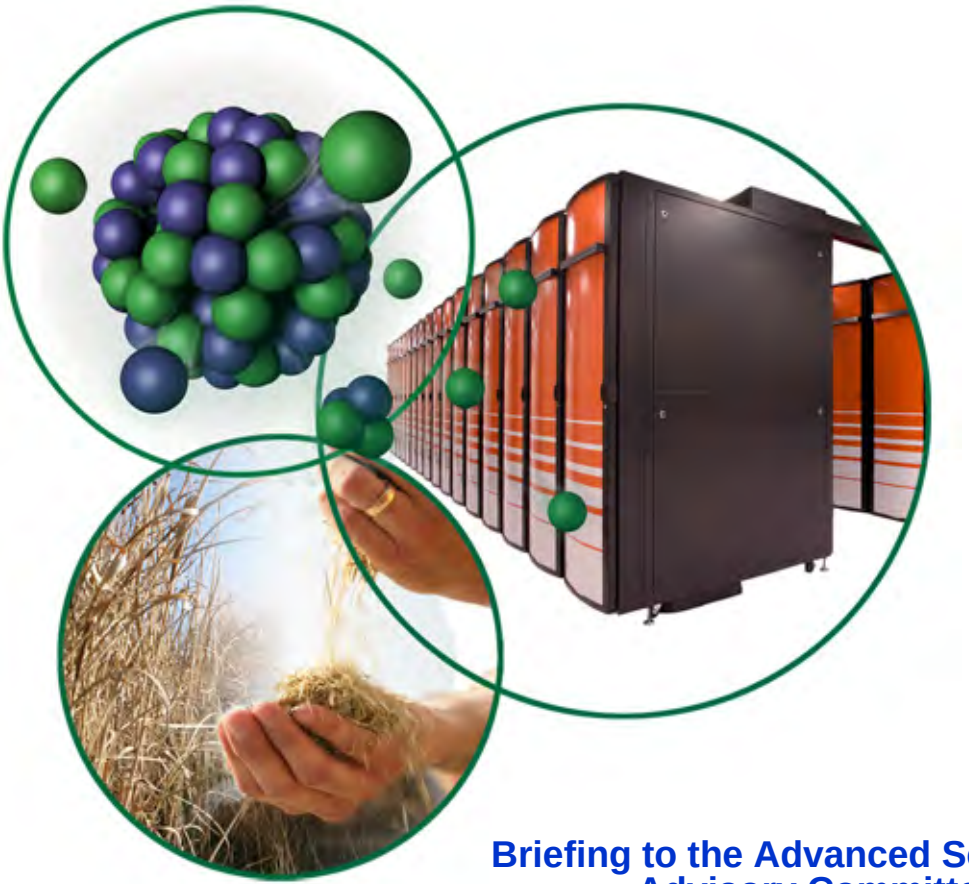
Early Access Pioneering Applications for the 250 TF Leadership System at the ORNL Leadership Computing Facility



Douglas B. Kothe

Director of Science

Leadership Computing Facility
National Center for Computational Sciences
Oak Ridge National Laboratory

Briefing to the Advanced Scientific Computing Advisory Committee (ASCAC)

