Early Access Pioneering Applications for the 250 TF Leadership System at the ORNL Leadership Computing Facility

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Briefing to the Advanced Scientific Computing Advisory Committee (ASCAC)
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Outline

- ORNL Roadmap for Leadership Computing
- ORNL LCF Cray “Jaguar” leadership platform
  - Status today and after imminent 250 TF upgrade
  - Current acceptance process
- Introduction of a new Transition to Operations (T2O) period for leadership systems at the ORNL LCF
- Pioneering applications for the 250 TF T2O
  - Definition and selection process
  - Science plans and impact
  - Readiness preparations and current status
  - Performance and scalability
- Simulation plans during the 250 TF T2O
# Near term HPC roadmap

<table>
<thead>
<tr>
<th>Mission: Deploy and operate the computational resources needed to tackle global challenges</th>
<th>Vision: Maximize scientific productivity and progress on the largest scale computational problems</th>
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</thead>
</table>
| • Understanding earth’s life-support systems  
• Understanding biology  
• Global epidemics  
• Revolutionizing medicine  
• Understanding the universe  
• Future energy | • Providing world class computational resources and specialized services  
• Providing a stable hardware/software path of increasing scale to maximize productive applications development  
• Educating and training the next generation of computational scientists |

### FY2007
- Cray XT4: 119 TF  
  World’s fastest open computer

### FY2008
- Cray XT4: 250 TF  
  Track 2: 170 TF  
  Both AMD quad-core

### FY2009
- Cray Baker: 1 PF  
  leadership class system for science  
  AMD multi-core  
  Track2: 1PF

### FY2011
- Cray Cascade: 20 PF  
  leadership class sustained PF system for science  
  AMD multi-core
The Jaguar Cray XT4 Leadership System

Today

- 11,508 compute nodes
  - 2.6 GHz dual-core AMD Opteron processors with 4 GB memory
  - 23,016 compute cores
- 396 service & I/O nodes
- ~750 TB local storage
- 3D Torus interconnect
- 46 TB aggregate memory
- 119 TF peak performance

After Upgrade*

- 7,824 compute nodes
  - 2.2 GHz quad-core AMD Opteron processors with 8 GB memory
  - 31,296 compute cores
- 240 service & I/O nodes
- ~750 TB local storage
- 3D Torus interconnect
- 63 TB aggregate memory
- 275 TF peak performance

*Planned to commence in mid Dec, 2007

Currently #2 on Top 500 List (www.top500.org)
Leadership System Acceptance
Current Practice at ORNL

- Meet entry criteria prior to acceptance testing
  - System H/W & firmware configured, correctly functioning
  - Contractual performance rates achieved for agreed-upon apps (HPL, LSMS)
  - I/O performance verified and achieved
  - All critical and urgent tickets have been fixed or resolved

- Meet exit criteria after acceptance testing
  - Functionality tests
    - Test that H/W & S/W have the functionality required for successful operation
    - Rebooting, networking, job launch/completion, MPI, I/O, programming env
  - Performance tests
    - Test H/W & S/W performance and scalability required by DOE-SC applications
    - Test and measure interconnect, I/O, & application performance and scalability
  - Stability tests
    - Can system sustain a production workload?
      - Code development and batch workloads for a number of days
    - 95% of the apps submitted complete, 100% complete correctly at least once, and
      100% of the completed apps generate correct answers

- Document formal acceptance test plan and subject it external peer review
  (bread & depth of acceptance testing improves as a result)
Align Applications Where Possible

- Applications for 250 TF system acceptance (not exhaustive)
  - Entrance: LSMS, HPL
  - Functionality: DCA++, Global Arrays (GA), MPI, IOR, CCSM
  - Performance: CHIMERA, S3D, GTC, POP, AORSA, FLASH, GA
  - Stability: Many (expanded set)

- Applications for FY07 Joule metric
  - CHIMERA, GTC, S3D

- Applications for 250 TF T2O period
  - CHIMERA, GTC, S3D
  - POP, DCA++, MADNESS

