SciDAC Application Projects Poster Blitz

September 11, 2012

Poster Session

4:05-5:35pm in Roosevelt/Madison

Format

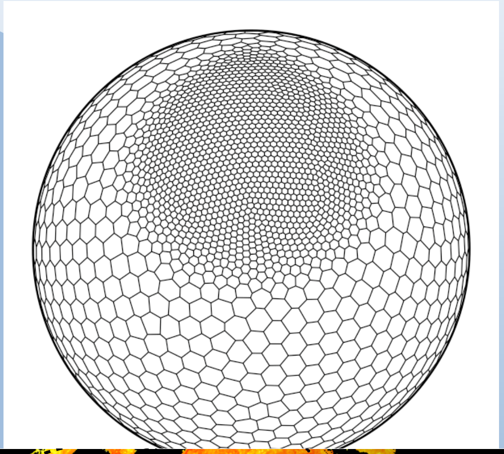
- 26 Posters
- 13 Projects, 5 Offices (BER, BES, FES, HEP, NP)
- 1 slide each
- 60 seconds
  - ***A bell's not a bell until you ring it*** -Sound of Music

....Ready Kate?

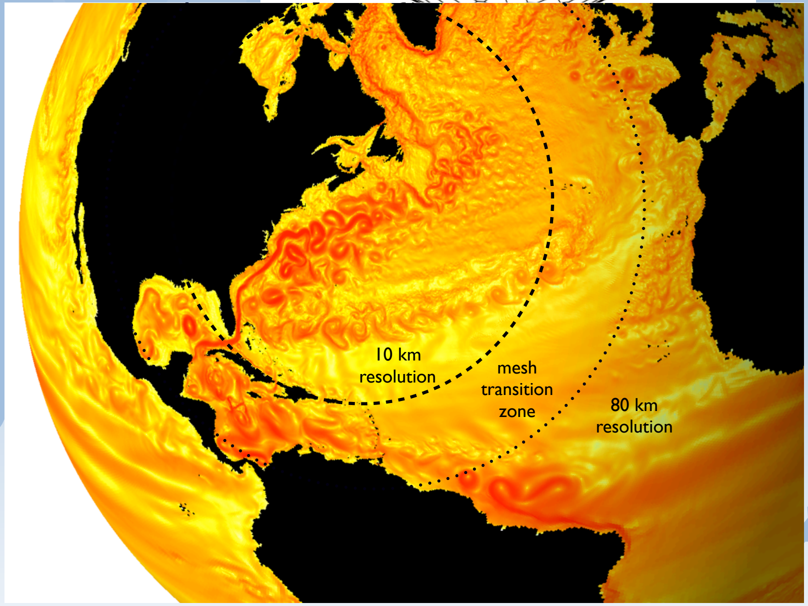
Multiscale Methods for the Earth System

Parameterization and Performance in Multiscale Ocean Models

T. Ringler, Q. Chen, D. Jacobsen (LANL)
L. Oliker, S. Williams (LBL/SUPER)



- New Ocean Model
  - MPAS-O
  - Variable resolution unstructured grids
- Ocean eddies
  - 50km scale (mesoscale)
  - Resolved vs parameterized
  - New scale-aware approaches
- Performance
  - Work with SUPER
  - Operators, unstructured grids on advanced architectures



Berkeley Lab · Los Alamos National Laboratory EST. 1943 · Lawrence Livermore National Laboratory · Oak Ridge National Laboratory · Pacific Northwest National Laboratory · Sandia National Laboratories

Introducing scale awareness into a subgrid parameterization

Vincent E. Larson, David P. Schanen, Minghuai Wang, Mikhail Ovchinnikov, and Steve Ghan

We wish to develop a statistical cloud model that works well over a variety of horizontal grid spacings.

Mathematical and computational challenges:

1. *Parameter estimation*. We want to choose a parameter value that works well over a range of grid spacings.

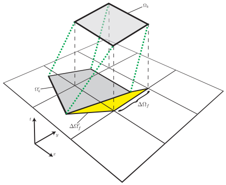
2. *Numerical discretization*. We want the numerics to work well over a range of grid spacings and time steps.

Computational Challenges of the Applying Computationally Efficient Schemes for BioGeochemical Cycles (ACES4BGC) Project

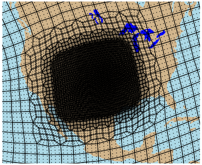
Forrest M. Hoffman (PI) and the Multi-Laboratory ACES4BGC Team

Goal: Advance the predictive capabilities of Earth System Models (ESMs) by reducing two of the largest sources of uncertainty, aerosols and biospheric feedbacks, utilizing a *highly efficient computational approach*.

ACES4BGC will implement and optimize advection algorithms for large numbers of tracer species using Conservative Semi-Lagrangian Multi-tracer (CSLAM) and Characteristic Discontinuous Galerkin (CDG) methods.



Spatio-temporal geometry of approach used to update the tracer in cell Ω_k, over a time step.



Unstructured CAM-SE variable resolution grid that increases 8-fold over the DOE ARM SGP site.

FASTMath's MOAB technology will provide parallel mesh infrastructure to enable CSLAM and CDG on unstructured variable resolution grids while delivering efficient performance. SUPER's performance engineering technology will assure optimal performance on DOE's Leadership Class supercomputers.

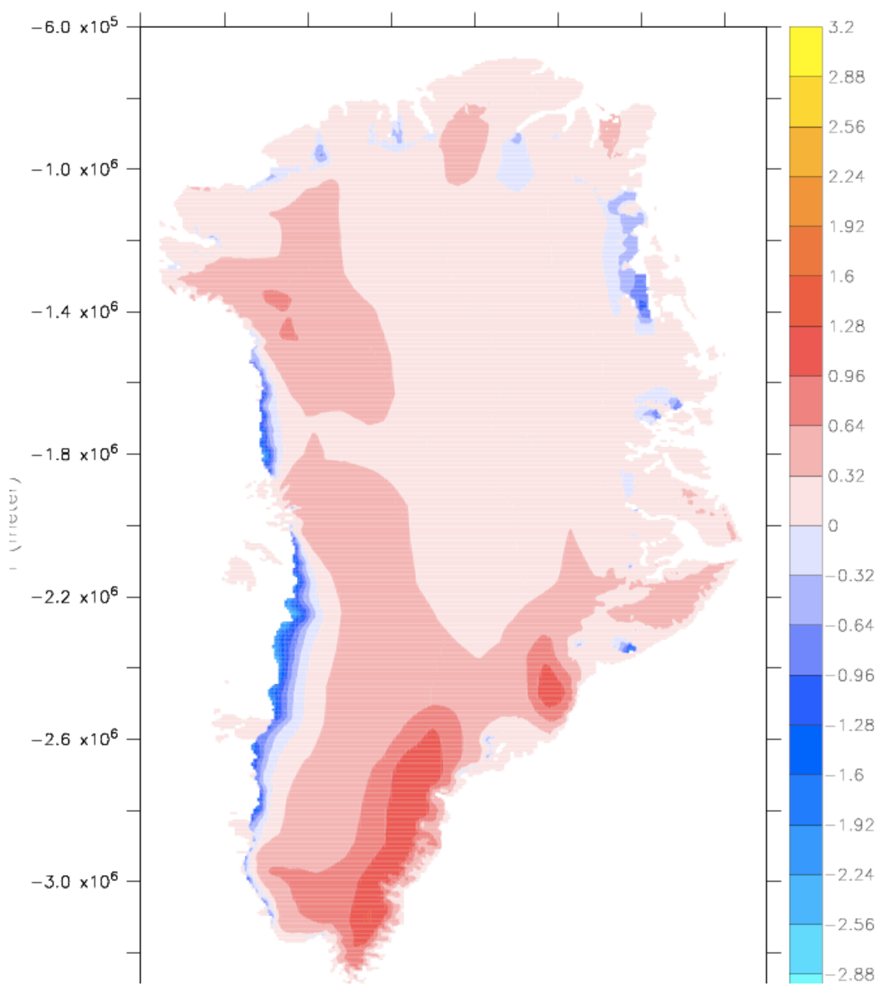
Important biogeochemical interactions between the atmosphere, land, and ocean models will be added and UQ techniques will be employed to constain process parameters and evaluate feedback uncertainties.

http://www.aces4bgc.org/

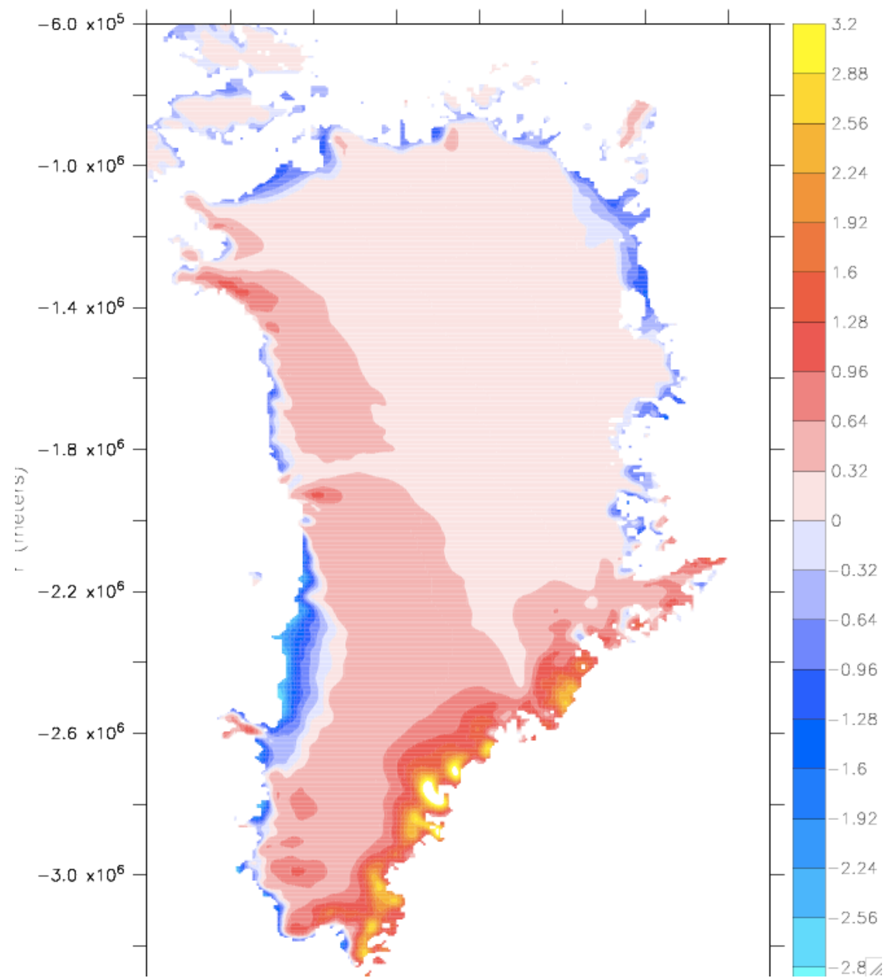
Verification, Validation, and Uncertainty Quantification for PISCEES

Charles Jackson (U. Texas) and Katherine Evans (ORNL)

CESM surface mass balance



Observed surface mass balance



Ice Sheet Model Dynamical Core Development for PISCEES

Dan Martin (LBNL), Stephen Price (LANL)

- **NEED:** Better dynamical cores ("dycores") for ice sheet modeling
  - Better spatial resolution (sub-kilometer)
  - Better physical fidelity ("full-Stokes" models)
  - Better computational efficiency and scaling (dominated by nonlinear solves)

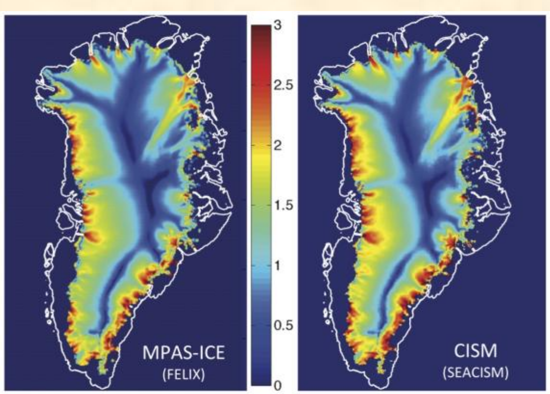
- PISCEES is developing **2** dynamical cores, based on different numerical approaches.