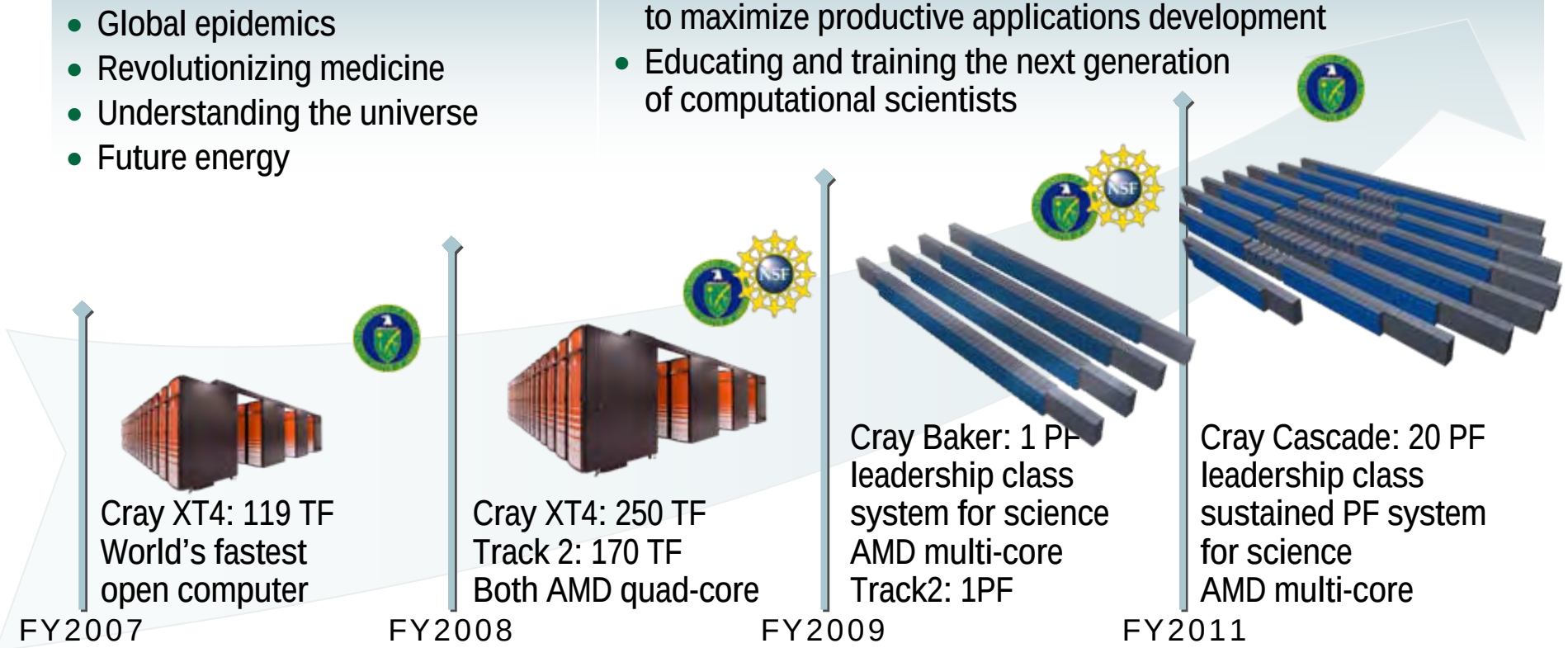
Nov 7, 2007

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

Mission: Deploy and operate the computational resources needed to tackle global challenges	Vision: Maximize scientific productivity and progress on the largest scale computational problems
• 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



The Jaguar Cray XT4 Leadership System

Currently #2 on Top 500 List (*www.top500.org*)

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

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

POC
Anthony
Mezzacappa, ORNL

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?

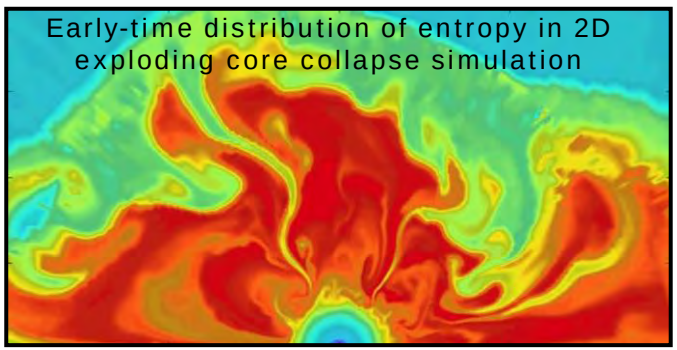
Science Impact

- 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



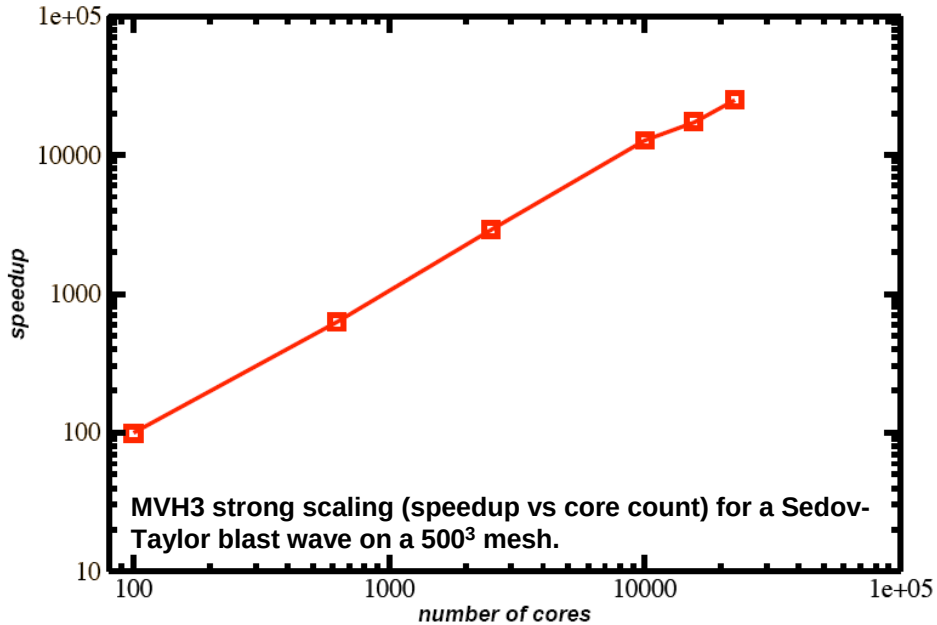
Numerical Algorithms

- 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

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

LCF liaison contributions
- Implementing efficient, collective I/O
- Pencil decomposition of 3D flow algorithm
- Preconditioning of the neutrino transport equation

