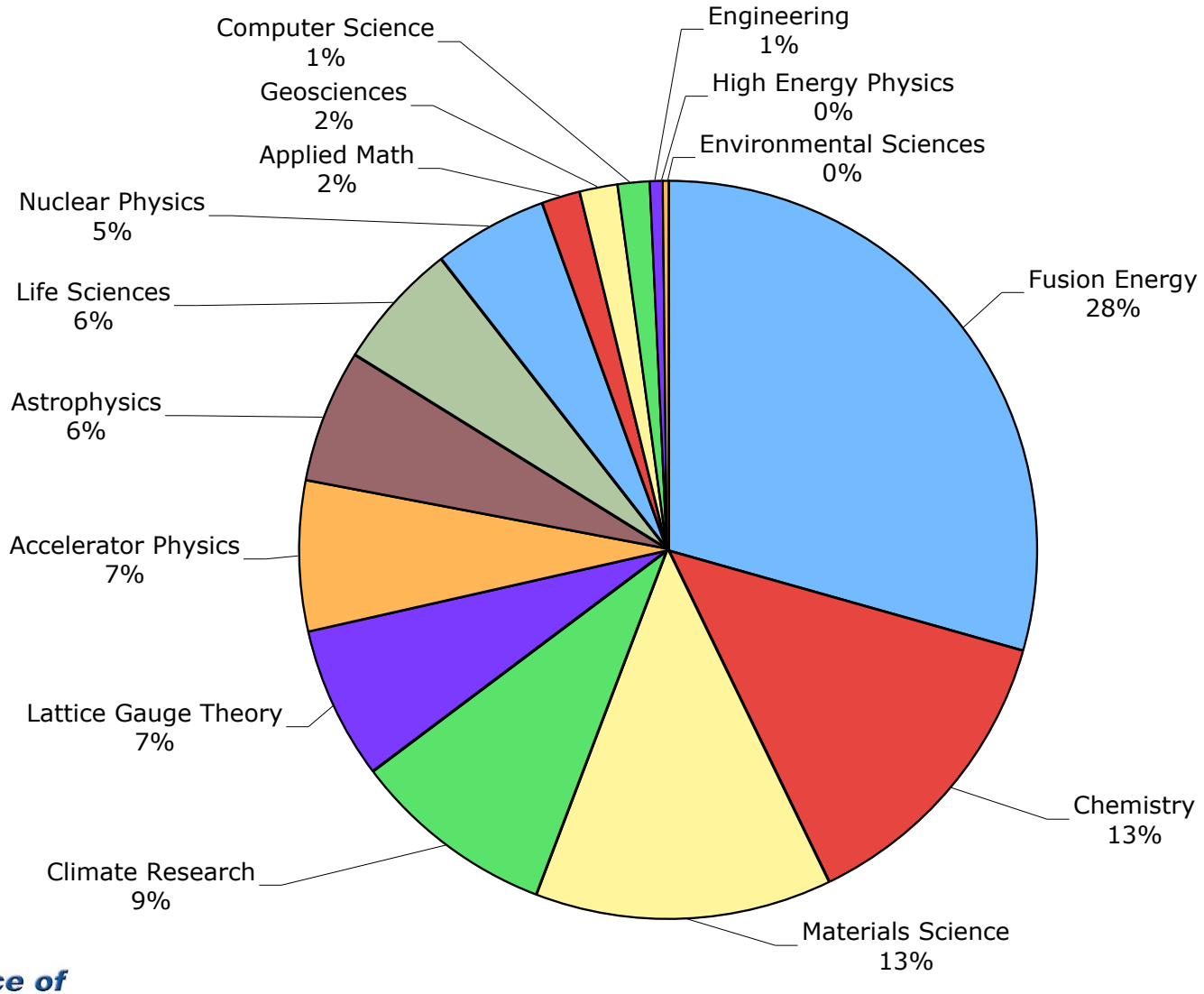
**Awards by DOE Office**



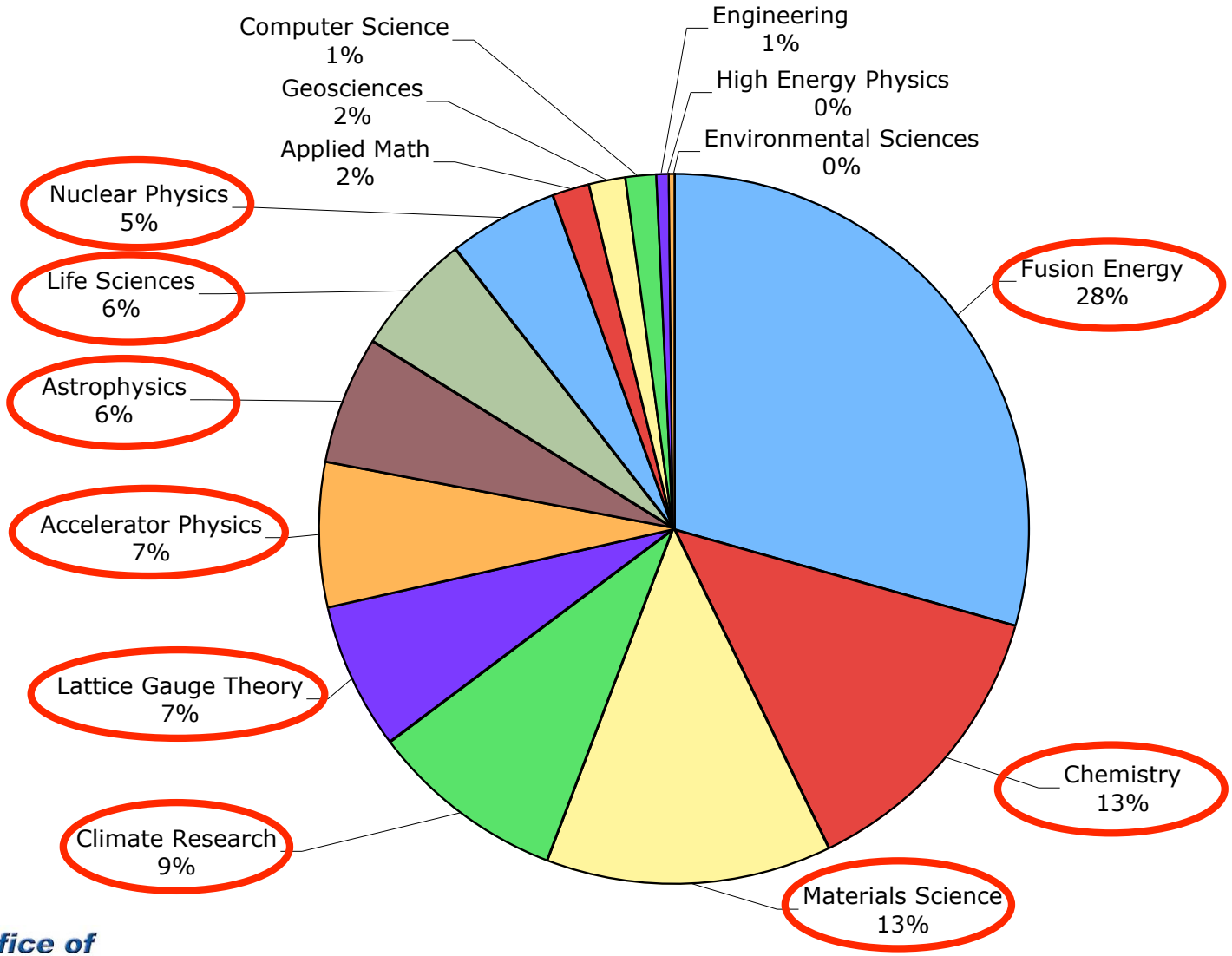

**Awards By Science Area**



# Focus on Science Areas



# Focus on Science Areas



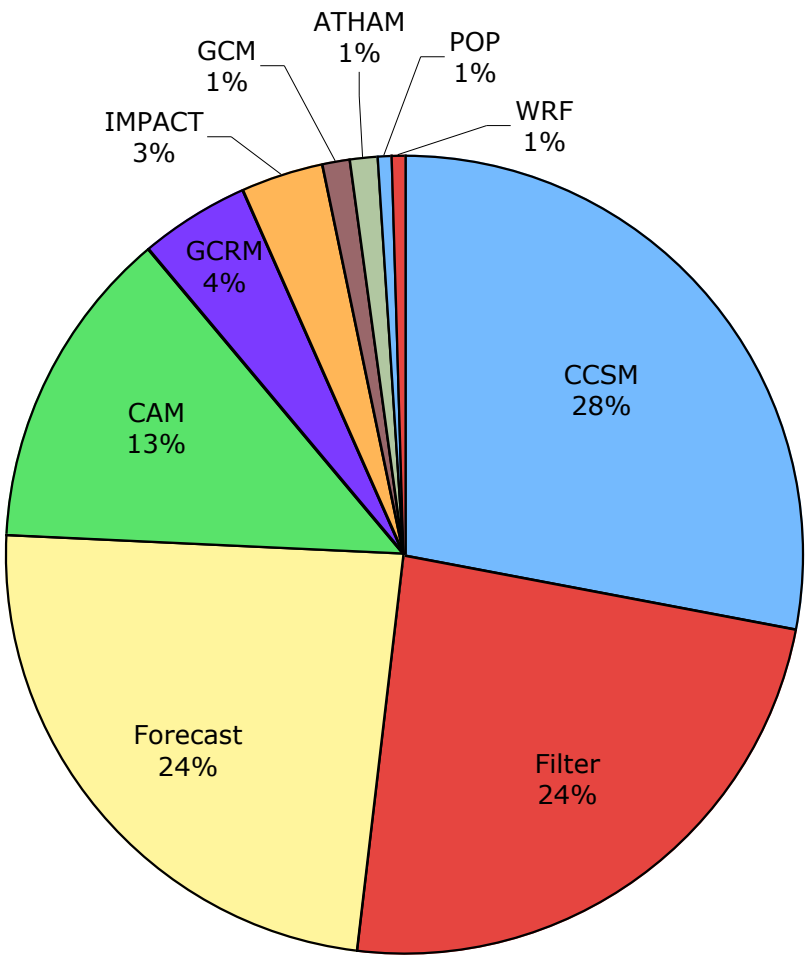
# Modeling the NERSC Workload

| Science Category | Award MPP Hours | Number of Projects |
|---|---|---|
| Fusion Energy | 16,509,000 | 51 |
| Chemistry | 7,405,000 | 41 |
| Materials Science | 7,385,000 | 58 |
| Climate Research | 4,911,000 | 29 |
| Lattice Gauge Theory | 3,812,500 | 6 |
| Accelerator Physics | 3,650,000 | 16 |
| Astrophysics | 3,319,000 | 16 |
| Life Sciences | 3,149,000 | 20 |
| Nuclear Physics | 2,790,000 | 16 |
| Applied Math | 930,000 | 10 |
| Geosciences | 920,000 | 6 |
| Computer Science | 731,500 | 13 |
| Engineering | 390,000 | 4 |
| High Energy Physics | 70,000 | 1 |
| Environmental Sciences | 24,000 | 1 |