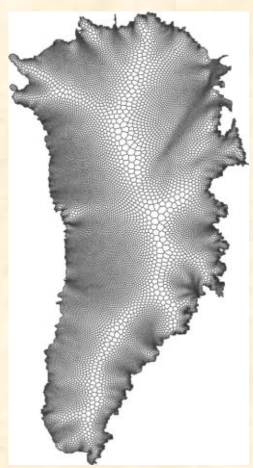
FELIX

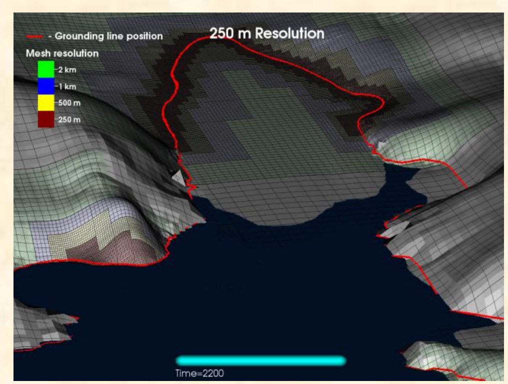
- Unstructured-mesh finite-elements
- Uses the Model for Prediction Across Scales (MPAS) to achieve variable spatial resolution.
- Uses FASTMath-supported Trilinos
- Range of physical models

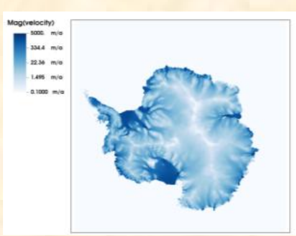
BISICLES

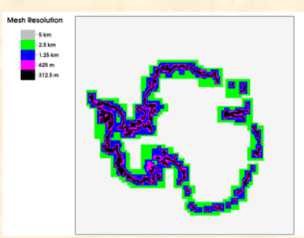
- Block-structured Adaptive Mesh Refinement
- Dynamically adaptive
- Built on Chombo framework (FASTMath)
- Range of physical models under development.





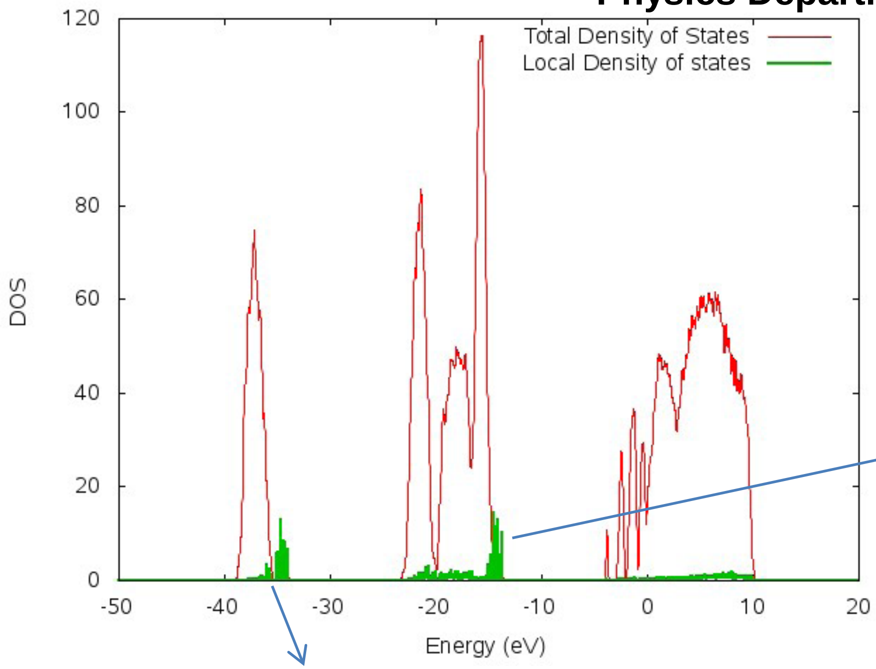


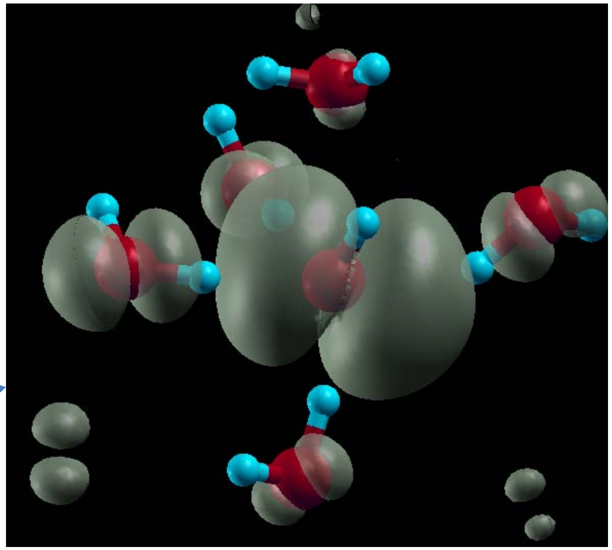


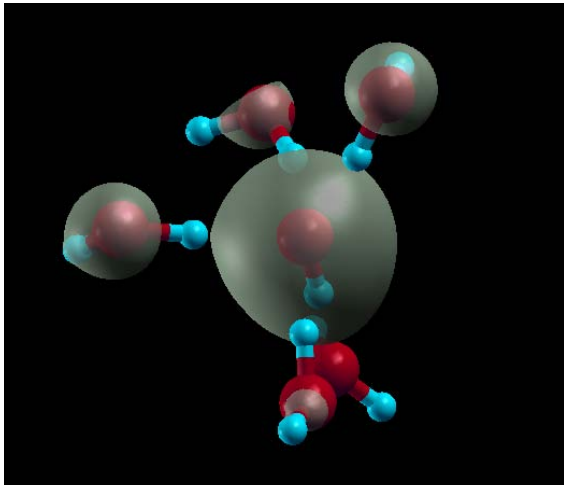


Electric binding energies of hydrated OH- and H3O+: ab initio molecular dynamics combined with GW quasiparticle theory

Charles W. Swartz VI, Xifan Wu
Physics Department, Temple University





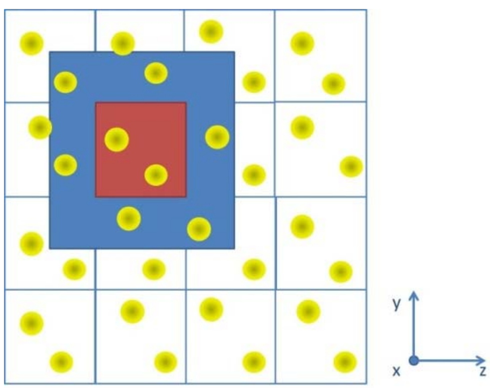


- Solvation structrure of OH- and H+ based on Car-Parrinello molecular dynamics
- Quasiparticle theory : Static GW inculding local field
- OH- and H+ binding energies
- Molecular origin

New computational methodologies for accelerating *ab initio* molecular dynamics simulation

Lin Lin, Lawrence Berkeley National Laboratory

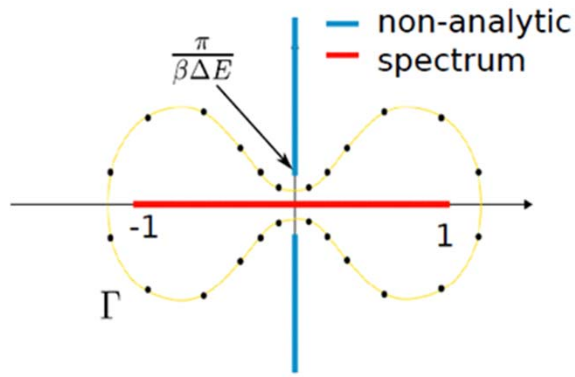
ALB-DG: Systematic reduction of the number of basis functions starting from a complete basis set.



Team: J. Pask, V. Lordi, L. Lin, C. Yang, E.W. Draeger

Discontinuous methods for accurate, massively parallel quantum molecular dynamics: Lithium ion interface dynamics from first principles

PEXSI: Accurate evaluation of the electron density, energy and atomic force with at most $O(N^2)$ scaling.

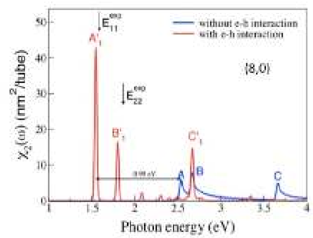


Team: R. Car, W. E, M. Klein, X. Wu, E. Ng, C. Yang, L. Lin

Advanced Modeling of Ions in Solutions, on Surfaces, and in Biological Environments

Numerical Algorithms for Accelerating GW and Bethe-Salpeter Equation Calculations

Team member: Chao Yang, Andrew Canning, Jack Deslippe, Jeff Neaton, Steven Louie (LBNL), Yousef Saad (University of Minnesota), Alex Demkov , Jim Chelikowsky (University of Texas at Austin)



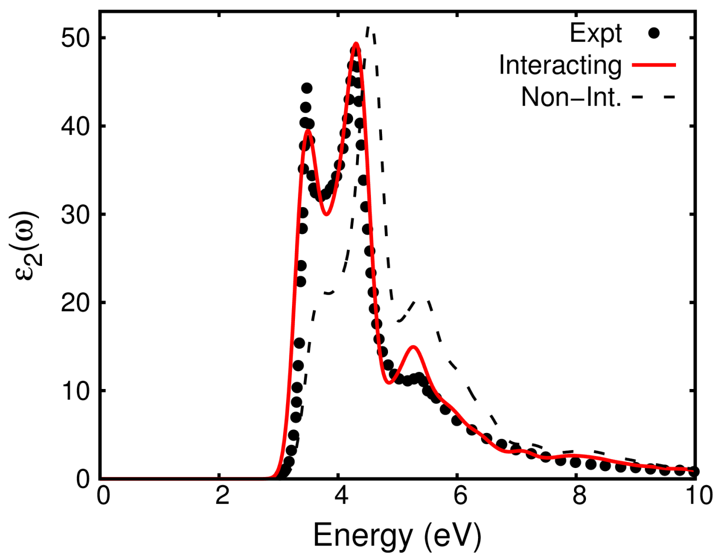
- **Goals**:
  - ✓ Develop efficient algorithms and implementations to accelerate excited and ground state electronic structure calculations on leadership class machines
  - ✓ Leverage the development in SciDAC FASTmath institute on linear and nonlinear eigensolvers, linear equations solver to improve the performance of PARSEC and BerkeleyGW software packages

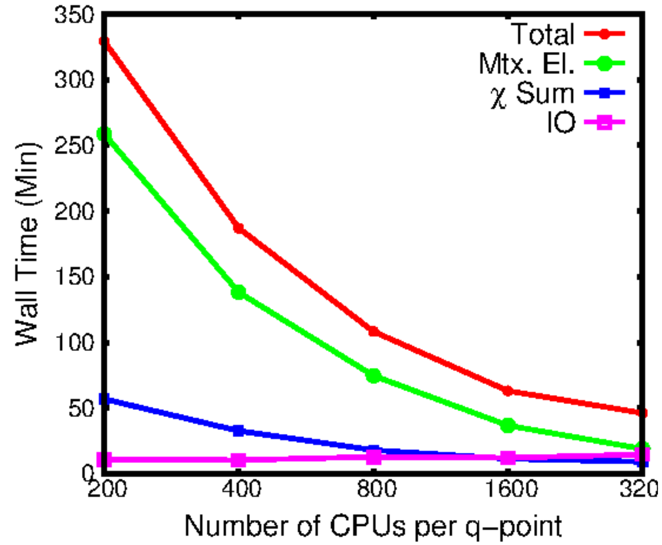
- **Approaches:**
  - ✓ Spectrum slicing for computing a large number of eigenpairs need for polarizability operator
    - ❖ Polynomial transformation
    - ❖ Shift-invert
    - ❖ Contour integral
  - ✓ Polarizability without unoccupied eigenstates

