Quo Vadis Computational (Condensed Matter) Physics?

- Unifying Themes of Computational Physics
- A Brief Look Backward (Gordon Bell Awards)
- Lattice Gauge Theory and Hubbard Models
- Renaissance of Diagrammatic Methods
- Combining Electronic Structure and Molecular Dynamics
- Some Algorithmic Challenges
- Computational Physics Education
- Outlook

Unifying Themes of Computational Physics

Driven by desire to solve major scientific problems

Shared Strategies

- Choose theoretical approximations/models to represent phenomena
- Devise algorithms to solve equations
- Choose numerical techniques (hardware architecture important)
  - [APS Tutorial 8: GPU Computing in Physics, Duane Johnson]
- Write quality programs
- Verify and validate: integrate experiment and theory
- Educate a new generation of computational physicists

Shared Connections

- Applied Math (algorithms and numerical techniques)
- Computer Science (parallelization, data management)

A Brief Look Backward

Gordon Bell Performance Prize Winners

2000 Molecular Dynamics simulation for NaCl

2001 Simulation of black holes in a galactic center

2002 Global Atmospheric Simulation

2003 14.6 Billion Degrees of Freedom, 5 Tflop, 2.5 Tbyte Earthquake Simulation

2004 Simulation of Geodynamos

2005 Solidification Simulations

2006 1. Large-Scale Electronic Structure Calculations of High-Z Metals
2. The BlueGene/L Supercomputer and Quantum Chromodynamics

2007 Kelvin-Helmholtz instability in molten metals

2008 1. 400+ TFlop/s Simulations of Disorder Effects in High-Tc
2. Electronic Structure for Thousand Atom Nanostructures.

2009 Simulations of Magnetic Systems and Curie Temperature

2010 Electronic Structure Simulations of Excited States in Materials

Computational Physics is well, and broadly, represented in Gordon Bell Awards.

Peak Performance of Gordon Bell Prize Winners

year	peak performance	
1987	450	Mflops
1988	1	Gflops
1989	6	Gflops
1990	14	Gflops
1996	111	Gflops
1999	1.2	Tflops
2001	11.4	Tflops
2005	107	Tflops
2006	207	Tflops
2007	103.9	Tflops
2008	1.352	Pflops
2009	2.33	Pflops

Recent Progress in Lattice Gauge Theory

Last five years: computation of parameters of Standard Model

Cabibbo, Kobayashi, Maskawa (CKM) matrix elements.

Examine effects of QCD on weak interactions.

LGT: Quarks and gluons on a lattice.