- Aligning applications exploits synergies to focus PIs and their teams, Center support, SciDAC projects, and the DOE/SC base program
  - Toward a common goal: the application’s ability to achieve science
  - Maximizes the return on investment in the applications
  - Accelerates evolution of the application
Transition to Operations
A New Period After Acceptance, Before General Availability

- ORNL LCF systems enter a Transition to Operations (T2O) period
  - Upon passing Acceptance in that system’s Acceptance Test Plan
  - A short period pre-negotiated with DOE ASCR Program Management

- The T2O has three principal goals
  - Achieve at-scale “science on day one” with early access pioneering apps
  - Address any outstanding system problems found during acceptance
  - Subject system to a real production workload, thereby increasing stability

- The T2O period is a limited availability period
  - Only pre-defined pioneering applications are scheduled on the system
  - Only those users associated with the pioneering applications have access
    - Other users may gain access as needed during this time

- The actual T2O phase for a given LCF system
  - Lasts for a period that depends upon pre-defined completion criteria
    - The criteria for completion is system dependent and negotiated in advance

- System enters General Availability after the T2O period
  - All INCITE users allowed on system at this time

- T2O plans are documented in advance for each LCF system
  - T2O Execution Plan for the 250 TF system is available
Transition to Operations
Execution Plan for 250 TF System

- A set of six pioneering applications have been selected, prioritized, and readied for exclusive, early access science-at-scale simulations
  - Tier 1: CHIMERA, GTC, S3D
  - Tier 2: POP, MADNESS, DCA++
  - Multiple (6) applications selected to
    - Increase the probability of achieving significant science result prior to General Availability
    - Ensure broad coverage of science, algorithm & software commitments by Center

- Data for pioneering app selection collected and submitted by Center to DOE/ASCR (for decision) at least 12 months in advance
  - Allows ample time for coordinated readiness activities

- Pioneering application readiness
  - Application team: scaling, tuning, optimization, and algorithm/model development
  - Support team: I/O, end-to-end workflow, applications-driven OS issues, math libraries, and multi-core programming and algorithms
  - ORNL LCF has been coordinating and supporting these activities this past year
    - Biweekly meetings with rigorous, formal tracking of all readiness progress
    - One LCF liaison assigned per pioneering application

- 6 week period currently planned for 250 TF T2O
  - Planning for ~6 full-machine days per application (~4.5M hours)
    - Each app does not have to consume entire system at once, but this is encouraged
  - Assume 1 day aggregate out of every week for problem resolution
  - Applications are hand scheduled: Tier 1 first, then Tier 2
  - Each application team has POC who is on-call 24x7
  - Stability and performance tests continue to run during this time if system is ever idle
Pioneering Applications
250 TF Selection Process

- ORNL LCF collected data in an open call from science application teams
  - Physics models
    - What physical models are in your code and what changes are planned in the near future?
  - Algorithms
    - What algorithms are in your code and what changes are planned in the near future?
  - Scaling
    - How does your code currently scale and what bottlenecks preclude improved performance?
  - If chosen for acceptance
    - How might your code be used to test and accept a leadership system?
  - If chosen for science on day one
    - What science would you explore and what simulations would you do with a 250 TF-month?
  - Functional software requirements
    - What system software and math libraries are required by your code?

- Over 20 application teams delivered written responses
  - Broad email requests sent out to user groups
  - Predominant response from INCITE, SciDAC, and NSF Projects
  - Documented in Appendix E of NCCS 2007 Requirements Document
  - *Computational Science Requirements for Leadership Computing*
  - Data delivered in fall 2006 to DOE/ASCR for decision

- Pioneering applications for the 1 PF T2O period
  - Web-based form available online by 12/31/07; accept applications through Spring 07
  - Each application could potentially access 50M hours during the 1 PF T2O period!
Pioneering Application: CHIMERA
Science Goals and Impact