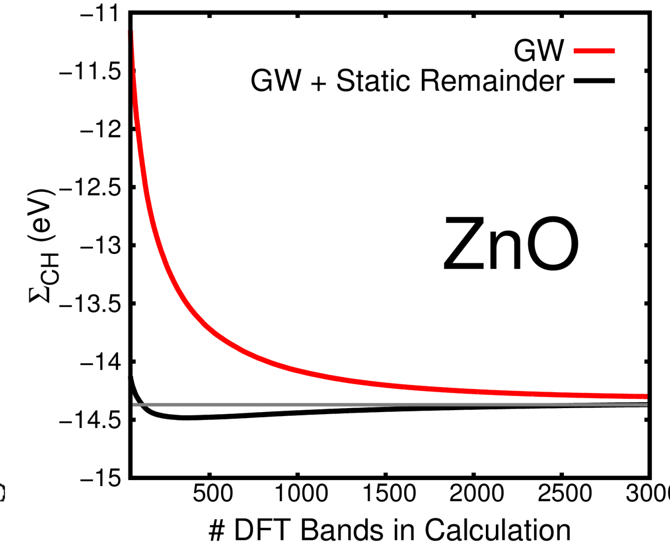
BerkeleyGW: A massively parallel computer package for calculating excited state properties of materials

Jack Deslippe, Steven Louie, Jeff Neaton, Andrew Canning, Chao Yang, Yousef Saad, Alex Demkov, Jim Chelikowsky

Feature Overview and Performance Characteristics:



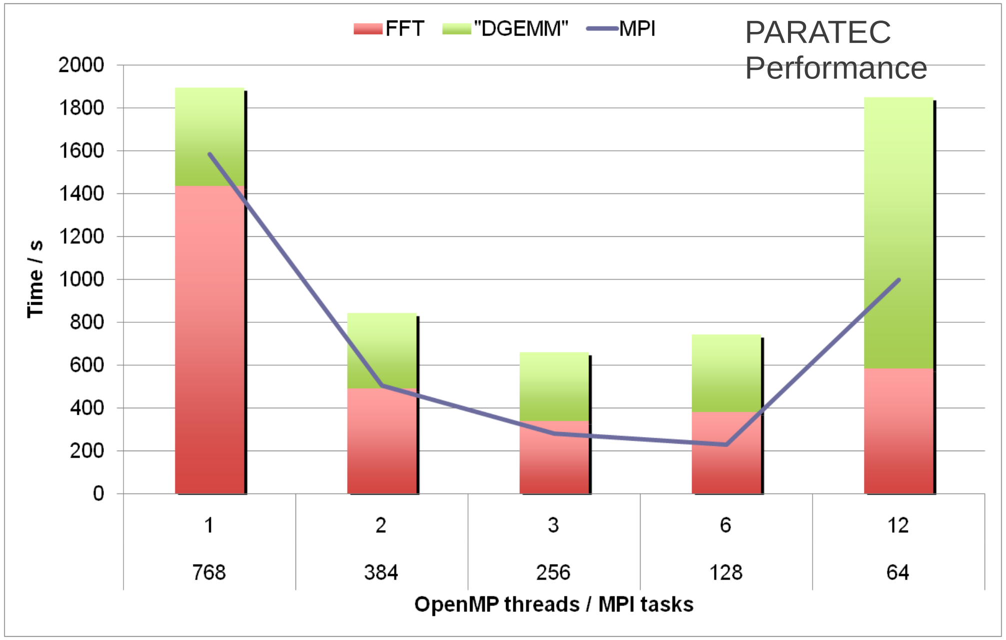




Ongoing Developments:

- Empty State Approximations
- GW Starting Points
- Full-Frequency
- New Levels of Parallelism with OpenMP and Accelerators
- ...

BerkeleyGW




Chris Cramer

Bert de Jong

Laura Gagliardi

Challenges Associated with the Development of Electron-Correlated Methods for Excited State Structure and Dynamics

Laura Gagliardi

Department of Chemistry and Chemical Theory Center, University of Minnesota, Twin Cities MN

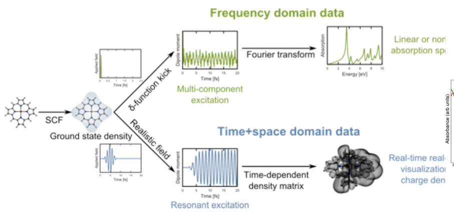

Niri Govind

Ilja Siepmann

Don Truhlar

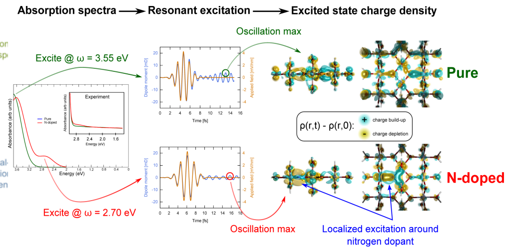
Challenges with Excited States

Real-time TDDFT in a nutshell

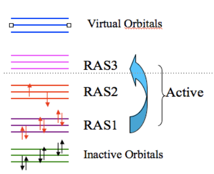


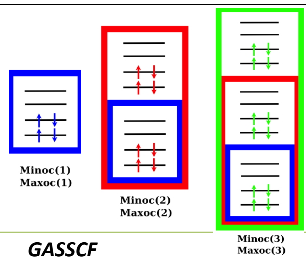
- Full response beyond perturbation limit
- Real-time, real-space ➔ full dynamical information
- Insight into ultrafast and nonlinear processes

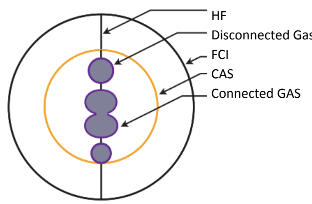
Real-Time TDDFT Calculations



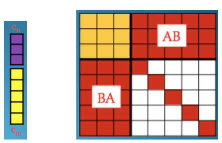
Multiconfigurational QM: New Developments







RASSCF ***GASSCF*** ***Various wavefunctions***



How to solve the system of Secular Equations?

$$\sum_{n=1}^{N}(H_{mn} - E\delta_{mn})c_n = 0 \quad m = 1,2,\ldots,N$$

$$\begin{pmatrix} H^{AA} & H^{AB} \\ H^{BA} & H^{BB} \end{pmatrix} \rightarrow \left(U^{AA}\right)$$

$$\left\{ \begin{array}{ll} \sum_{n}^{A}(U_{mn} - E\delta_{mn})c_n = 0 & m \in (A) \\ c_m = \sum_{n}^{A} \frac{U_{mn}}{E - H_{mm}} c_n & m \in (B) \end{array} \right.$$

No Configurations neglected!

$$U_{mn} = H_{mn} + \sum_{\alpha}^{B} \frac{H'_{m\alpha} H'_{\alpha n}}{E - H_{\alpha\alpha}} + \sum_{\alpha}^{B}\sum_{\beta}^{B} \frac{H'_{m\alpha} H'_{\alpha\beta} H'_{\beta n}}{(E - H_{\alpha\alpha})(E - H_{\beta\beta})} + \{\ldots\}$$


Esmond Ng

Why NWChem?

- DOE's Premier computational chemistry software
- Scalable with respect to scientific challenge and compute platforms
- From molecules and nanoparticles to solid state and biomolecular systems
- Open-source (ECL 2.0)

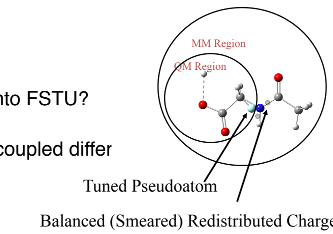
Electronically nonadiabatic and ultrafast dynamics

ANT (Adiabatic and Nonadiabatic Trajectories) program
Two methods for non-Born-Oppenheimer dynamics:
FSTU: surface hopping by fewest switches with time uncertainty
CSDM: coherent switches with time-uncertainty

Tuned and balanced (smeared) redistributed charge schemes in (QM/MM)

Implement FSTU with decoherence into NWChem

Mathematical issue: Is it physically correct to add decoherence onto FSTU?
Scientific issue: How accurate is FSTU with decoherence?
Algorithmic Issue: What is the most efficient way to integrate the coupled differ equations?

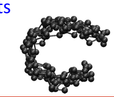


Challenge: Polar bonds across the the QM/MM boundary.

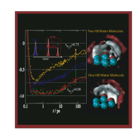
Method:
Charge Balancing: Adjust the MM charges to conserve the total charge of the entire QM/MM system.
Charge Redistribution: Move the charges that are close to the boundary away from the boundary.
Charge Smearing: Place the redistributed charges in Slater-type orbitals.
Tuned Pseudoatom: Use Fluorine as the link atom but add a pseudopotential *U(r)* to it to mimic the original MM atom.

Multiscale approaches for explicit local solvation environments and conformational sampling of chromophores

Automatic generation of a large number of uncorrelated explicit-solvent configurations and chromophore conformations
Development of a fitness function to measure whether a subset of these configurations/conformations is representative of the entire ensemble
Monte Carlo simulated annealing/genetic evolution algorithm for pruning of subsets



NWChem program
Computation of ground- and excited-state wave functions and convergence control



FASTMath SciDAC Institute

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE

Large-scale simulation of vortex liquid pinning in high-temperature superconductors

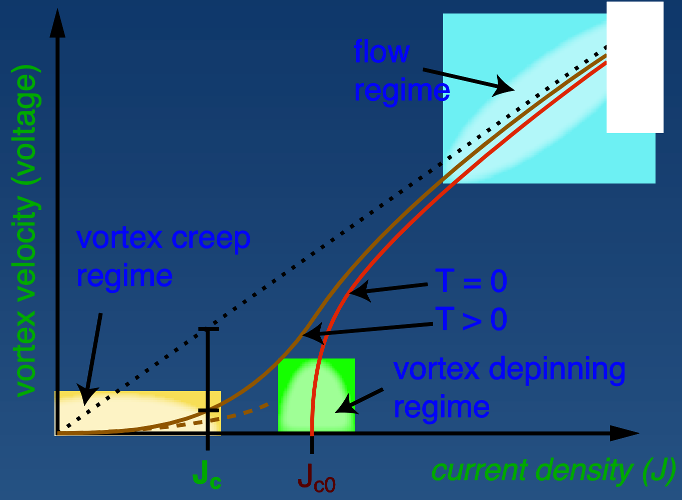
Dmitry Karpeev[1] , Igor Aronson[2] , George Crabtree[2] , Andreas Glatz[2], Alexei Koshelev[2], Todd Munson[1], Jason Sarich[1], Stefan Wild[1]
[1]Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, USA
[2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

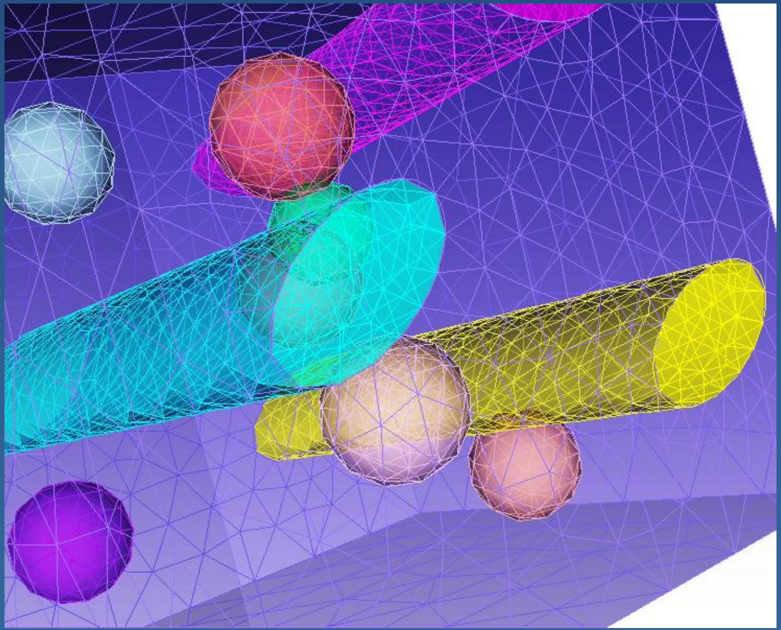
- Critical current determined by vortex movement
- Modeled by Time-dependent Ginzburg-Landau eqns.