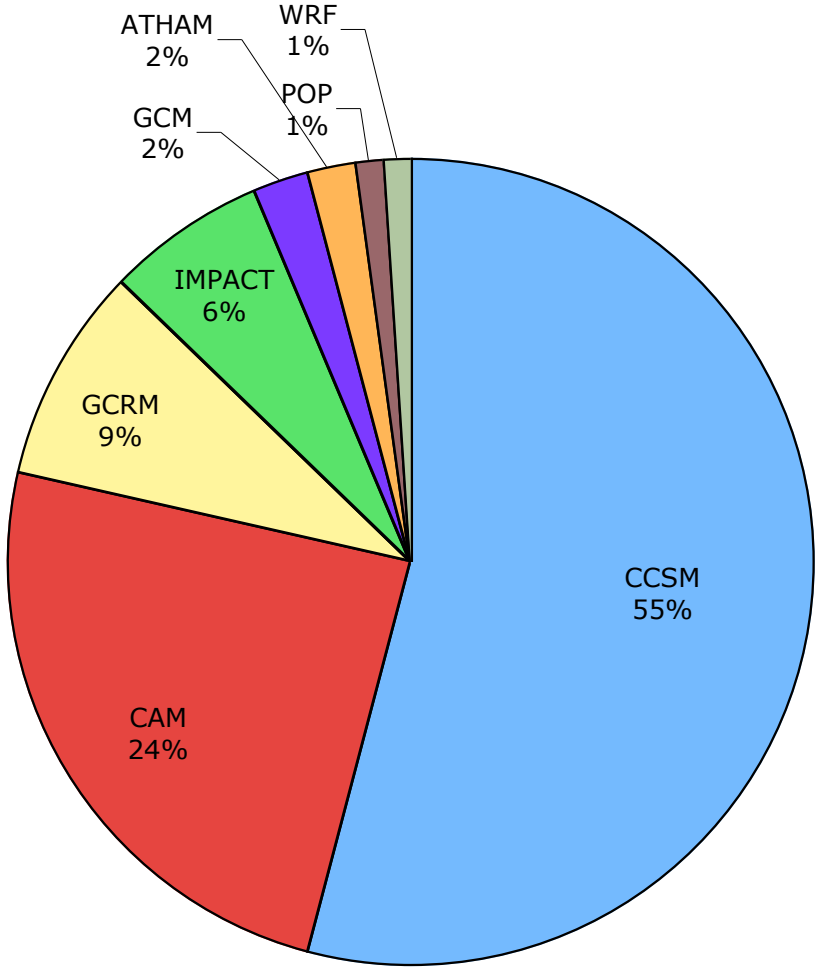
- **Target: choose 6 representative applications from 288 projects, 684 code descriptions**