Science Goals

- Investigate the 3D multi-physics core-collapse of a non-rotating, 11 solar mass progenitor star
  - Include all important physics except B fields (neutrino transport and interactions)
- Probe the first 500 ms after stellar core bounce, when a supernova explosion is expected to be initiated in this progenitor
  - Use 256 radial zones, 128 latitudinal zones, and 256 longitudinal zones.
- Many questions to answer
  - Does an explosion occur?
  - If so, is it robust (the explosion energy)?
  - How does the SASI develop in 3D and what impact does it have on the asphericity of the explosion?
  - How aspherical is the explosion?
  - What implications does the asphericity of the explosion have for neutron star kicks?
  - What implications does the asphericity of the explosion have for pulsar spins?
  - What is the element synthesis?

Science Impact

- Core collapse supernovae mechanism cannot be understood without accounting for all relevant physical processes
  - Multi-frequency (and multi-angle) neutrino transport with neutrino interactions
  - Magneto-hydrodynamics
  - Self gravity
  - Realistic nuclear equation of state
- The supernova explosion mechanism is sensitive to the neutrino energy spectra
  - Inclusion of multi-frequency neutrino transport is therefore critical
  - No such inclusion has been achieved in 3D
- Realistic 3D core collapse models do not exist prior to these planned simulations
- Anticipated simulation outcomes
  - First 3D multi-physics core collapse supernova simulation to include multi-frequency neutrino transport
  - Genesis of development of realistic 3D core collapse supernova models
  - Fill significant voids in supernova theory surrounding element synthesis and gravitational wave generation
Pioneering Application: CHIMERA
Physical Models and Algorithms

**Physical Models**

- A "chimera" of three separate yet mature codes
  - Coupled into a single executable
- Three primary modules ("heads")
  - MVH3: Stellar gas hydrodynamics
  - MGFLD-TRANS: "ray-by-ray-plus" neutrino transport
  - XNET: thermonuclear kinetics
- The heads are augmented by
  - Sophisticated equation of state for nuclear matter
  - Self-gravity solver capable of an approximation to general-relativistic gravity

**Numerical Algorithms**

- Directionally-split hydrodynamics with a standard Riemann solver for shock capturing
- Solutions for ray-by-ray neutrino transport and thermonuclear kinetics are obtained during the radial hydro sweep
  - All necessary data for those modules is local to a processor during the radial sweep
  - Computed along each radial ray using only data that is local to that ray
- Physics modules are coupled with standard operator-splitting
  - Valid because characteristic time scales for each module are widely disparate
- Neutrino transport solution
  - Sparse linear solve local to a ray
- Nuclear burning solution
  - Dense linear solve local to a zone

Early-time distribution of entropy in 2D exploding core collapse simulation
Pioneering Application: CHIMERA
Code Readiness, Scalability, and Performance

Readiness Activities

- Physical Models
  - Alpha network
- Algorithms
  - Spherical polar coordinate singularity workaround
  - Poisson solver
- Scalability & performance
  - Multi-core ray-by-ray solves
  - Replace domain decomposition from slab to pencil
  - Parallel I/O
  - Joule metric benchmark studies

Scalability/Performance

- Good weak and strong scaling
- Initial Barcelona quad-core testbed performance promising
  - Currently using 1 MPI task/core, with plans to implement OpenMP for threading of transport and nuclear burning solves

MVH3 strong scaling (speedup vs core count) for a Sedov-Taylor blast wave on a $500^3$ mesh.
Pioneering Application: GTC

Science Goals

- Use GTC-C (classic) to analyze cascades and propagation in Collisionless Trapped Electron Mode (CTEM) turbulence
  - Resolve the critical question of $\rho^*$ scaling of confinement in large tokamaks such as ITER; what are consequences of departure from this scaling?
  - Avalanches and turbulence spreading tend to break Gyro-Bohm scaling but zonal flows tend to restore it by shearing apart extended eddies: a competition

- Use GTC-S (shaped) to study electron temperature gradient (ETG) drift turbulence & compare against NSTX experiments
  - NSTX is a spherical torus with a very low major to minor radius aspect ratio and a strongly-shaped cross-section
  - NSTX exps have produced very interesting high frequency short wavelength modes - are these kinetic electron modes?
    - ETG is a likely candidate but only a fully global nonlinear kinetic simulation with the exact shape & exp profiles can address this.