$$\Gamma\left(\partial_t + i\frac{2e}{\hbar}\mu\right)\psi = a_0\epsilon(\mathbf{r})\psi - b|\psi|^2\psi + \frac{1}{4m}\left(\hbar\nabla + \frac{2e}{ic}\mathbf{A}\right)^2\psi + \zeta(\mathbf{r},t)$$

$$\nabla\times(\nabla\times\mathbf{A}) = \frac{4\pi}{c}\left(\mathbf{J}_n + \mathbf{J}_s + \mathcal{I}\right),$$

- Calculated via very long-time dynamic simulation
- Optimized over many pinning configurations





Poster will discuss:

- Meshing and mesh adaptation
- Time-integration strategy
  - Implicit, fully coupled
- Preconditioning
  - Physics-based, multigrid
- Scaling issues
- Pinning configuration optimization strategy
  - Derivative-free
  - Including robust optimization

General block-tensor library for high-level electronic structure calculations

Evgeny Epifanovsky (UC Berkeley, USC), Michael Wormit, Andreas Dreuw (Heidelberg), Anna Krylov (USC)

Current functionality

Special block structure of large tensors

Divide-and-conquer approach to storing and operating on tensors

Single node out-of-core implementation

Applications

Post-Hartree-Fock methods: coupled cluster theory, equation-of-motion theory

Future functionality

1. Support for complex tensor entries

Complex scaled post-Hartree-Fock methods for resonance electronic states

2. Tensor factorization

Reduced-rank tensor approximations

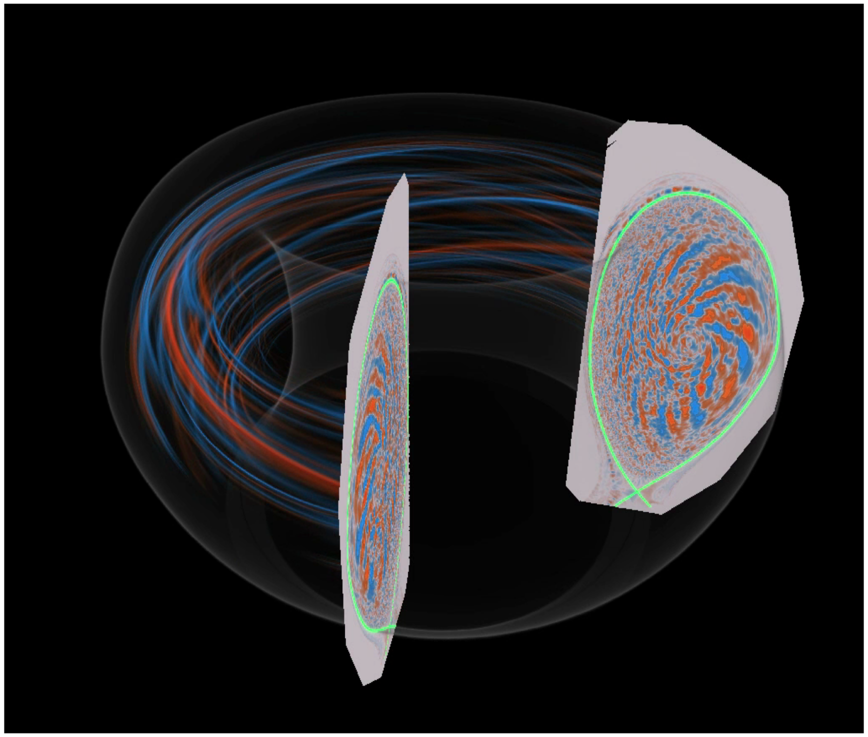
3. Parallel implementation over MPI
4. Extension to heterogeneous architectures

Open possibilities to study larger problems

Building an extreme scale, first-principles, fusion edge physics code

EPSI
Edge Physics Simulation

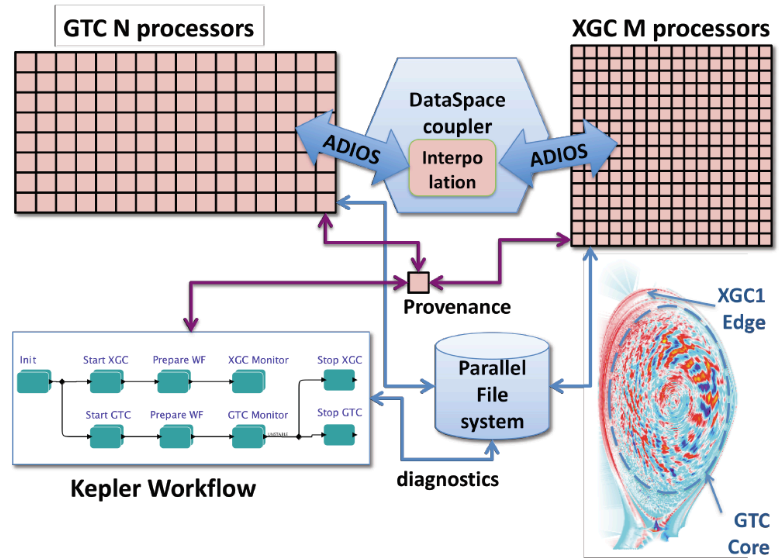
- Essential physics tool for fusion reactor design and operation
- Inseparable multi-scale edge physics
- Effort builds on success - XGC0 and XGC1
  - Embarrassingly parallel, utilizes maximal Jaguarpf capability
- Main goal - more complete XGC for ab initio modeling
- Challenges
  - Applied Mathematics: multi-scale/ multi-physics
  - Verification, Validation & UQ of nonlinear self-organization of ab initio physics
  - Performance engineering: extreme scale, heterogeneous
  - Computer science: extreme scale data, I/O, and multiscale coupling → in-situ/in-memory

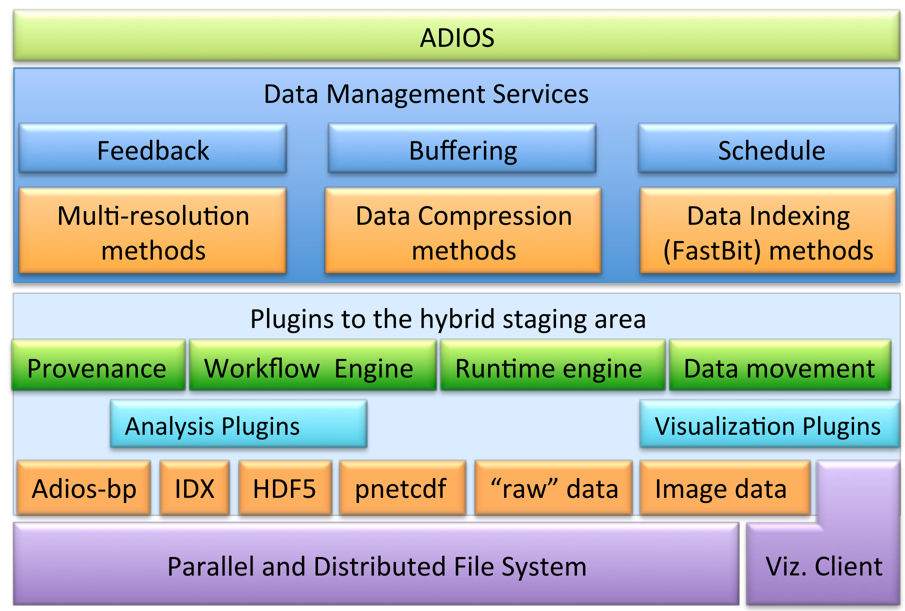


EPSI
Edge Physics Simulation

On-the-fly data management for high performance multiscale fusion simulation on Titan

- Goal: To create essential physics tool for fusion reactor design and operation
  - Support inseparable multi-scale edge physics and complete XGC for ab initio modeling
- Challenges:
  - Tight Coupling:
  - Large scale Data Management
  - Minimizing Data Movement
- Key components
  - Programming models, abstraction and systems
  - Runtime mechanism to manage and schedule in-situ execution
  - Dynamic deployment of plugins within the staging area
- Build on CPES Successes
  - ADIOS, DataSpaces, eSimon

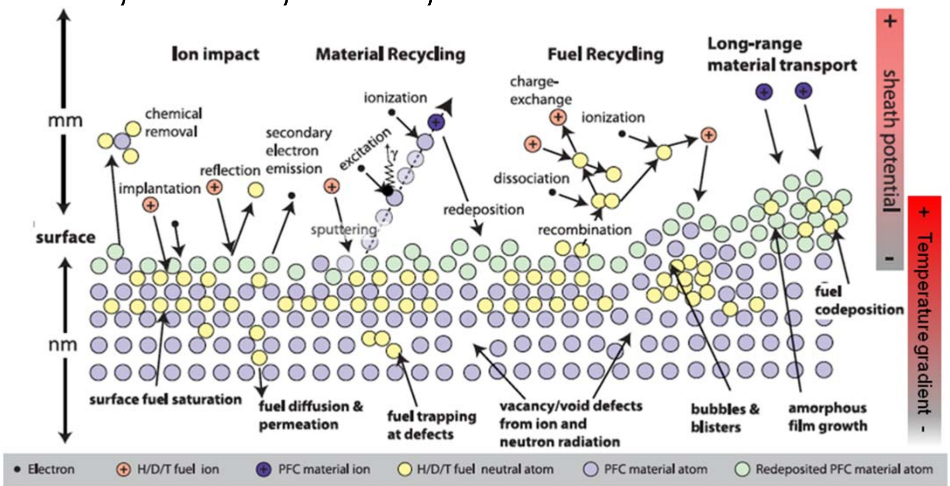




Plasma Surface Interactions (PSI): Bridging from the Surface to the Micron Frontier through Leadership Class Computing

ANL, GA, LANL, **ORNL**, PNNL, UCSD, UIUC, UMass

- Performance of plasma-facing components of fusion reactors is critical to commercial viability