Pioneering Application: GTC
Science Goals and Impact

POC
Wei-li Lee, PPPL

Science Goals

- **Use GTC-C (classic) to analyze cascades and propagation in Collisionless Trapped Electron Mode (CTEM) turbulence**
  - **Resolve the critical question of ρ* 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**

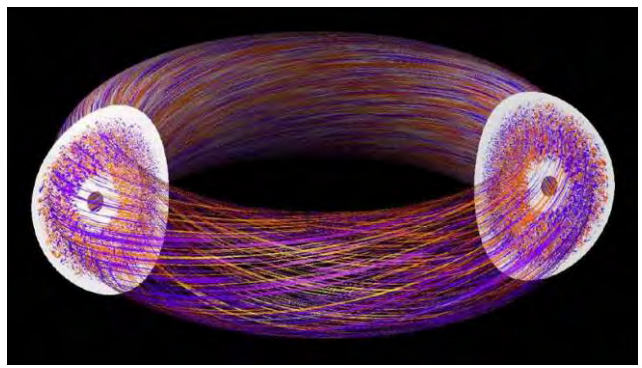
Pioneering Application: GTC
Physical Models and Algorithms

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

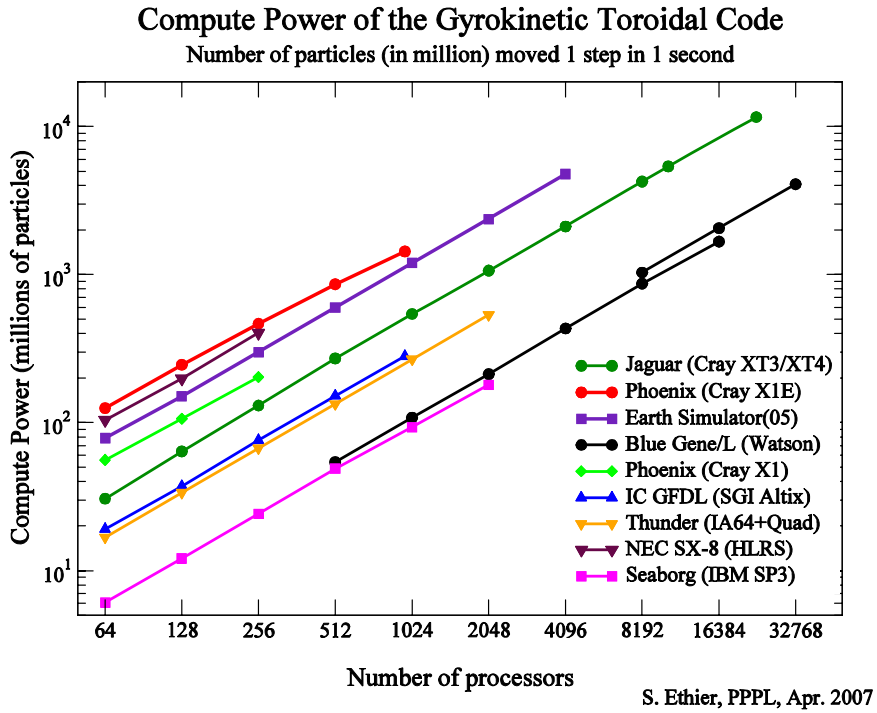


Pioneering Application: GTC
Code Readiness, Scalability, and Performance

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

LCF liaison contributions
- Asynchronous I/O
- Automated end-to-end workflow
- Porting/scaling new shaped plasma version