Science Impact

- Further the understanding of CTEM turbulence by validation against modulated ECH heat pulse propagation studies on the DIII-D, JET & Tore Supra tokamaks
  - Is CTEM the key mechanism for electron thermal transport?
  - Electron temperature fluctuation measurements will shed light
  - Understand the role of nonlinear dynamics of precession drift resonance in CTEM turbulence

- First-time for direct comparison between realistic global simulation & experiment on ETG drift turbulence
  - GTC-S possesses right geometry and right nonlinear physics to possibly resolve this
  - Help to pinpoint micro-turbulence activities responsible for energy loss through the electron channel in NSTX plasmas
Pioneering Application: GTC
Physical Models and Algorithms

Physical Models

- GTC is a global code for turbulence transport simulations
  - Uses a shaped plasma in general geometry with electrostatic electron dynamics based on the δh scheme for nonadiabatic part of δf
- Based on the Particle-In-Cell method for solving the gyrokinetic Vlasov-Maxwell equations.
- GTC-C version of GTC uses a circular cross-section model geometry in the large-aspect ratio limit and can accommodate both kinetic ions & electrons
- GTC-S version of GTC can simulate more realistic plasmas where shaping effects are important
  - Global general geometry interfaced with realistic fusion plasma experimental profiles through the TRANSP fusion data tool

Numerical Algorithms

- Gyrokinetic Vlasov equation is solved with standard PIC method
  - Scatter-and-add operation is used for charge and current deposition on the grid
  - Gather operation is used to calculate the fields associated with each particle
- Gyrokinetic Poisson’s equation and the associated continuity equation are solved using an iterative method
- Finite element solutions to the Gyrokinetic-Darwin-Maxwell equations are found with multi-grid and other linear solvers
Pioneering Application: GTC
Code Readiness, Scalability, and Performance

Readiness Activities

- **Physical Models**
  - Implement split-weight scheme for kinetic electrons in shaped plasma component (GTC-S)

- **Algorithms**
  - Port and optimize GTC-S

- **Scalability & performance**
  - Implement radial and particle domain decomposition in GTC-S
  - Implement asynchronous I/O
  - Data flow automation
  - Joule metric benchmark studies

Scalability/Performance

- Excellent full system weak scaling with ~20% of peak performance realized
  - Parallelized with MPI and OpenMP

- Initial Barcelona quad-core testbed performance promising
  - OpenMP threads perform well
  - Reduced memory B/W may not be an issue

- Needs to vectorize better

LCF liaison contributions
- Asynchronous I/O
- Automated end-to-end workflow
- Porting/scaling new shaped plasma version
Pioneering Application: S3D
Science Goals and Impact

Science Goals

- Turbulent lifted flames occur in diesel engines and gas turbines
  - Fuel is injected into a hot gas environment and flame is stabilized through the recirculation of hot air and combustion products
- What are the mechanisms that stabilize the flame base?
  - Explore the role of auto-ignition, flame propagation, and large eddies
- Analyze a lifted turbulent slot jet flame with a heated coflow
  - Extend a recent H2/air lifted jet flame configuration in ambient coflow to more realistic chemistry (ethylene) and higher pressures representative of compression ignition engine operating regimes
- Detailed of proposed simulation
  - 15 um grid spacing, 2 mm nozzle jet height, 2.4 cm axial length, 3.2 cm transverse width, 0.6 cm spanwise
  - 200 m/s jet velocity (Re = 11,000)
  - Simulate 3 flow-through times (0.36 ms) for stationary statistics at lifted flame base

Science Impact

- Fundamental insight into lifted-flame stabilization mechanisms in auto-ignitive environments
- Provision of data for ignition and combustion model validation
- Acceleration of the evolution of a validated, predictive, multiscale, combustion modeling capability
- Optimize design and operation of evolving fuels in advanced engines for transportation applications.