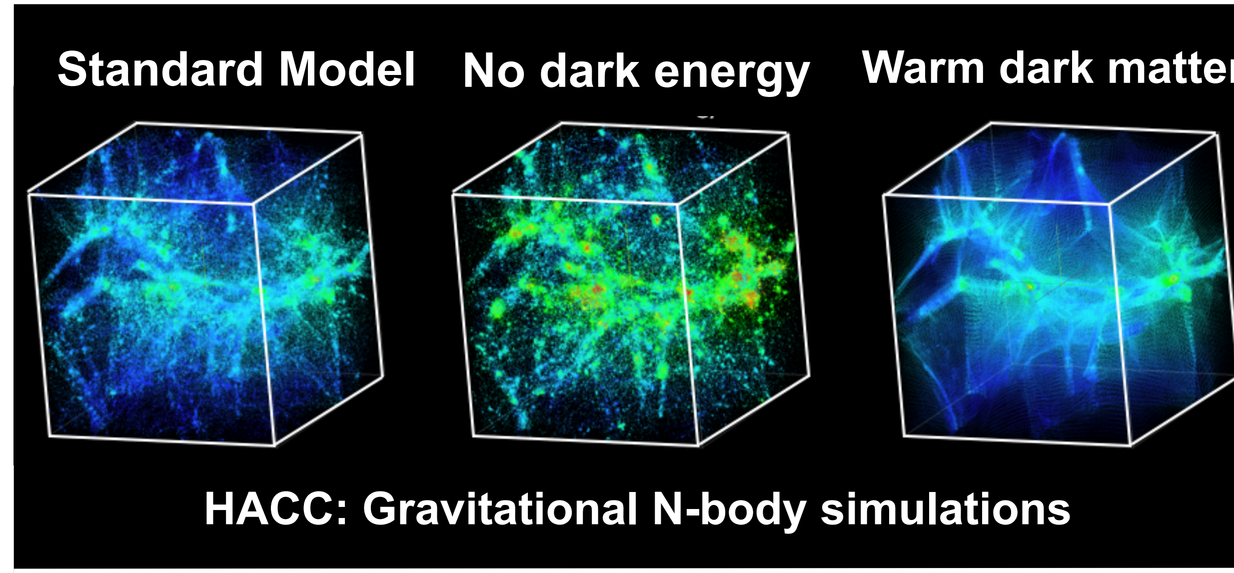


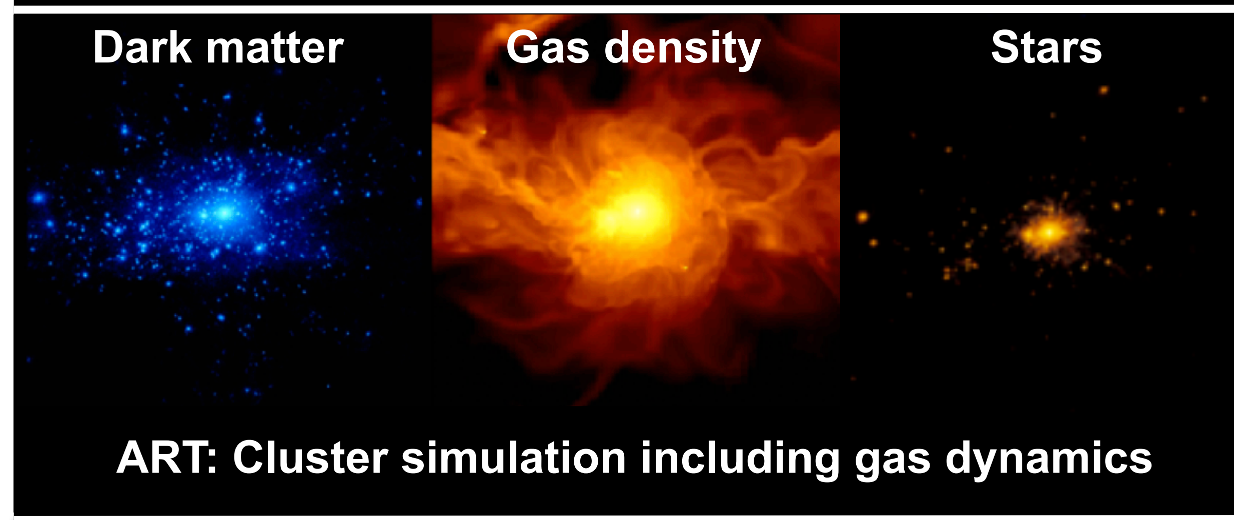
- Materials science questions:
  - Evolution of near-surface morphology and composition in re-deposition layer?
  - Effects of neutron damage on near-surface evolution and tritium permeation/retention?
  - Impact of dilute impurities on surface morphology evolution?
  - Impact of bulk microstructure on thermal properties?

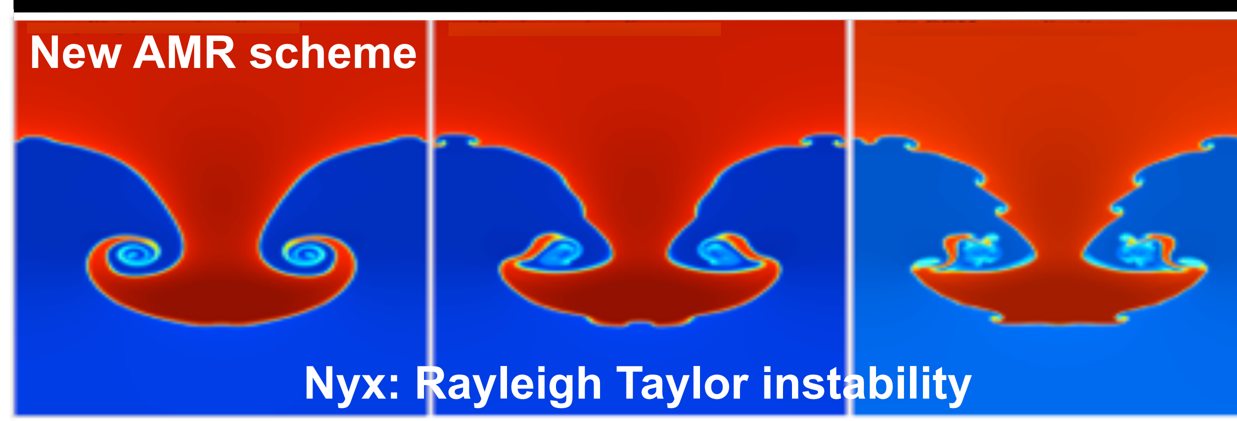
- Computer science and applied math questions:
  - Scalable multigrid methods, solvers, integrators for diffusion problems?
  - Uncertainty quantification?
  - Performance engineering?
  - Data analytics?

Computation-Driven Discovery for the Dark Universe

- **Aims for New SciDAC-3 Project**
  - Build next-generation computational cosmology prediction and analysis frameworks for current and future surveys
  - Explore the physics of dark energy, dark matter, neutrinos, and the early Universe via large-scale structure probes
  - Further development of three large-scale high-performance cosmology simulation codes: HACC (@ANL), ART (@Fermilab), Nyx (@LBNL)
  - Make full use of DOE's Leadership class systems: Mira (ANL), Jaguar/Titan (ORNL), Hopper (NERSC)
- **Connections to ASCR SciDAC Instititutes**
  - FastMath (AMR), SDAV (analysis, I/O), QUEST (UQ)







Argonne National Laboratory · Berkeley Lab · Brookhaven National Laboratory · Fermilab · Los Alamos National Laboratory EST. 1943 · SLAC National Accelerator Laboratory

The Search for Beyond-the-Standard-Model Physics at the Intensity Frontier

Heechang Na (ALCF, ANL) for the USQCD collaboration

- The Intensity Frontier experiments search for the unknown signals of physics beyond-the-Standard-Model.

- The signals might be very week, so High-precision Lattice QCD calculations are very important to understand the experiments.

- The most highly optimized programs on the highest capable computers available are required for the Lattice QCD calculations.

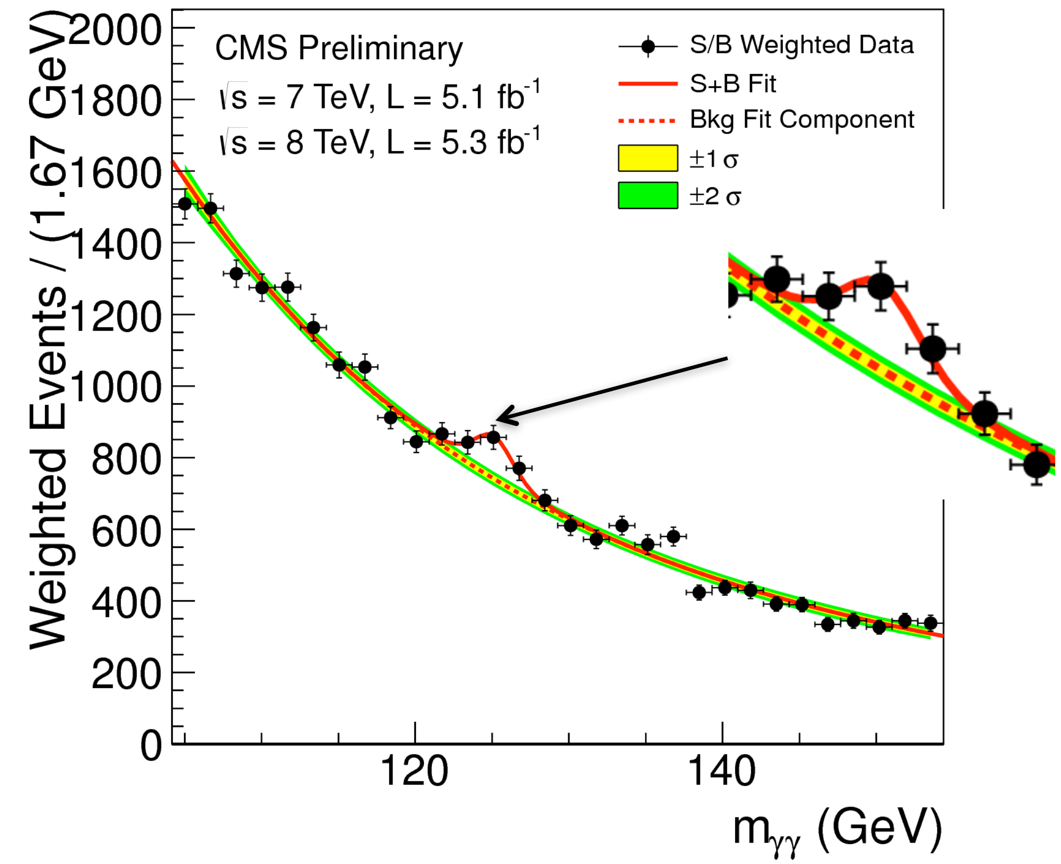
- This poster presents:
  - Hot issues on the physics
    - CKM unitarity triangle, $K \to \pi\pi$ ($I=2$ and $I=0$) decays, $B \to D\tau\nu$ decays, and muon g-2 measurement
  - Contributions of the Lattice community in designing and using the Blue Gene family
  - MIRA, 48 rack BG/Q machine at ALCF

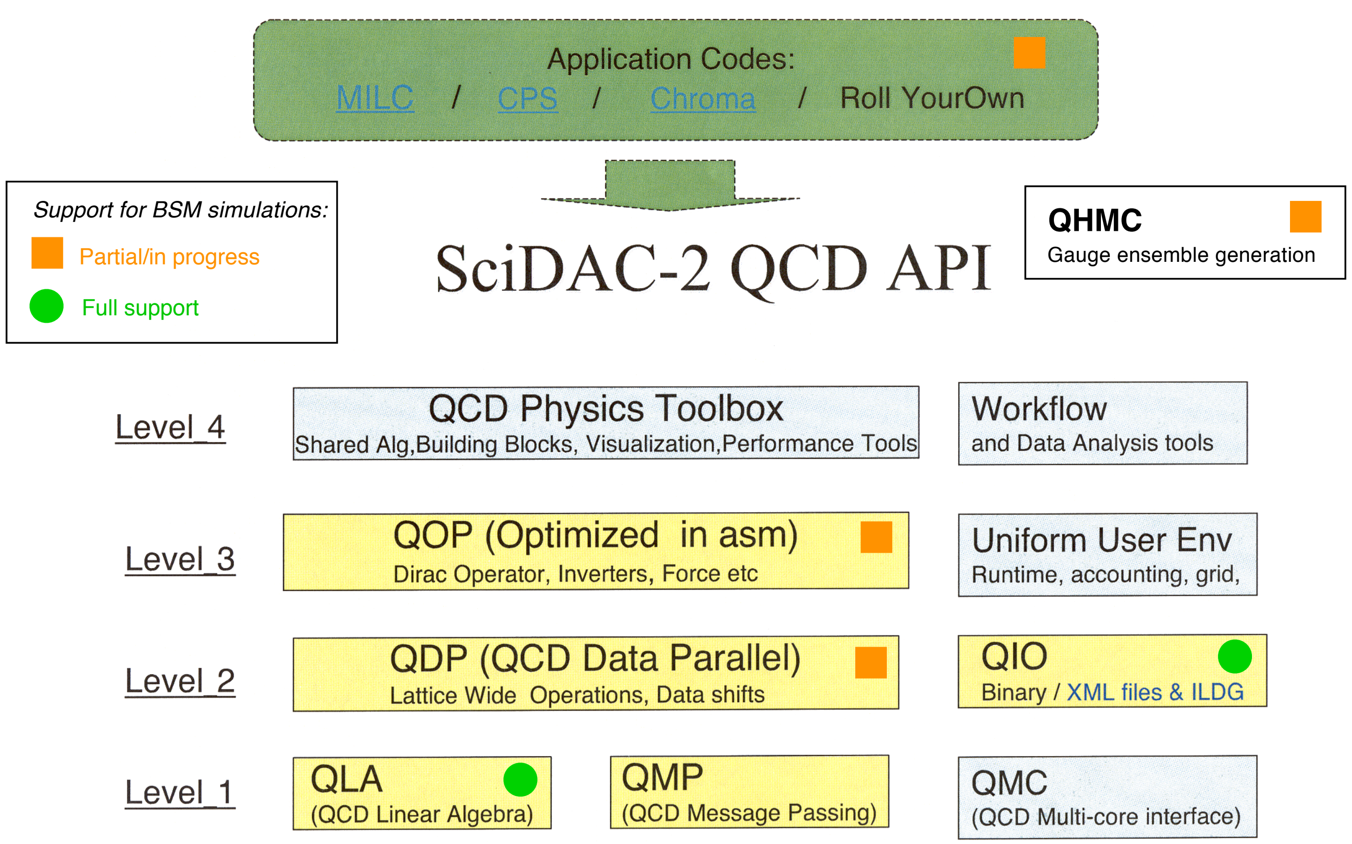
Strongly Coupled Field Theories at the Energy Frontier

Ethan T. Neil (Fermilab), for the USQCD Collaboration

LHC discovers a Higgs-like particle!
Last piece of the Standard Model?
Or first hints of something beyond?