# Climate Modeling (BER)

**Climate with INCITE**



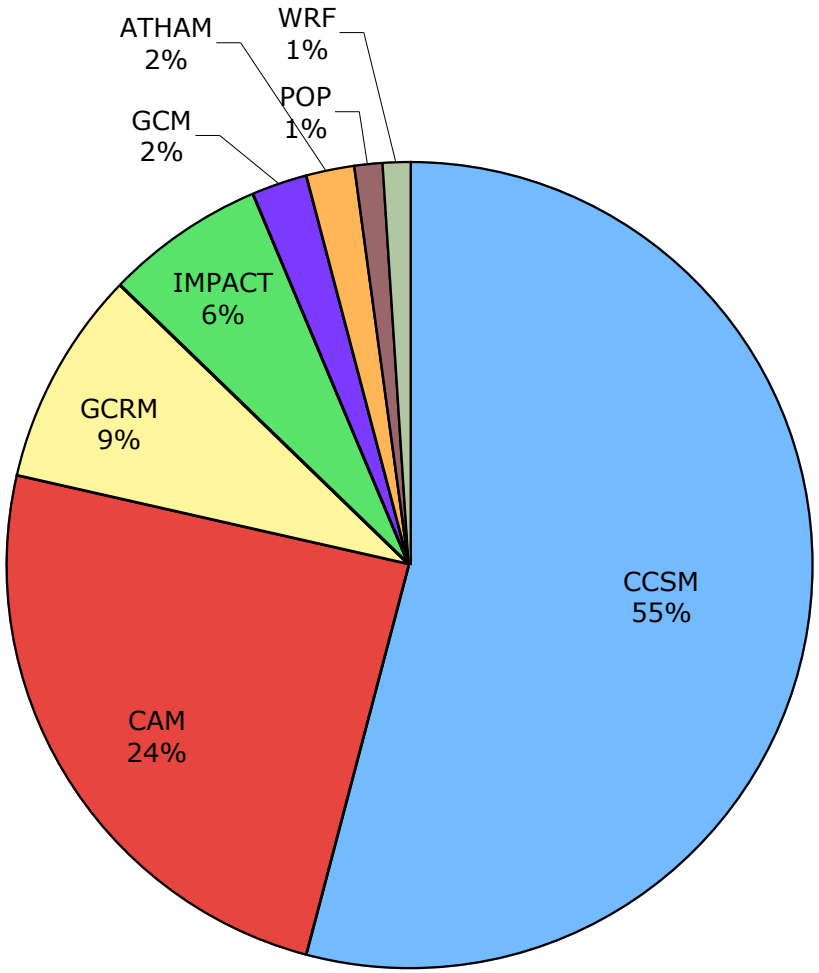

**Climate without INCITE**



# Climate Modeling (BER)

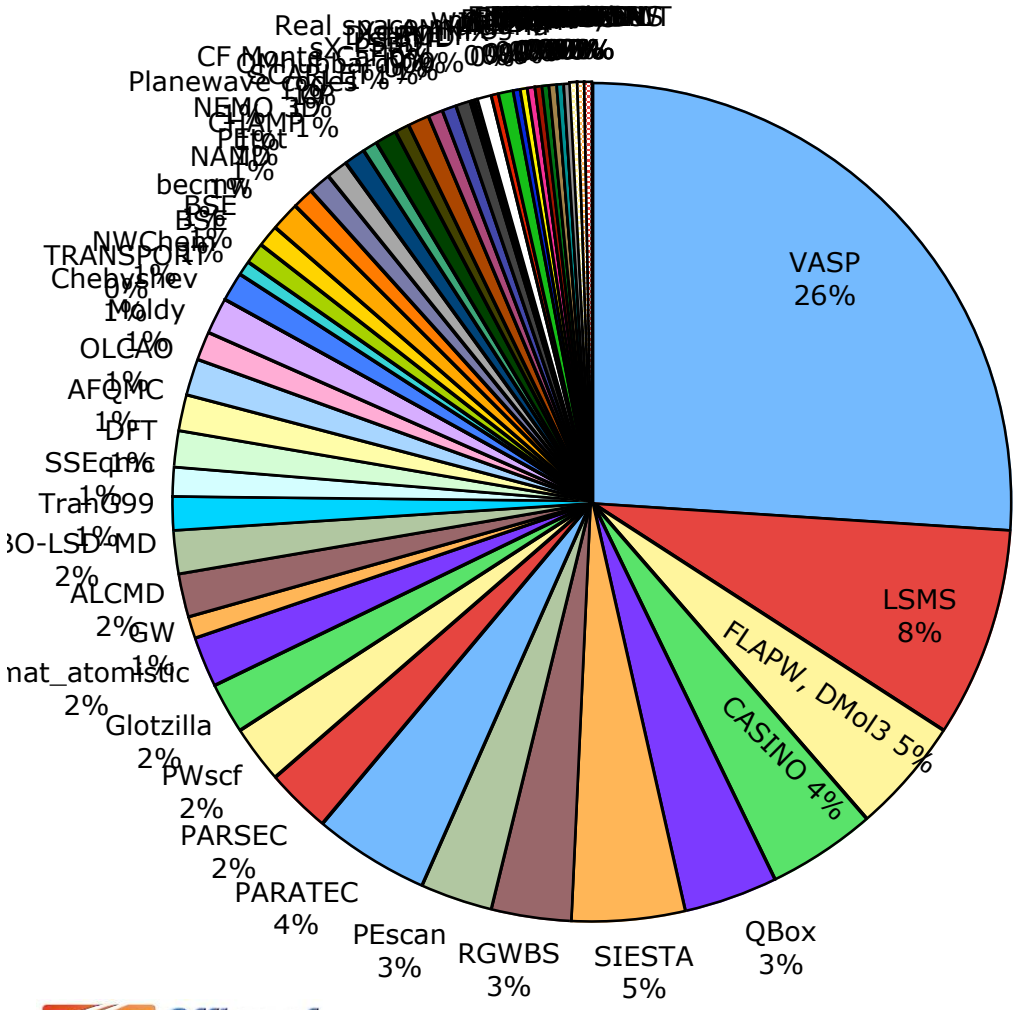
| | Code | MPP Award | Percent | Cumulative% |
|---|---|---|---|---|
| 1 | CCSM | 2,342,000 | 51% | 51% |
| 2 | CAM | 2,000,000 | 23% | 74% |
| 3 | GCRM | 2,000,000 | 8% | 82% |
| 4 | IMPACT | 1,085,000 | 6% | 88% |
| 5 | GCM | 375,000 | 2% | 90% |
| 6 | ATHAM | 280,000 | 2% | 92% |
| 7 | POP | 100,000 | 1% | 93% |
| 8 | WRF | 80,000 | 1% | 94% |

**Climate without INCITE**




- **CAM and POP dominate CCSM computational requirements**
- **FV-CAM increasingly replacing Spectral-CAM in future CCSM calculations**
- **FV-CAM with D-Mesh selected (coordinate w/NCAR procurement)**