S. Ethier, PPPL, Apr. 2007

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**

Pioneering Application: S3D
Science Goals and Impact

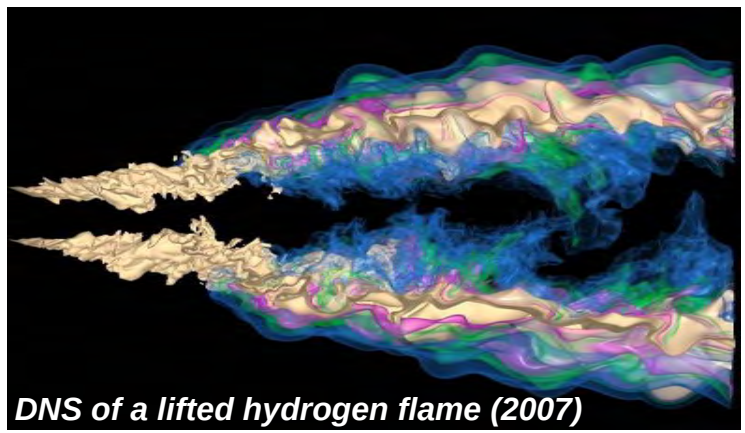
POC
Jackie Chen, SNL

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 to 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

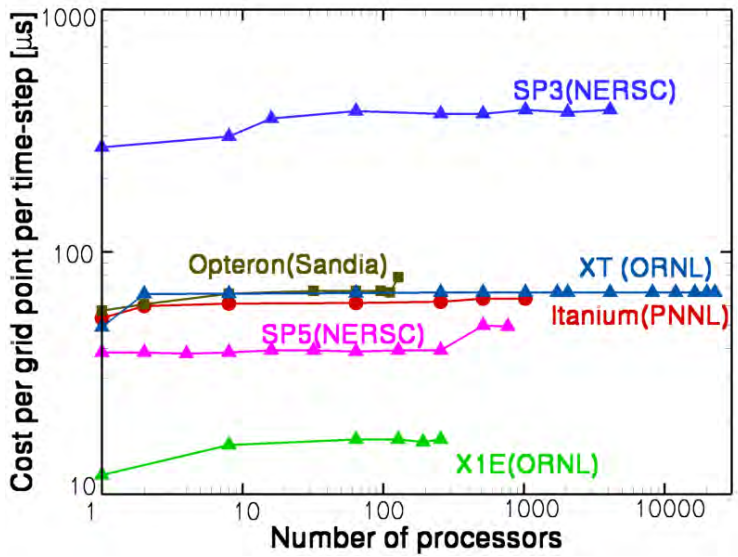
- Parallel DNS compressible Navier-Stokes solver with total energy, species and mass continuity coupled with detailed chemistry
- Chemical reactions and species diffusion rates in optimized library based on SNL’s Chemkin package
- 3D domain partitioned rectilinear mesh in Cartesian geometry
- High-order 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

LCF liaison contributions
- Implement Lagrangian tracers
- I/O rework with NW University
- Scaling studies identified processors burdened by memory corrections