What if the Higgs is a composite - a bound state of some new, strong force, like QCD? Lattice simulations allow us to study the possibilities!





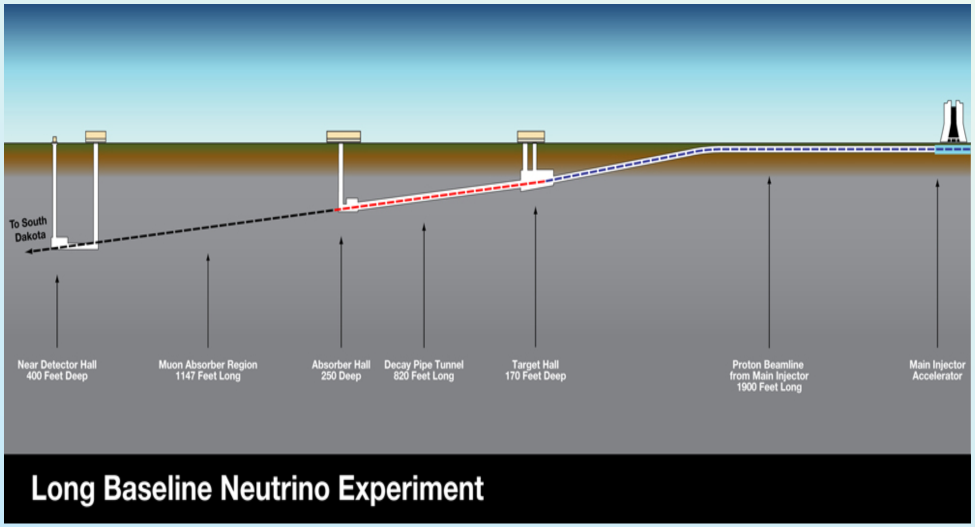
Current lattice code is heavily optimized (and sometimes hard-coded) for QCD. Work so far mostly relies on "hacked" versions.

Modification of SciDAC-2 QCD API for optimized support of general strongly-coupled models is underway.

ComPASS SciDAC-3

Advanced Computational Tools for the Intensity Frontier

High intensity accelerators are needed for precision measurements of rare processes, which challenge the Standard Model



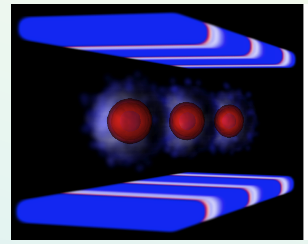
ComPASS SciDAC-3 will improve our ability to model high intensity accelerators

New algorithms increase the range of physics covered

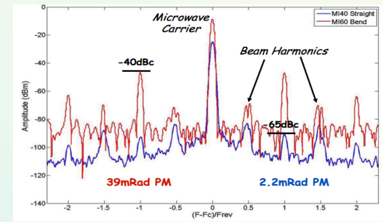
And take us to higher fidelity simulations

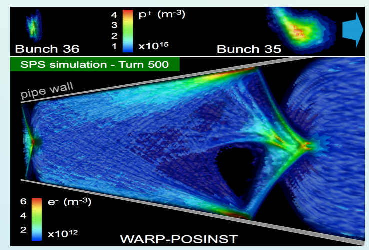
Integration with performance optimization to improve use of GPUs and parallelism

At high intensity feedback effects become increasing problematic

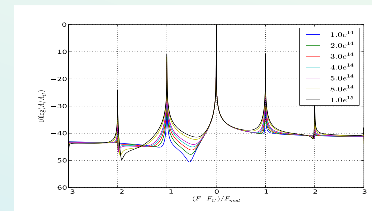


Self-consistent fields

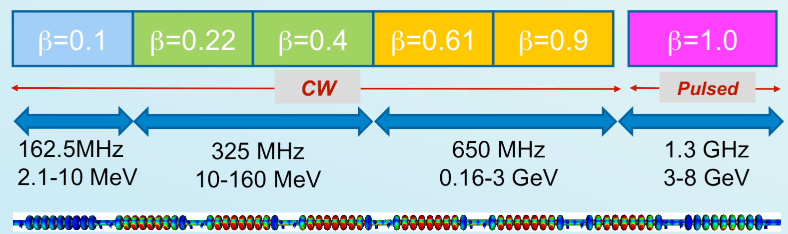




Electron cloud formation



Electron cloud diagnosis



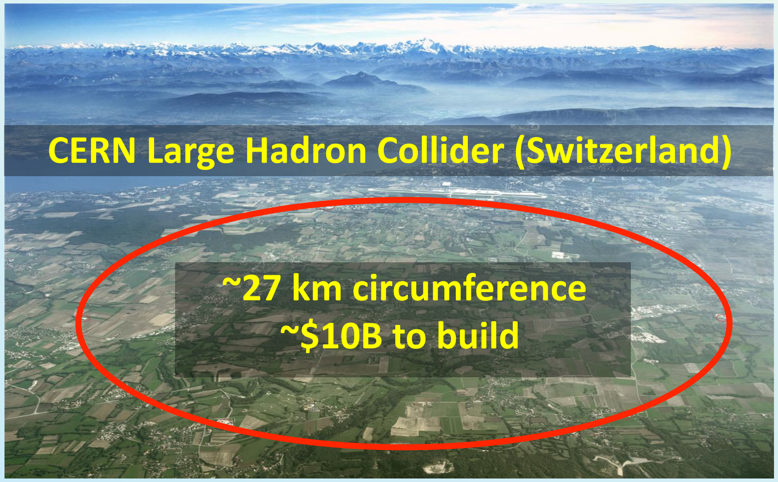
Wakefield and HOM effects

Argonne National Laboratory · Berkeley Lab · Fermilab · SLAC National Accelerator Laboratory · Tech-X · UCLA · The University of Texas at Austin

ComPASS SciDAC-3

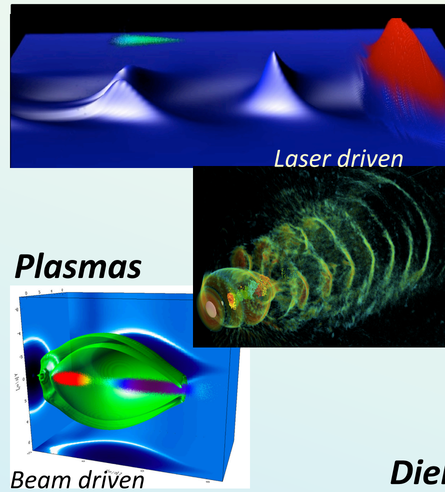
Advanced Computational Tools for the Energy Frontier

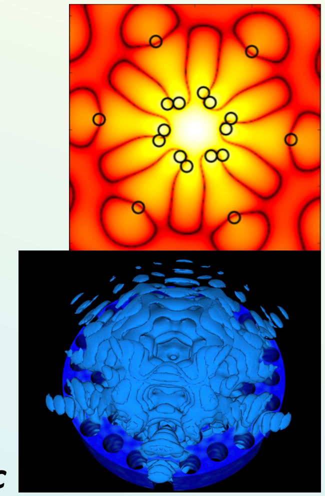
Large accelerators of particles are among the ***most complex & expensive*** tools for ***scientific discovery***.



Courtesy S. Myers (IPAC 2012)

New technologies (plasmas, dielectric) offer great promise for ***smaller & cheaper accelerators***.





ComPASS SciDAC-3 *will* ***push further*** *the* ***state-of-the-art*** *in* ***modeling of accelerators****, using/developing:*

- the **most advanced algorithms** & **performance optimization** on the **latest most powerful supercomputers**,
- **cutting-edge non-linear parameter optimization** and **uncertainty quantification (UQ)** methods.

New tools *will provide* ***unprecedented capabilities*** *that will be used for:*

- **understanding** and **optimizing existing accelerators**,
- **developing new acceleration technologies**.

Argonne National Laboratory | Berkeley Lab | Fermilab | SLAC National Accelerator Laboratory | Tech-X | UCLA | The University of Texas at Austin

Nuclear Density Functional Theory

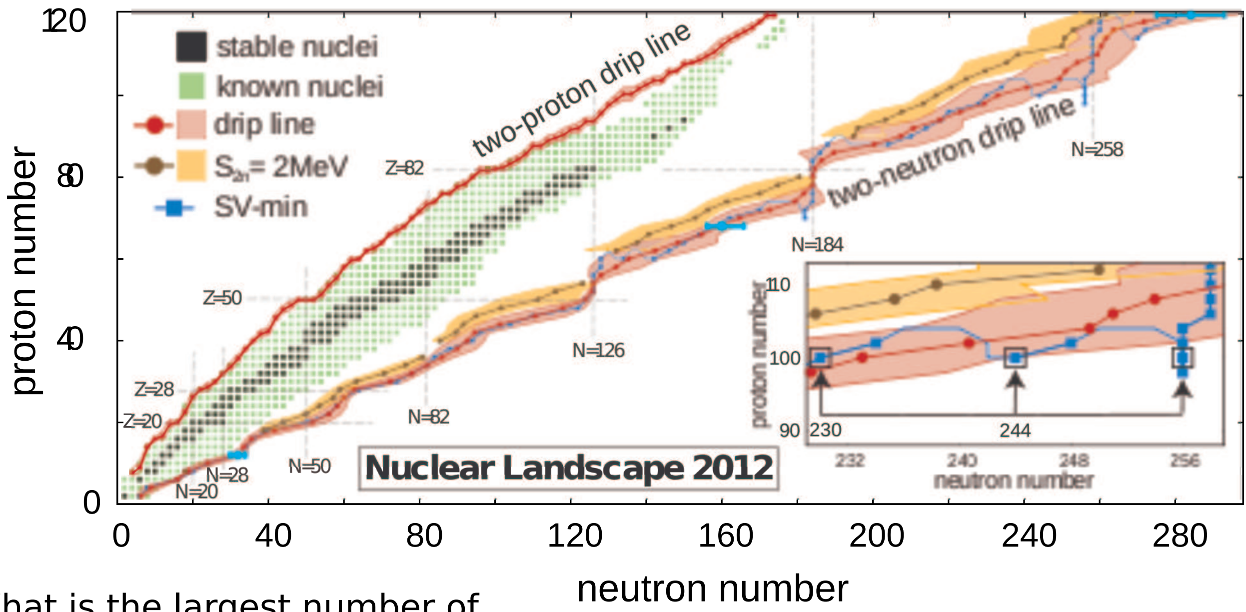
Exploring Fission and the Limits of the Nuclear Landscape