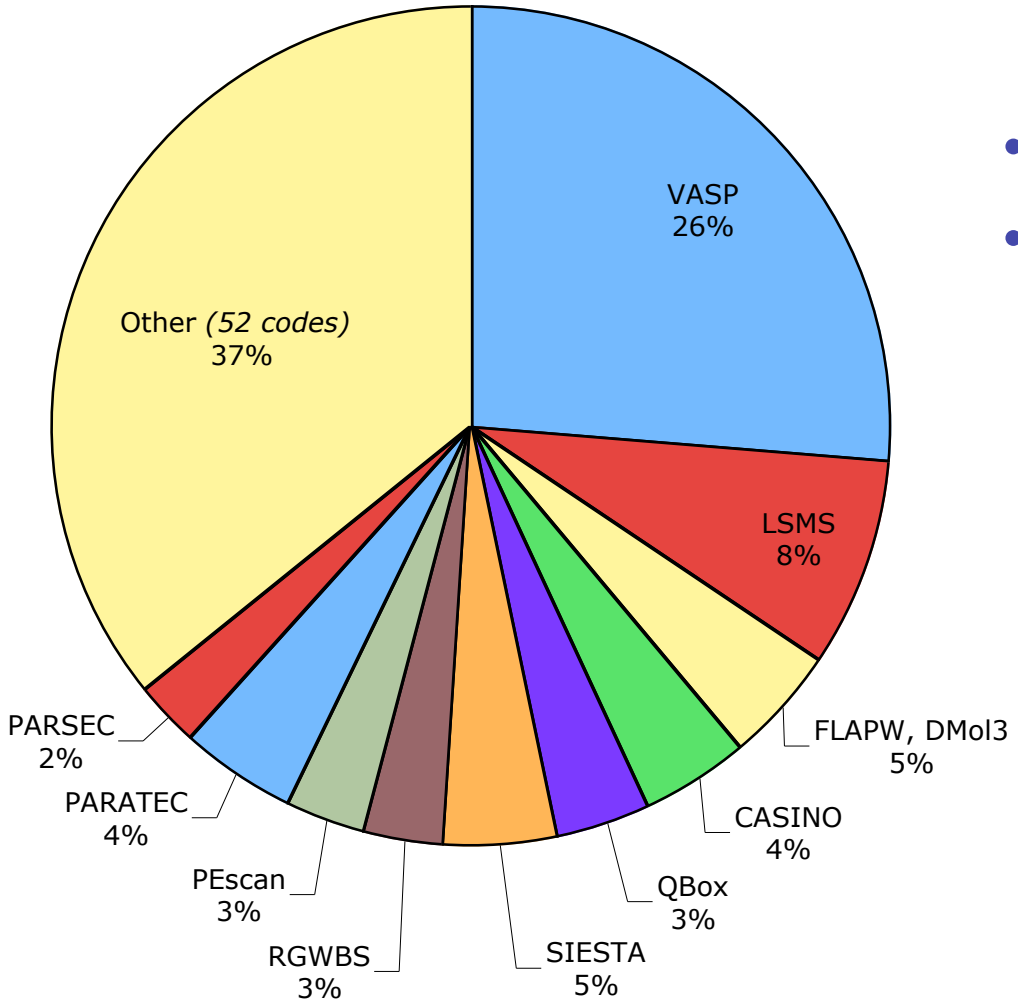
# Material Science




- **7,385,000 MPP hours awarded**
- **62 codes, 65 users**
- **Typical code used in 2.15 allocation requests**

| | Code | MPP Hours | Percent | Cumulative% |
|---|---|---|---|---|
| 1 | VASP | 1,992,110 | 26% | 26% |
| 2 | LSMS | 600,000 | 8% | 34% |
| 3 | FLAPW, DMol3 | 350,000 | 5% | 39% |
| 4 | CASINO | 312,500 | 4% | 43% |
| 5 | QBox | 262,500 | 3% | 46% |
| 6 | SIESTA | 346,500 | 5% | 51% |
| 7 | RGWBS | 232,500 | 3% | 54% |
| 8 | PEscan | 220,000 | 3% | 57% |
| 9 | PARATEC | 337,500 | 4% | 61% |
| 10 | PARSEC | 182,500 | 2% | 64% |
| | Other | 167,300 | 34% | 66% |

# Material Science

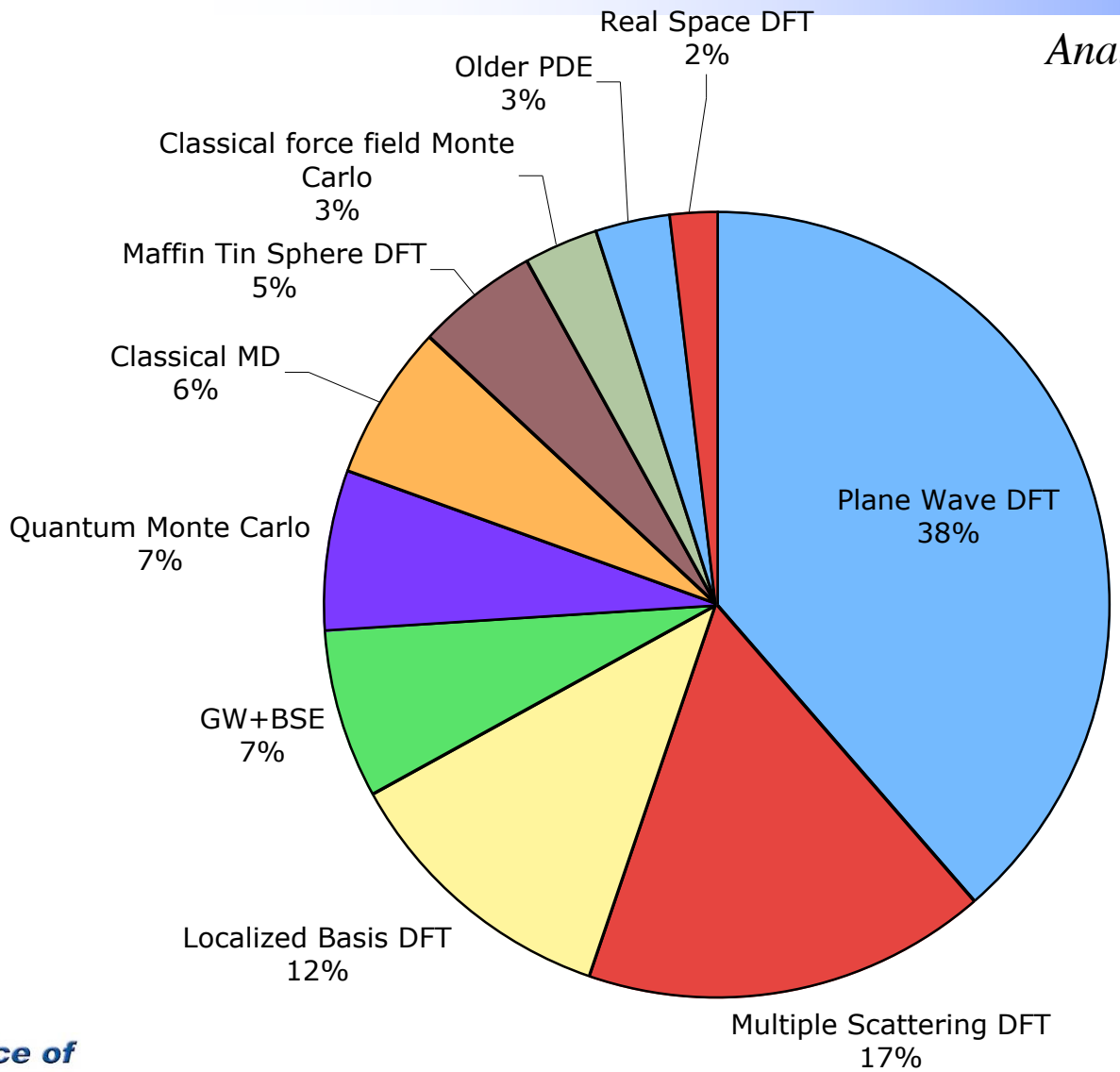



- 7,385,000 MPP hours awarded
- 62 codes, 65 users
- Typical code used in 2.15 allocation requests