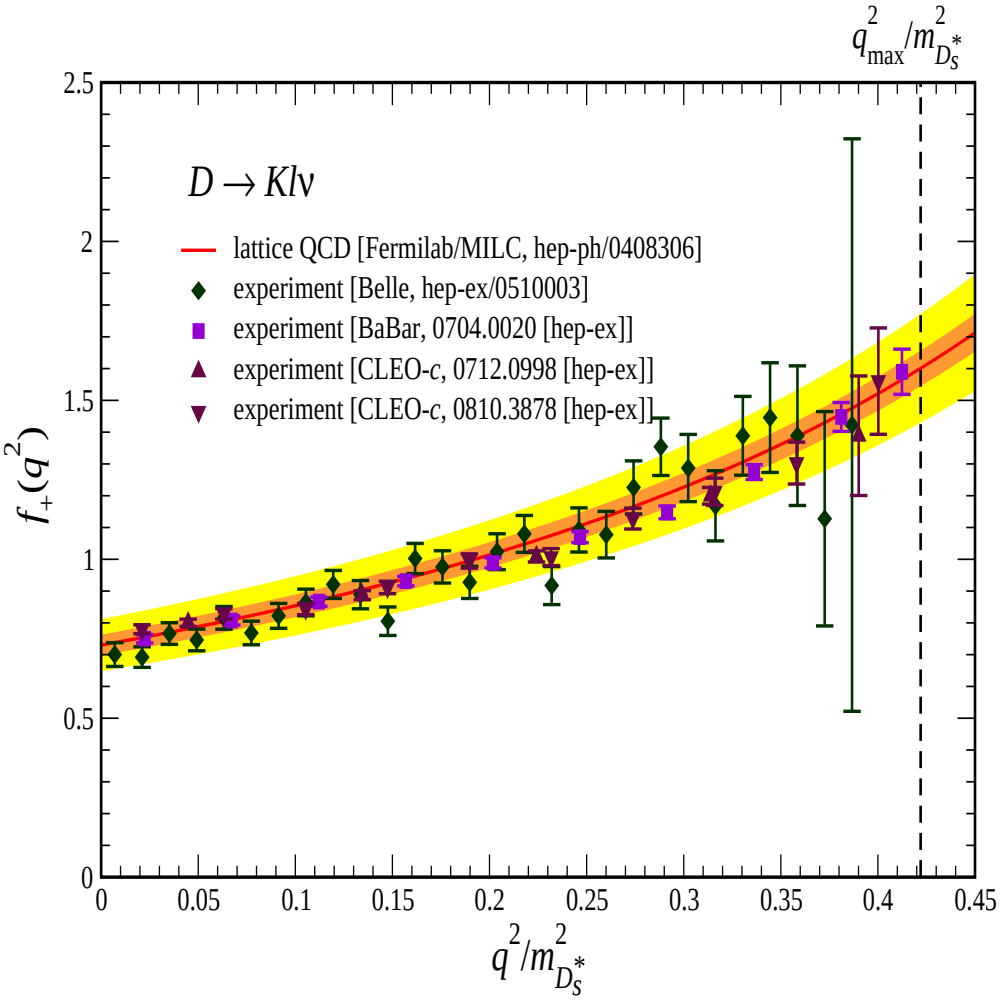
CM: Electrons and phonons (or Hubbard-Stratonovich field) on a lattice.

Close methodological connections to "Determinant Quantum Monte Carlo"

and other approaches to condensed matter physics.

- Sign problem
- Linear Scaling Algorithms
- Molecular Dynamics

Decay of D meson (charmed + light quark)
to K meson (strange + light quark), lepton, and neutrino



- Overall normalization measures CKM matrix elements.
- Functional dependence on q^2 (outgoing lepton momentum) matches between LGT (2004) and experiment (2005-2008).

High energy physics looking for breakdown of Standard Model.

- Experimentally by going to higher energy (LHC).
- Very accurate numerics at existing energies, look for deviations.

Future of Lattice Gauge Theory will follow both these approaches.

- Higher resolution data, e.g. the preceding CKM matrix elements.
- Coding up LGT variants of standard model.

A big Computational Challenge is LGT at finite density.

Needed for modeling of experiments on quark-gluon plasma (RHIC)

Similar issues to simulations of Hubbard model (sign problem).

Other large scale computational effort in high energy physics:

Data storage and analysis for the LHC.

Lattice (Hubbard) Models in Condensed Matter

Interest driven by solid state materials

- Cuprate and iron-pnictide superconductors
- Heavy fermion systems
- Transition metal oxides/lanthanides (eg volume collapse transitions)

And also, recently, "optical lattice emulation" using ultracold atoms.