DNS of a lifted hydrogen flame (2007)
Pioneering Application: S3D
Physical Models and Algorithms

Physical Models

- DNS directly solves the continuum equations for turbulent reactive flows with detailed descriptions of chemical kinetics and molecular transport
  - Requires time and space resolution for all relevant physical and chemical scales
  - Compute-limited by moderate turbulence intensities and to simple lab configurations
- Preferred method for fundamental studies of fine-scale turbulence-chemistry interactions in combustion
- Framework for the development and validation of subgrid turbulence and combustion models for engr design
- Turbulence is “model-free” since fluid scales are resolved
  - Still reliance on models for chemical kinetics & molecular transport properties
- Accurate and computationally efficient chemical mechanisms used in the range of thermo-chemical states traversed

Numerical Algorithms

- Parallel DNS compressible Navier-Stokes solver with total energy, species and mass continuity coupled with detailed chemistry
- Chemical reactions and species diffusion rates in optimized library based on SNL’s Chemkin package
- 3D domain partitioned rectilinear mesh in Cartesian geometry
- High-order accurate, non-dissipative numerical scheme ensures turbulence not swamped by numerical error
  - Spatial discretization achieved with eighth-order finite differences and tenth-order filters to damp spurious oscillations
  - Temporal discretion via an explicit six-stage, fourth-order Runge-Kutta method
- Differencing and filtering require nine and eleven point centered stencils
- Navier-Stokes characteristic boundary condition treatment used boundaries
Pioneering Application: S3D
Code Readiness, Scalability, and Performance

**Readiness Activities**

- **Physical Models**
  - Develop reduced chemical mechanism for n-heptane and ethylene; developed reduced efficient transport model

- **Algorithms**
  - Test n-heptane model for stiffness; develop additive RK integration scheme if stiffness limits integration time step
  - Implement massless Lagrangian tracers

- **Scalability & performance**
  - Tune multi-core performance
  - Develop and test collective I/O
  - Finalize run parameters (e.g. spatial resolution, domain size)
  - Joule metric benchmark studies

**Scalability/Performance**

- Excellent full system weak scaling with ~15% of peak performance
- Initial Barcelona quad-core testbed performance promising
  - Good vectorization
  - Reduced memory B/W may not be an issue
  - Addition of OpenMP threads still of interest
- Efforts of SciDAC-PERI and Cray COE @ ORNL helpful

LCF liaison contributions
- Implement Lagrangian tracers
- I/O rework with NW University
- Scaling studies identified processors burdened by memory corrections
Pioneering Application: POP
Science Goals and Impact

Science Goals

- Fundamental understanding of how the global ocean responds to the biogeochemistry feedback mechanism
  - Also facilitates model calibration in preparation for full CCSM coupling at the petascale
- Addition of biogeochemistry to the ocean model is a critical step toward prediction of the Earth system and its carbon, nitrogen, and sulphur cycles
- Simulate effects of biogeochemistry in current leading-edge eddy-resolving global ocean circulation models
  - A 20-year POP run is needed to resolve the time scales of interest
  - 0.1° resolution with tripole grid to keep coordinate singularities on land
  - Use of partial bottom cells to give more accurate bathymetry
- Sea ice model not included in current planned simulations
- 23 passive tracers will be used

Science Impact

- First-ever global eddy-resolving simulation with ocean biogeochemistry
  - A number of regional studies (Ross sea, Arabian Sea) have been performed but nothing global finer than 1°
- Combine the most realistic ocean simulation with a comprehensive ocean ecosystem and trace gas model
  - First attempt at a realistic simulation of ocean ecosystems
  - Include eddy pumping of nutrients and realistic simulation of fronts that are necessary for ocean ecology
Pioneering Application: POP
Physical Models and Algorithms