| | Code | MPP Hours | Percent | Cumulative% |
|---|---|---|---|---|
| 1 | VASP | 1,992,110 | 26% | 26% |
| 2 | LSMS | 600,000 | 8% | 34% |
| 3 | FLAPW, DMol3 | 350,000 | 5% | 39% |
| 4 | CASINO | 312,500 | 4% | 43% |
| 5 | QBox | 262,500 | 3% | 46% |
| 6 | SIESTA | 346,500 | 5% | 51% |
| 7 | RGWBS | 232,500 | 3% | 54% |
| 8 | PEscan | 220,000 | 3% | 57% |
| 9 | PARATEC | 337,500 | 4% | 61% |
| 10 | PARSEC | 182,500 | 2% | 64% |
| | Other | 167,300 | 34% | 66% |

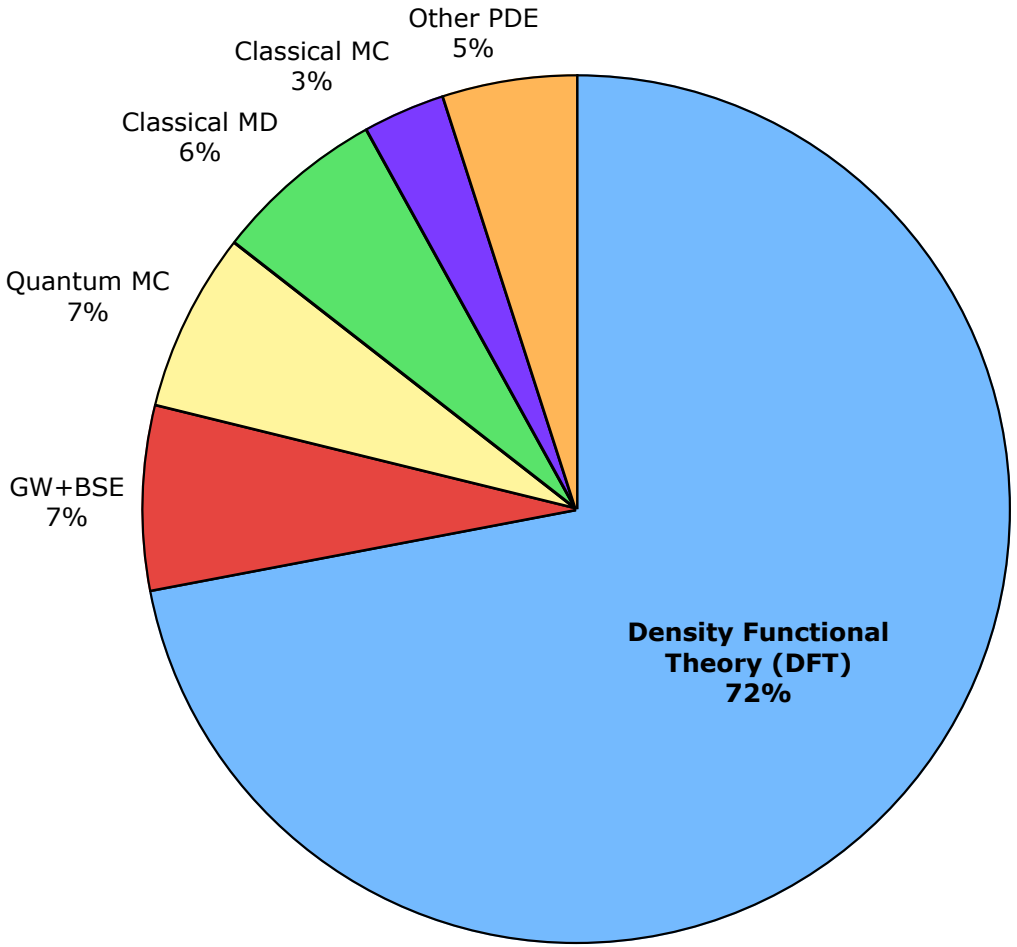
# Materials Science *(by algorithm)*

*Analysis by Lin-Wang Wang*

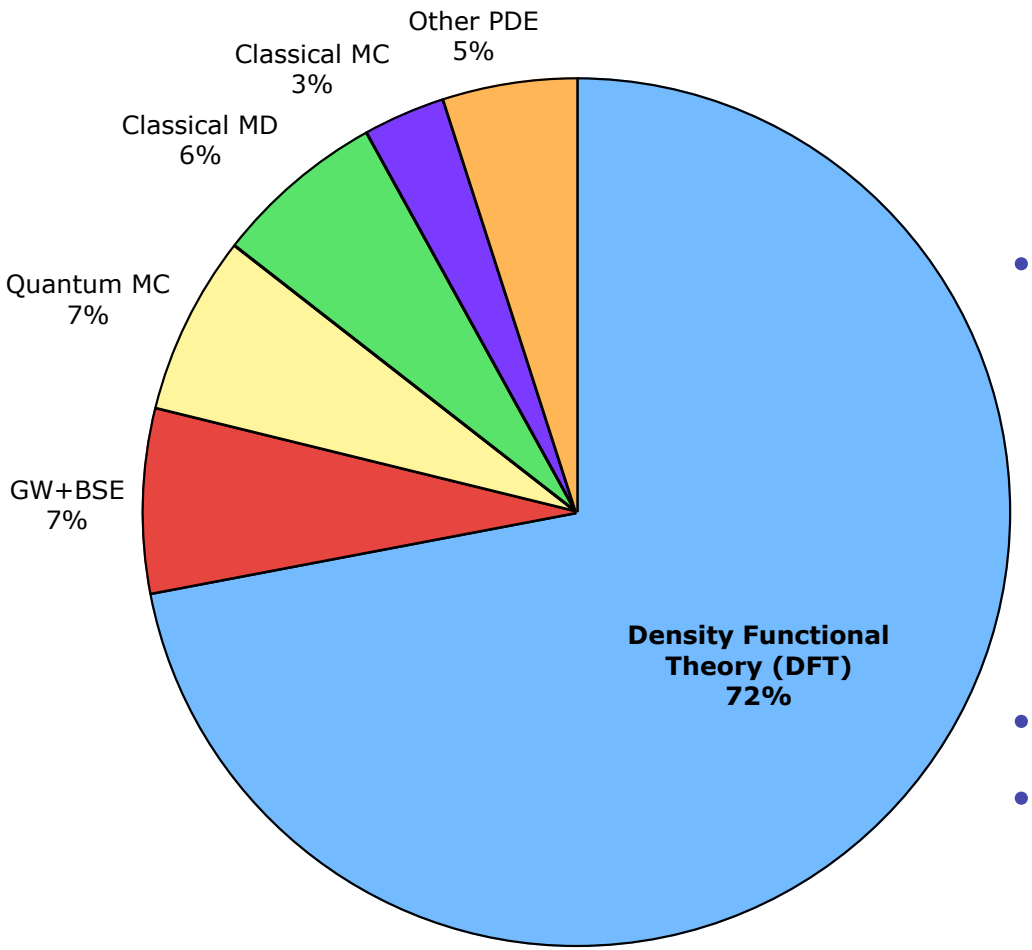


# Materials Science
## *(by algorithm category)*

*Analysis by Lin-Wang Wang*

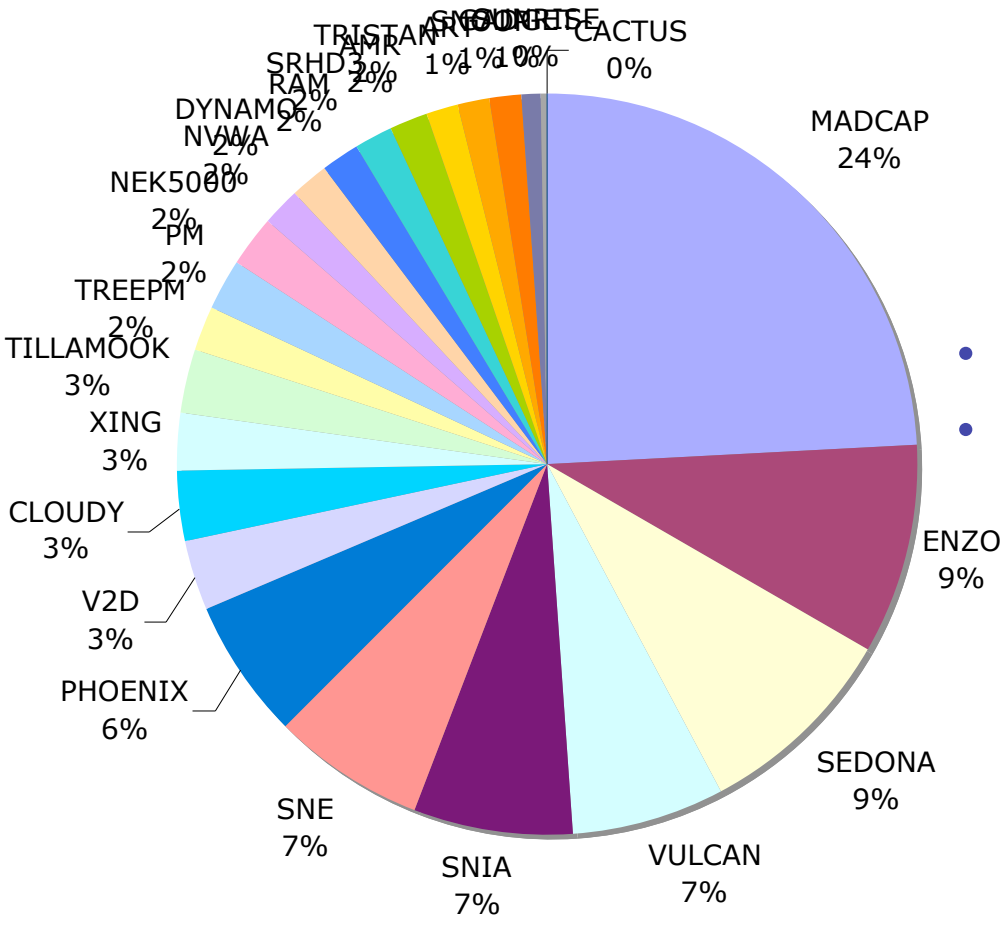


# Materials Science *(by algorithm category)*




- Density Functional Theory codes
  - >70% of the workload!
  - Majority are planewave DFT!
- Common requirements for DFT
  - 3D global FFT
  - Dense Linear Algebra for orthogonalization of wave basis functions
  - Dense Linear Algebra calculating pseudopotential
- Dominant Code: VASP
- Similar Codes (planewave DFT)
  - QBox
  - PARATEC
  - PETOT/PESCAN

# Astrophysics




- **MADCAP: CMB Analysis Suite**
  - **Dominates allocations even though it is not INCITE**
  - **I/O dominated: Now covered in separate I/O benchmarking tests**
- **ENZO: INCITE AMR code**
- **SciDAC Astrophysics Codes dominant**
  - **Coverage of MHD + combustion**
  - **Suggested to look at codes that use implicit methods rather than explicit timestepping (better representative of future codes)**
  - **Might help with Fusion coverage**