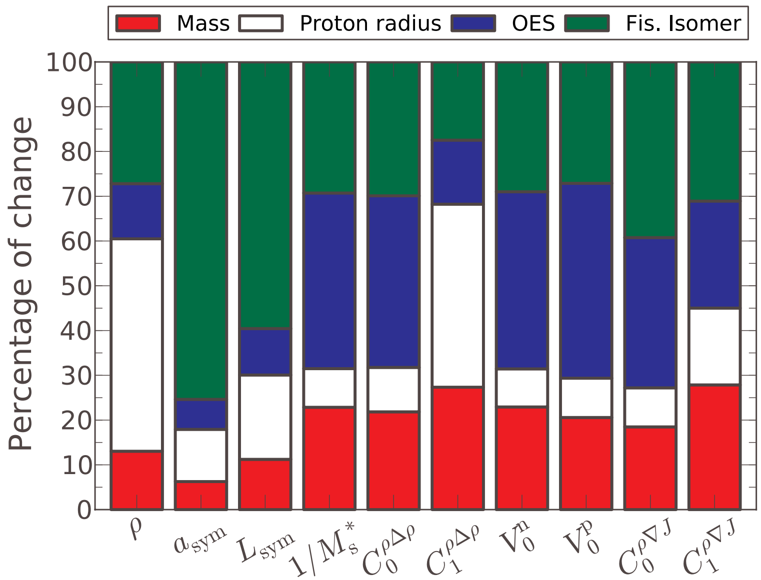
J.D. McDonnell, E. Olsen, W. Nazarewicz, N. Schunck, S. Wild, *et al*

NUCLEI
Nuclear Computational Low-Energy Initiative

- With advances in computational power, our theoretical picture of the nucleus is becoming increasingly clearer

- Through density functional theory, we aim to predict the properties of medium, heavy, and super-heavy nuclei.



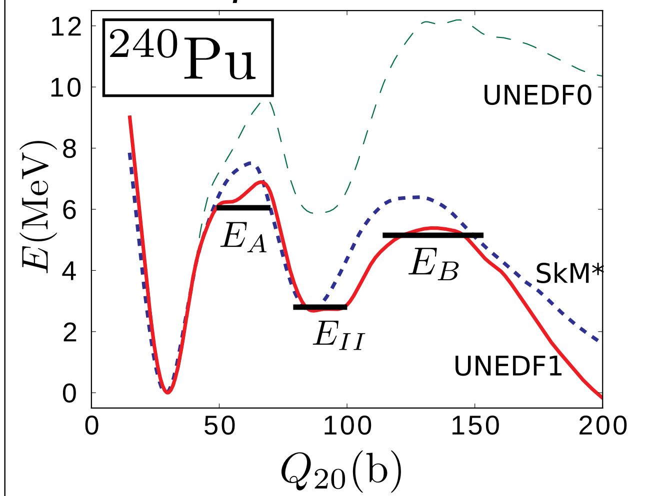


- What is the largest number of protons and neutrons that can be bound together in a nucleus? What are the properties of these extreme nuclei?

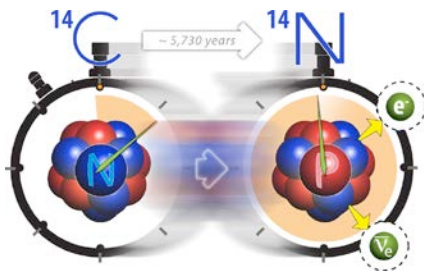
- How can we understand nuclear fission better, from a fully microscopic standpoint?

- How can we control and quantify the uncertainty in our predictions? How can we identify data that will pose the strongest constraints on our model?

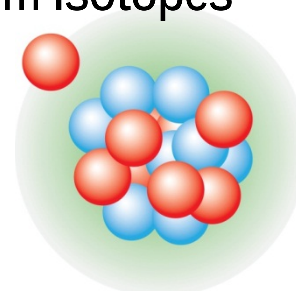
Potential Energy Curve for plutonium-240



- NUCLEI leadership-class applications are advancing scientific discovery at DOE's leadership-class facilities
  - MFDn [Many Fermion Dynamics – nuclear]
    - What is the nuclear structure of ^{14}C that leads to its anomalously long half-life?

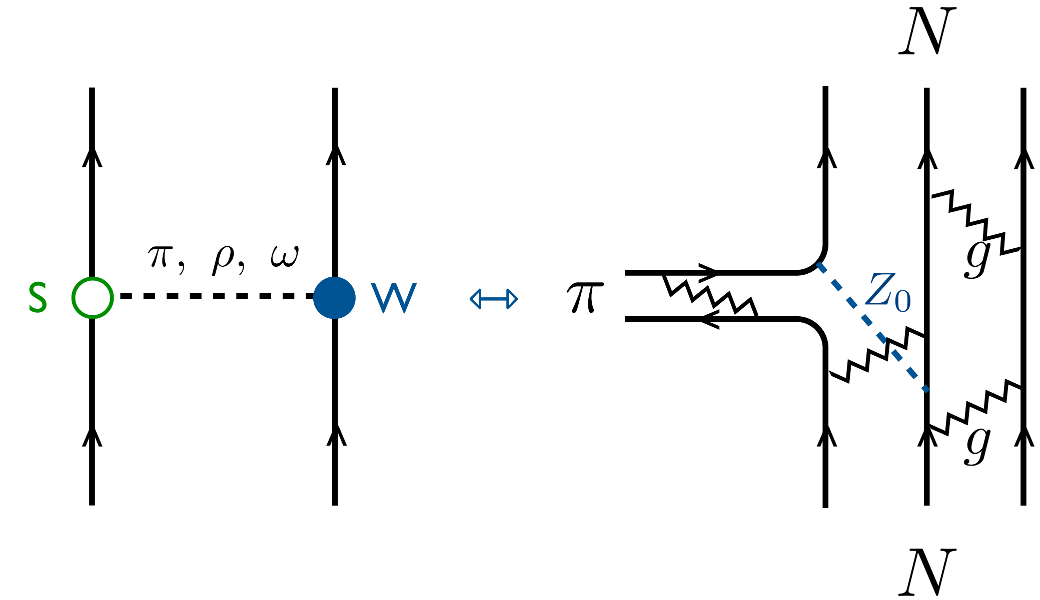


  - NUCCOR-j [Nuclear Coupled-Cluster Oak Ridge]
    - State-of-the-art predictions of neutron-rich calcium isotopes
  - AGFMC [Argonne Green's Function Monte Carlo]
    - Ab initio reaction calculations for ^{12}C



- To the next generation
  - NUCLEI members are addressing the challenges created by the change in computing architectures to push the frontiers of scientific discovery

Hadronic Parity Violation and Lattice QCD
Wick Haxton and Joe Wasem for CalLat



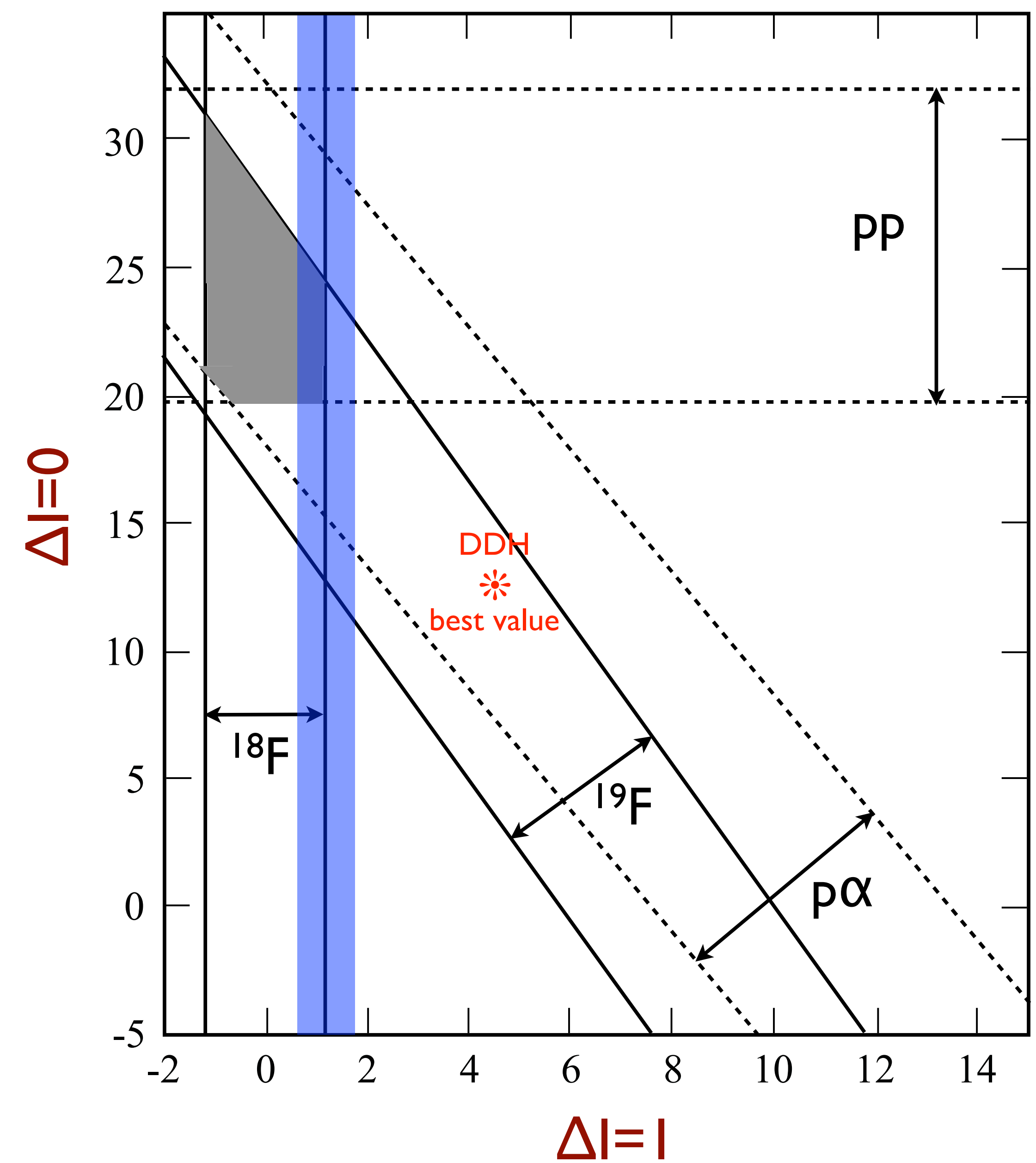
- **Motivation:** To isolate the one SM interaction not yet measured, the weak force between hadrons mediated by the neutral current

- **Experimental technique:** Observation of parity violation in the NN interaction

- **Theory progress:** A new global analysis showing consistency among existing measurements but an anomalous behavior in isospin: ΔI=0/ΔI=1 ~ 6

  First LQCD calculation confirming a weak ΔI=1 amplitude (connected only)

- **CalLat goal:** Completion of the ΔI=1 work and evaluation of ΔI=2 contribution in anticipation of new results from the ongoing cold-neutron SNS experiment

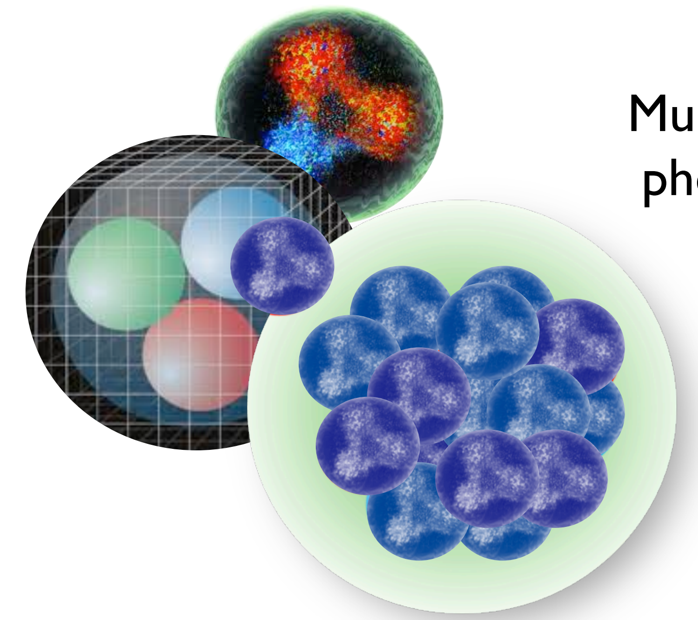


Connecting Cold QCD to Nuclear Many-body Physics

T. Luu for CalLat

Goal: Link *Nuclear Observables* calculated from *QCD* (using *LQCD*) to *Nuclear Many-body Effective Theories*