Physical Models

- An ocean circulation model derived from earlier models of Bryan, Cox, Semtner and Chervin in which depth is used as the vertical coordinate
  - Solves 3D primitive equations for fluid motions on the sphere under hydrostatic and Boussinesq approximations
  - Possesses a wide variety of physical parameterizations and other features
- Sea ice model features
  - Energy conserving thermodynamics model with four layers of ice and one layer of snow in each of five ice-thickness categories
  - An energy-based ridging scheme, an ice strength parameterization, elastic-viscous-plastic ice dynamics, and horizontal advection via incremental remapping
  - Prognostic variables for each thickness category include ice area fraction, ice volume, ice energy in each vertical layer, snow energy, and surface temperature
  - Can accommodate four wavelengths of radiation and have four associated albedos

Numerical Algorithms

- Spatial derivatives approximated with finite-difference discretizations formulated for any generalized orthogonal grid on a sphere
  - Including dipole and tripole grids which shift the North Pole singularity into land masses to avoid time step constraints due to grid convergence
- Time integration is split into two parts
  - 3D vertically-varying (baroclinic) tendencies are integrated explicitly using a leapfrog scheme
  - Very fast vertically-uniform (barotropic) modes are integrated using an implicit free surface formulation in which a preconditioned conjugate gradient solver is used to solve for the two-dimensional surface pressure.
- Lagrangian particles
- Passive tracer transport
  - Lax-Wendroff advection (w/ limiting)
Pioneering Application: POP
Code Readiness, Scalability, and Performance

Readiness Activities

- **Algorithms**
  - Implement more scalable barotropic solver with improved CG preconditioner
    - Block Jacobi (additive Schwartz), with plans for multi-level enhancement
    - Trade extra flops for more iterations

- **Scalability & performance**
  - Tune for SSE and OpenMP parallelism
  - Implement parallel I/O and test

Scalability/Performance

- **Ever-improving strong scaling with ~10% of peak performance**
  - Tackle scalability-limiting barotropic solver dominated by MPI all-reduce latency with new block Jacobi preconditioner
  - Should benefit more from QC SSE instructions

- **New preconditioner in barotropic solve is 1.78x faster on 15,000 cores**
  - Full benchmark 1.38x faster

- **Initial Barcelona quad-core testbed perf**
  - Good vectorization
  - Memory B/W an issue unless high processor counts are used to ensure small subgrid size
  - Improved speedup needed w/ OpenMP threads

- **Addition of biogeochemistry creates more independent work, improving scalability**

- **Issue with global gather for I/O on CNL**
  - Currently being addressed in multiple ways

**LCF liaison contributions**

- New preconditioner for barotropic solver
- Contributed bug fixes to POP 2.0
- Represent needs at OBER/ESNET meeting
Pioneering Application: DCA++
Science Goals and Impact

Science Goals

- Study high temperature superconductivity (HTC) via simulations of inhomogeneous Hubbard models
  - Believed to describe the HTC cuprates

- Recent simulations have shown that the 2D homogeneous Hubbard model does have a superconducting state and pairing mechanism is now understood
  - The responsible pairing interaction arises from anti-ferromagnetic spin fluctuations

- Must address the effect of charge & spin inhomogeneities on the superconducting state in the Hubbard model
  - Their effect on the critical temperature $T_c$ and their role in the pairing mechanism

- Studies of both random and periodic inhomogeneities will be carried out

Science Impact

- Recent experiments have shown that nanoscale charge and spin inhomogeneities emerge in a number of cuprates

- Based on these findings, it was proposed in the literature that inhomogeneities play a major role in HTC

- Results will be used to study the role of inhomogeneities in the pairing mechanism of the 2D Hubbard model and address questions such as
  - Do inhomogeneities act to increase or decrease the critical temperature $T_c$?
  - Do they enhance, suppress or even modify the pairing mechanism?
  - Is there an optimal inhomogeneity that maximizes $T_c$?