# Other Application Areas

- **Fusion: 76 codes**
  - 5 codes account for >50% of workload: OSIRIS, GEM, NIMROD, M3D, GTC
  - Further subdivide to PIC (OSIRIS, GEM, GTC) and MHD (NIMROD, M3D) code categories
- **Chemistry: 56 codes for 48 allocations**
  - INCITE award (S3D) eclipses other chemistry codes: put in separate category
    - Planewave DFT: VASP, CPMD, DACAPO
    - Quantum Monte Carlo: ZORI
    - Ab-initio Quantum Chemistry: Molpro, Gaussian, GAMESS
  - Planewave DFT dominates (but already covered in MatSci workload)
  - Small allocations Q-Chem category add up to dominant workload component
- **Accelerator Modeling**
  - 50% of workload consumed by 3 codes VORPAL, OSIRIS, QuickPIC
  - Dominated by PIC codes

| code | MPP Award | Percent | Cumulative% |
|---|---|---|---|
| OSIRIS | 2,112,500 | 11% | 11% |
| GEM | 2,058,333 | 11% | 22% |
| NIMROD | 2,229,167 | 12% | 34% |
| M3D | 1,921,667 | 10% | 45% |
| GTC | 1,783,333 | 10% | 54% |

| Code | Award | Percent | Cumulative% |
|---|---|---|---|
| ZORI | 695,000 | 12% | 12% |
| MOLPRO | 519,024 | 9% | 21% |
| DACAPO | 500,000 | 9% | 29% |
| GAUSSIAN | 408,701 | 7% | 36% |
| CPMD | 396,607 | 7% | 43% |
| VASP | 371,667 | 6% | 49% |
| GAMESS | 364,048 | 6% | 56% |

| Code | MPP Award | Percent | Cumulative% |
|---|---|---|---|
| VORPAL | **1,529,786** | 33% | 33% |
| OSIRIS | **784,286** | 16% | 49% |
| QuickPIC | **610,000** | 13% | 62% |
| Omega3p | **210,536** | 4% | 66% |
| Track3p | **210,536** | 4% | 70% |

# Selecting Benchmarks

- Coverage
  - Cover science areas
  - Cover algorithm space
- Portable
  - Robust 'build' systems
  - Not architecture specific implementation
- Scalable
  - Do not want to emphasize applications that do not justify scalable HPC resources
- Distributable
  - No proprietary or export-controlled code
- Availability of Developer for Assistance/Support

# Narrowing Selection

**First Cut (Primary Secondary Kernel):**

| | |
|---|---|
| **Fusion PIC** | **GEM (4.9) / GTC (4.4) / XGC (3.7) / SUMMIT (1.5)** |
| **Accelerator modeling** | **OSIRIS (2.9) / VORPAL (2.6) / IMPACTZT / BeamB3D / QuickPIC** |
| **Fusion MHD** | **M3D / NIMROD / GS2 / GYRO / BOUT / Dynamo** |
| **DFT** | **VASP / LSMS / PWscf / CPMD / PARATEC /** |
| **Quantum Chem** | **NWChem / SIESTA / CASINO / GAMESS / Gaussian** |
| **Climate** | **CAM / Forecast Model / IMPACT** |
| **LG Physics** | **MILC / RHMC** |
| **Other astro** | **MADCAP / SN1A / VULCAN / SRH3D / FLASH/MAESTRO** |
| **Combustion** | **S3D** |
| ~~**LifeSci**~~ | ~~**BLAST / Forge / RepeatMasker**~~ |

# Narrowing Selection

**First Cut (Primary Secondary Kernel):**

| | |
|---|---|
| **Fusion PIC** | **GEM (4.9) / GTC (4.4) / XGC (3.7) / SUMMIT (1.5)** |
| **Accelerator modeling** | **OSIRIS (2.9) / VORPAL (2.6) / IMPACTZT / BeamB3D / QuickPIC** |
| **Fusion MHD** | **M3D / NIMROD / GS2 / GYRO / BOUT / Dynamo** |
| **DFT** | **VASP / LSMS / PWscf / CPMD / PARATEC /** |
| **Quantum Chem** | **NWChem / SIESTA / CASINO / GAMESS / Gaussian** |
| **Climate** | **CAM / Forecast Model / IMPACT** |
| **LG Physics** | **MILC / RHMC** |
| **Other astro** | **MADCAP / SN1A / VULCAN / SRH3D / FLASH / MAESTRO** |
| ~~**LifeSci**~~ | ~~**BLAST / Forge / RepeatMasker**~~ |

# Benchmark Summary

| Benchmark | Science Space | Algorithm Space | Proposed Concurrency | Parameters | Lang | Libraries |
|---|---|---|---|---|---|---|
| CAM | Climate (BER) | Navier Stokes CFD, FFT | 1024 | Nx, ny | F90 | netCDF |
| GAMESS | Quantum Chem (BES) | Dense linear algebra, DFT | 512 | # of electron/ atoms | F90 | DDI, BLAS |
| GTC | Fusion (FES) | PIC, finite difference | 512, 2048 | # of particles and grid points | F90 | FFT (opt) |
| MILC | LG Physics (NP) | Conjugate gradiant, sparse matrix | 2048 | # of grid points, steps per trajectory | C | None |
| PARATEC | Mat Science (BES) | DFT | 512, 2048, 4096 | # of atoms | F90 | Scalapack |
| IMPACTZ ?<br>VORPAL ? | Accelerator Physics (HEP) | Largely PIC, fft component<br>Finite difference, PIC | | # of particles, grid points | F90/ C++<br>C/C++ | H5Part (HDF5)<br>HDF5, aztec, lapack, petsc |
| FLASH ?<br>MAESTRO ? | Astrophysics (HEP) | PPM, AMR<br>Low Mach Hydro | 1024, 2048 | # of grid points | F90/C | HDF5, Para-mesh |