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

Pioneering Application: POP
Science Goals and Impact

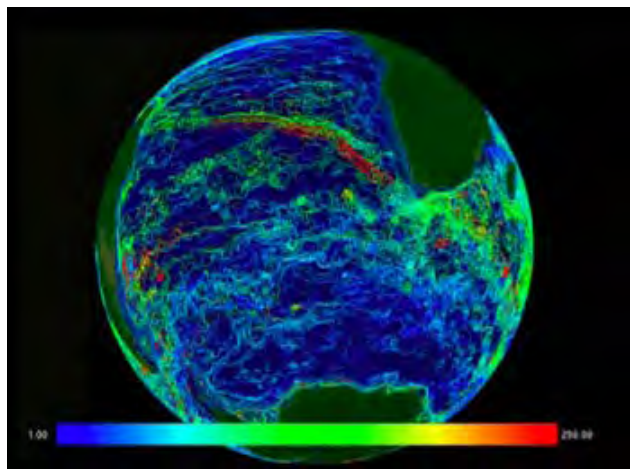
POCs
Mat Maltrud &
Phil Jones, LANL

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

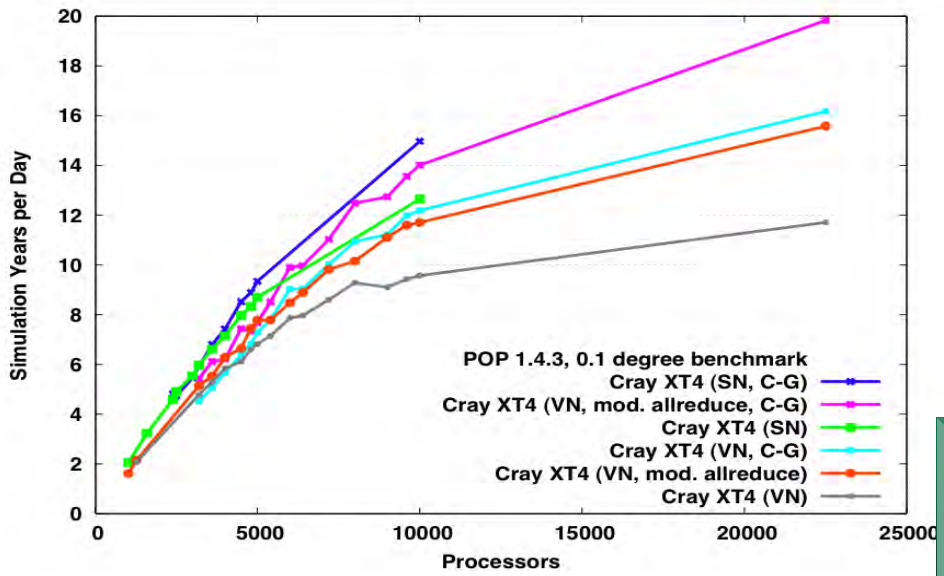
Numerical Algorithms

- 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

POC
Thomas
Schulthess, ORNL

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 Tc 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 Tc?
  - Do they enhance, suppress or even modify the pairing mechanism?
  - Is there an optimal inhomogeneity that maximizes Tc?
- 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

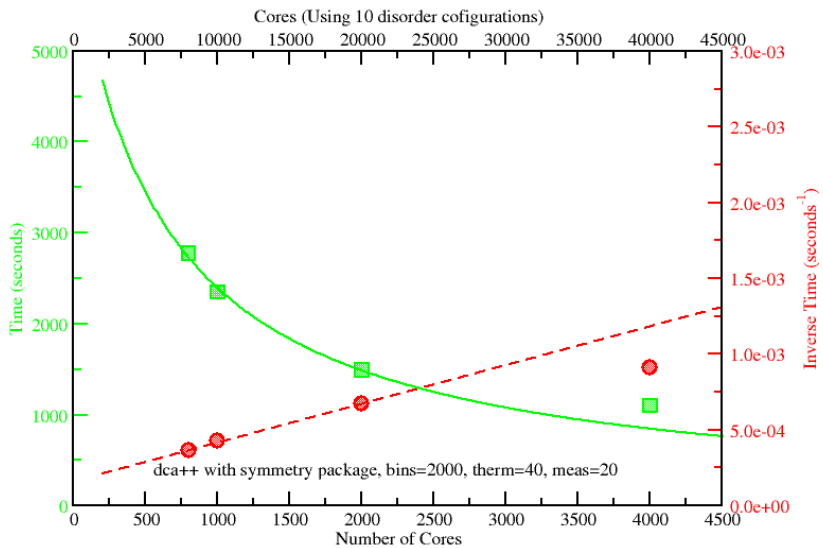
Pioneering Application: DCA++
Code Readiness, Scalability, and Performance

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

POC
Robert Harrison,
ORNL

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

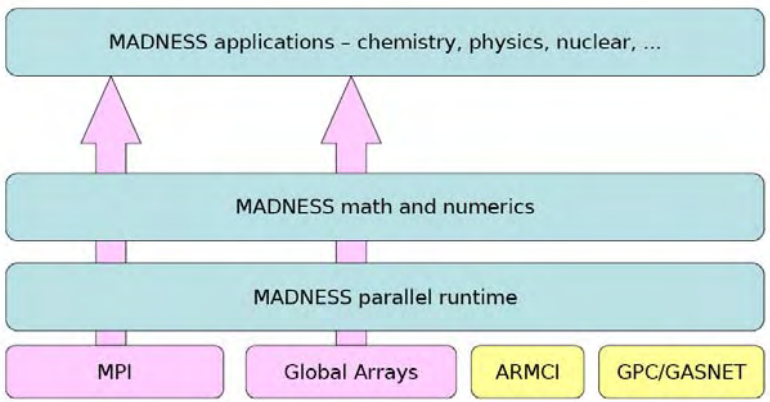
Science Impact

- 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**



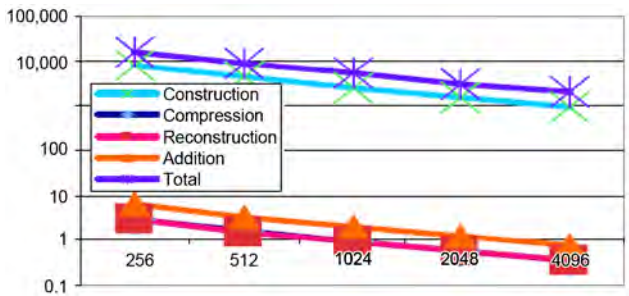
Numerical Algorithms

- **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

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

Astrophysics – Fusion – Combustion – Climate – Chemistry – Materials Science