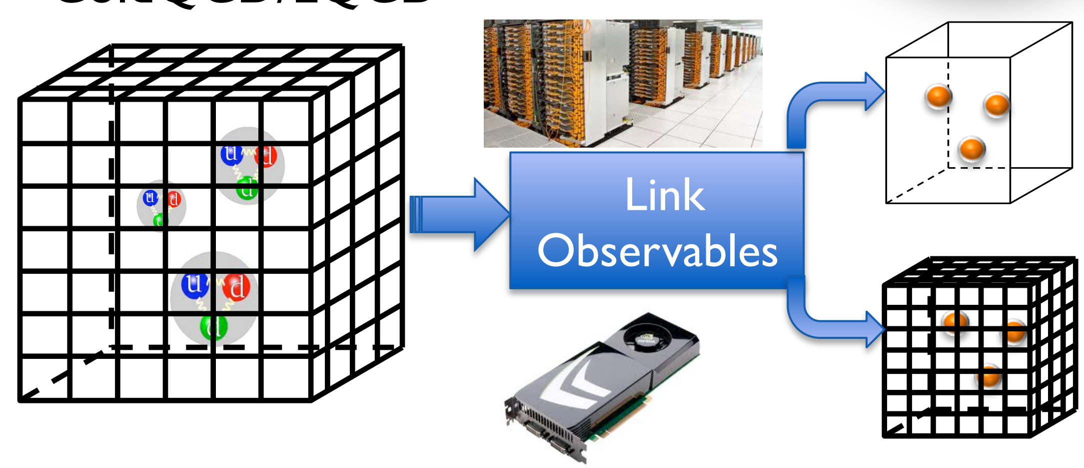
Quarks & Gluons



Multi-hadron phenomena

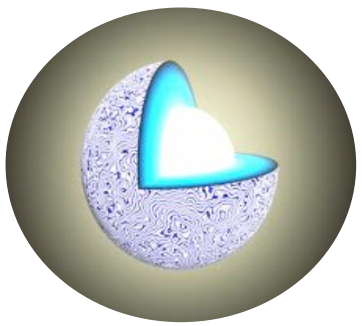
Requires: Formal developments in theory (e.g. finite-volume methods), algorithmic developments on capacity & capability (e.g. multi-grid, tensor contractions)

ColdQCD/LQCD



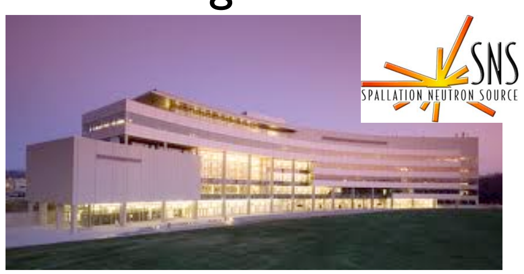
Nuclear Effective Theories

Impact: Extend applicability of LQCD to nuclear structure & reactions, root Nuclear Physics to fundamental QCD, make Nuclear Physics a *Predictive Science*



Neutron star composition

Complements DOE Exp. Programs



Computing Properties of Hot and Dense Nuclear Matter from Qunatum Chromodynamics

USQCD Nuclear Physics

Frithjof Karsch, Brookhaven National Laboratory

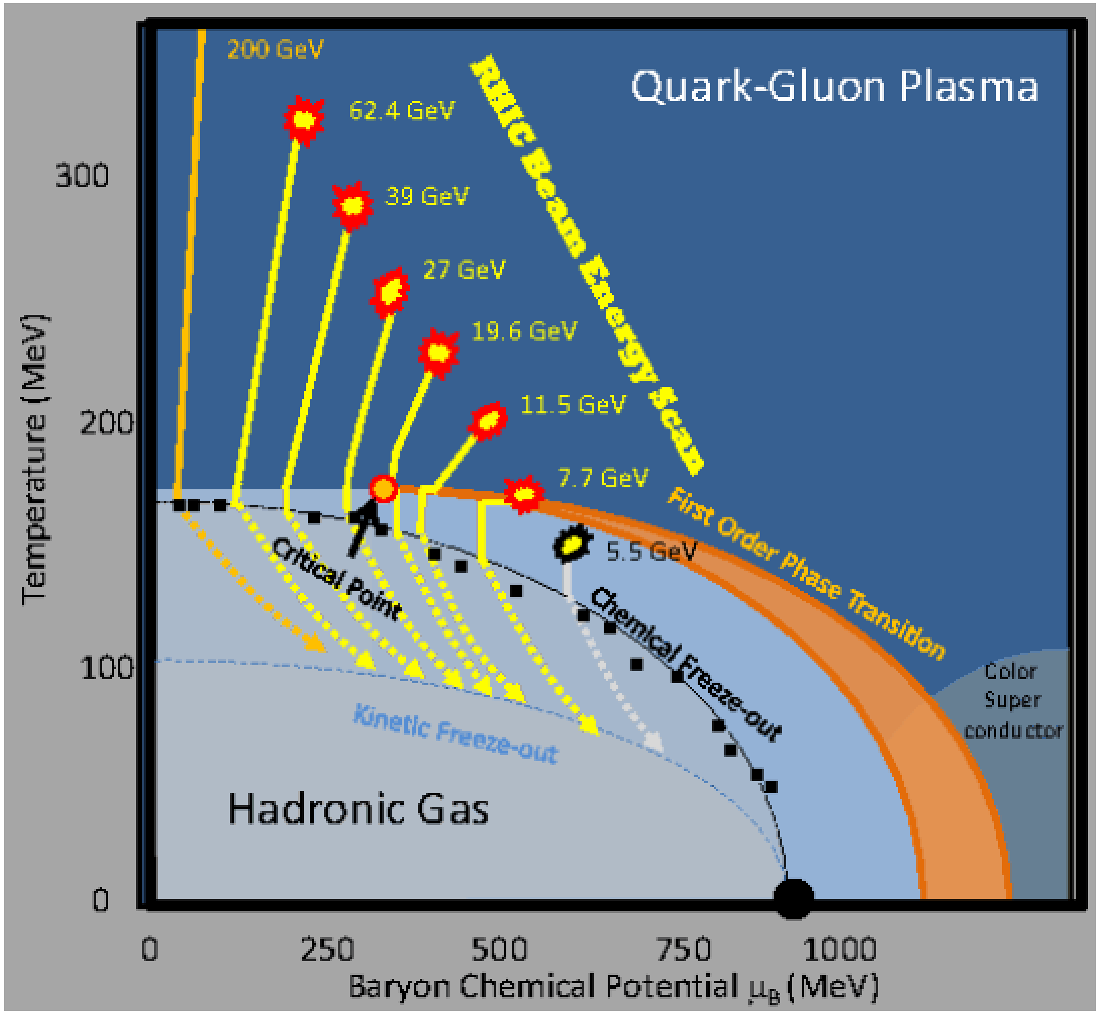


Figure: The phase diagram of QCD and the parameters of theRHIC Beam Energy Scan used to explore it.

Under conditions of extreme temperature or densities the constituents of protons and neutrons, quarks and gluons, get liberated and form a new, largely unexplored state of matter. **Numerical calculations based on lattice regularized Quantum Chromodynamics (QCD)** allow to study the transition from the hadronic phase to the quark gluon plasma phase. They **provide input to the interpretation of large experimental programs at the Relativistic Heavy Ion Collider (RHIC)** at Brookhaven National Laboratory and the Large Hadron Collider (LHC) at CERN, Switzerland.

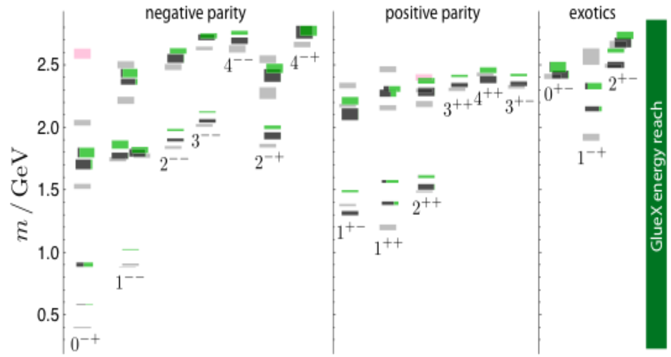
In the poster, **we describe recent successes at understanding the properties of hot and dense matter from lattice QCD, and future questions that will be addressed through our SciDAC activities.** In particular, we describe the computational challenges, and the likely impact of the resulting calculations on current and future experiments.

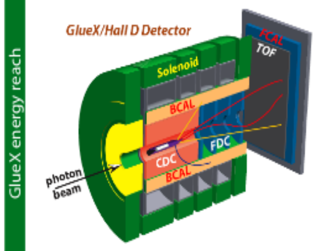
Understanding the structure and interactions of matter in Quantum Chromodynamics

Robert Edwards (Jefferson Lab) for the USQCD Collaboration

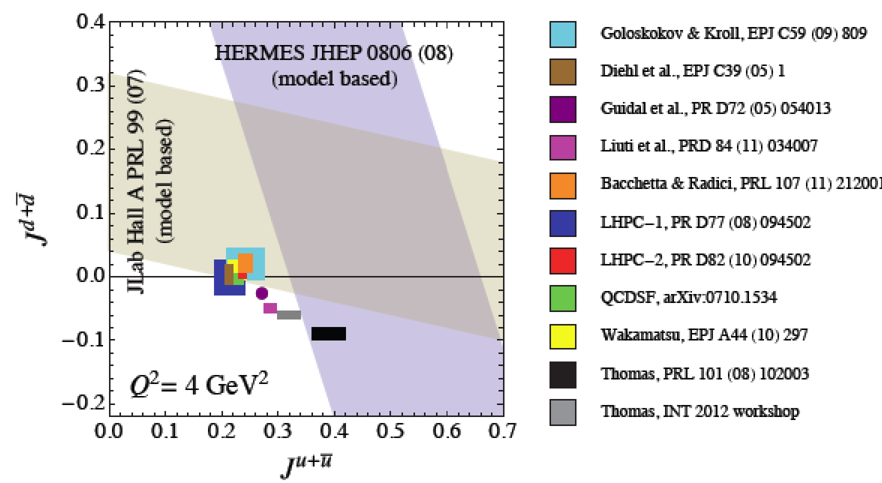
- Fundamental questions in Nuclear Physics
  - Can QCD predict the spectrum of hadrons? What is the role of gluons?
  - How do quarks and gluons make nucleons?
  - Can QCD explain light nuclei?
- Focus of experiments at BNL, JLab, and FRIB
- SciDAC 1 & 2
  - Large scale generation of gluon fields on leadership facilities
  - Exploitation of GPUs for capacity computing
- Significant impact on experimental searches
  - Spectroscopy, hadron and nuclear structure
- SciDAC 3 – confront new computational challenges
  - Support for heterogeneous and multi-core systems
  - New algorithms & techniques for "analysis" phase
- Collaboration with SUPER
  - Tuning, code generation, and performance portability analysis for heterogeneous and multi-core systems
  - Incorporate into development of a DSL for LQCD in out years
- Collaboration with industry
  - IBM, Intel Parallel Labs and NVIDIA

The search for exotic forms of matter @ JLab





The origin of the spin of a proton



Thank You!

Poster Session

4:05-5:35pm in Roosevelt/Madison