- Use the knowledge gained to artificially structure cuprate based materials with higher transition temperatures
Pioneering Application: DCA++
Physical Models and Algorithms

Physical Models
- Designed to simulate materials where electronic correlations are important using a dynamical cluster approximation (DCA) or other quantum cluster theories
- Approximates the effects of correlations in the bulk lattice with those of a finite-size quantum cluster
  - Enables mapping of the bulk lattice problem to an effective cluster embedded in a self-consistent bath designed to represent the remaining degrees of freedom.
- Invokes quantum Monte Carlo (QMC) or other quantum cluster solvers such as Lanczos
- Based on the extensible psimag toolkit for materials science
  - www.psimag.org
  - Present focus is on solving Hubbard models for superconducting cuprates
- Part of quantum models (QMOD) framework for the study of strongly correlated electrons

Numerical Algorithms
- Effective cluster problem is solved with a parallel Hirsch-Fye QMC algorithm
- Measurements are performed along the QMC Markov chain of physical quantities such as the single-particle Green’s function and two-particle correlation functions
  - Between measurements, the Green’s function is updated using a Dyson equation
- Majority of time is spent in the Green’s function updates and measurements
  - Performed efficiently with L3 BLAS DGEMM
- Other CPU intensive task is the two-particle correlation function measurement
  - These Fourier transforms are handled using the BLAS Level 3 CGEMM
- QMC algorithm is parallelized by distributing the Markov chain onto many processors
- Several independent, shorter Markov-chain walks on different processors are performed and the result for each disorder configurations is obtained by averaging the results of each walk
Pioneering Application: DCA++
Code Readiness, Scalability, and Performance

Readiness Activities

- **Physical Models**
  - Develop space group package for 2D/3D symmetry
  - Develop multi-band Hamiltonian concept and DFT

- **Algorithms & Software**
  - Rewrite current QMC/DCA code

- **Scalability & performance**
  - Implement additional parallelization over disorder configurations (order $10^2$)
  - Additional parallelizable loop over disorder configuration lies between the outer most self-consistency loop of the DCA and the Monte Carlo sampling loop
  - Enables ~10 disorder configurations in parallel on a total of up to 20K cores
    - Assuming individual QMC runs scale to 2000 cores at near optimal speedup

Scalability/Performance

- **Good weak scaling**
- **Single-node performance** relies on efficient execution of DGEMM on long thin rectangular matrices

Time to solution and speedup (inverse time) for a prototype DCA++ run of the 2D Hubbard model with 16 sites, 80 time slices, and 40,000 measurements, and two steps of MC updates between measurements
Pioneering Application: MADNESS
Science Goals and Impact

Science Goals

- Three applications - two based upon large-scale, all-electron, density functional simulations, and the third examining the dynamics of few-electron systems:

  1. Metal oxide surfaces in catalytic processes (in particular for heavier metals) with partially occupied f-shells
     - These systems require very large unit cells to describe both the adsorbed molecules and surface defects at which the chemistry occurs

  2. Investigate the neutron and x-ray spectra of cuprates and understand the significance of exact exchange in these systems
     - Explore approximate treatment of exchange which appears to be a limitation to current density functionals

  3. Interaction of few-electron systems with intense radiation
     - Confer the ability to describe the electronic structure of these systems essentially without approximation

Science Impact

- Ability to predict the structures, energetics, and reactions of molecules helps chemical industries to maintain their competitive position

- Fast, accurate and efficient treatments of general density functional theories for finite and periodic systems are essential to many topics in chemistry, physics & materials science
  - Must carefully benchmark and validation of these potentials against both more accurate theoretical models and exp data

- Provide detailed information and fundamental methodological benchmarks about catalytic systems and X-ray and neutron spectra

- Study electron dynamics in intense laser fields and will provide fundamental science information concerning electron correlation and interaction with strong fields
Pioneering Application: MADNESS
Physical Models and Algorithms

Physical Models

- MADNESS predicts the physical and chemical properties of molecules
  - Multiresolution ADaptive NumErical Scientific Simulation

Based on

- Multi-resolution analysis in multi-wavelet bases
- Separated representations of functions and operators
- Partitioned singular value representations
- Bandwidth-limited bases for efficient sampling in space and evolution in time

Numerical Algorithms

- Fully adaptive, multi-resolution solution, with guaranteed precision, of the all-electron density functional equations for polyatomic molecules

- Complete elimination of the basis error
  - One-electron models (e.g., HF, DFT)
  - Pair models (e.g., MP2, CCSD, ...)

- Correct scaling of cost with system size

- General approach
  - Readily accessible by students and researchers
  - Higher level of composition
  - Direct computation of chemical energy differences

- New computational approaches

- Fast algorithms with guaranteed precision
Pioneering Application: MADNESS
Code Readiness, Scalability, and Performance

Readiness Activities

- Dynamic load-balancing
  - Testing data redistribution
  - Commencing development on work stealing
- Multi-core
  - Testing design choices for threading of task queue
- Applications
  - Density functional theory – migrating from prototype to implementation
  - Dynamics – evaluating new time evolution scheme

Scalability/Performance

- Runtime objective: scalability to 1+M processors ASAP
- Runtime responsible for
  - scheduling and placement,
  - managing data dependencies,
  - hiding latency, and
  - Medium to coarse grain concurrency
- Compatible with existing models
  - MPI, Global Arrays
- Borrow successful concepts from Cilk, Charm++, Python
- Performance examples
  - Small matrix BLAS in x86 assembly
    - Tuned for target problems
    - 2-6x faster than existing libraries (ACML, ATLAS, Goto, MKL)
    - 50-87% of theoretical peak FLOP/s speed
  - Parallel scalability
    - Tested for correctness and performance on 4096 cores under CNL. Also functions on BG
## Current Planned Pioneering Application Runs

### Cursory Look at the Simulation Specs

<table>
<thead>
<tr>
<th>Code</th>
<th>Quad-Core Nodes</th>
<th>Global Memory Reqm (TB)</th>
<th>Wall-Clock Time Reqm (hours)</th>
<th>Number of Runs</th>
<th>Local Storage Reqms (TB)</th>
<th>Archival Storage Reqms (TB)</th>
<th>Resolution and Fidelity</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHIMERA</td>
<td>7824 4045</td>
<td>16 8</td>
<td>100 100</td>
<td>1 1</td>
<td>13</td>
<td>50</td>
<td>256x128x256 or 256x90x180 20 energy groups, 14 alpha nuclei</td>
</tr>
<tr>
<td>GTC-S GTC-C</td>
<td>3900 3900</td>
<td>40 60</td>
<td>36 36</td>
<td>2 2</td>
<td>350</td>
<td>550</td>
<td>600M grid points, 60B particles 400M grid points, 250B particles</td>
</tr>
<tr>
<td>S3D</td>
<td>7824</td>
<td>10</td>
<td>140</td>
<td>1</td>
<td>50</td>
<td>100</td>
<td>1B grid points, 15 μm grid spacing 4 ns time step, 23 transport vars</td>
</tr>
<tr>
<td>POP</td>
<td>2500</td>
<td>1</td>
<td>400</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>3600x2400x42 tripole grid (0.1°) 20-yr run; partial bottom cells; first with biogeochemistry at this scale</td>
</tr>
<tr>
<td>MADNESS</td>
<td>7824</td>
<td>48</td>
<td>12 2</td>
<td>10 12</td>
<td>5</td>
<td>50</td>
<td>600B coefficients</td>
</tr>
<tr>
<td>DCA++</td>
<td>2000 6000</td>
<td>16 48</td>
<td>12 to 24</td>
<td>20</td>
<td>1</td>
<td>1</td>
<td>Lattices of 16 to 32 sites 80 to 120 time slices O(10^2-10^3) disorder realizations</td>
</tr>
</tbody>
</table>

**Astrophysics — Fusion — Combustion — Climate — Chemistry — Materials Science**