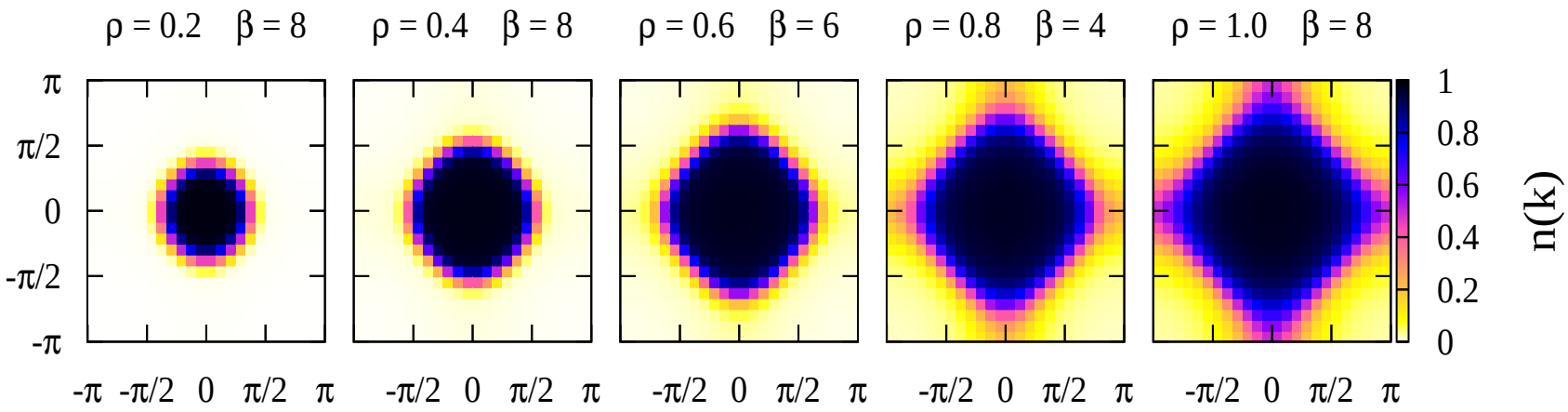
Computational Advances

- Improvements in Determinant QMC (close cousin of LGT):
  $10^2 \rightarrow 10^3$ fermions
- Renaissance of Diagrammatic Methods
  Dynamical Cluster Approximation
  Dynamical Vertex Approximation
  Diagrammatic Quantum Monte Carlo
  Novel, and intriguing, approach: diagrams are themselves sampled!

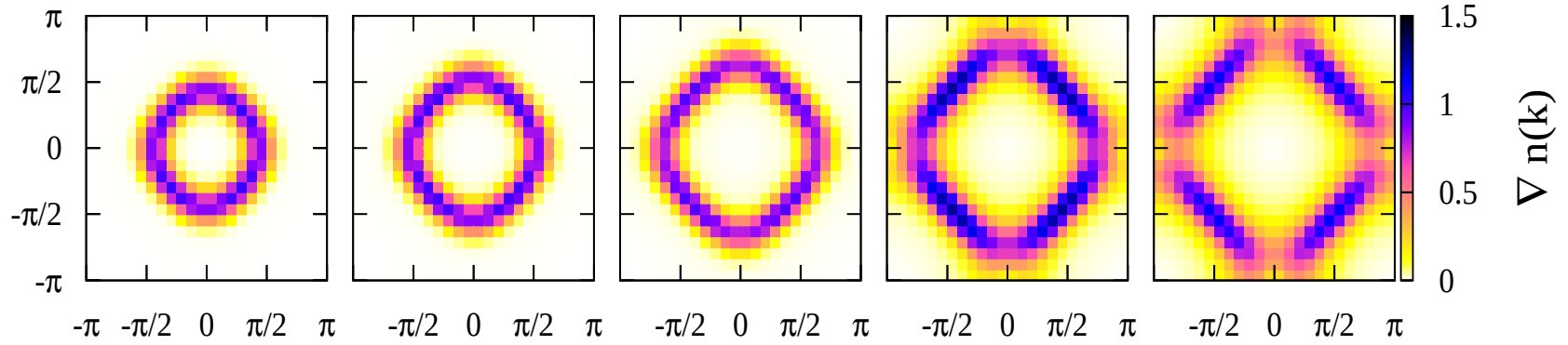
Combination with LDA.

Increased DQMC lattice size: resolution of Fermi surface of homogeneous systems.

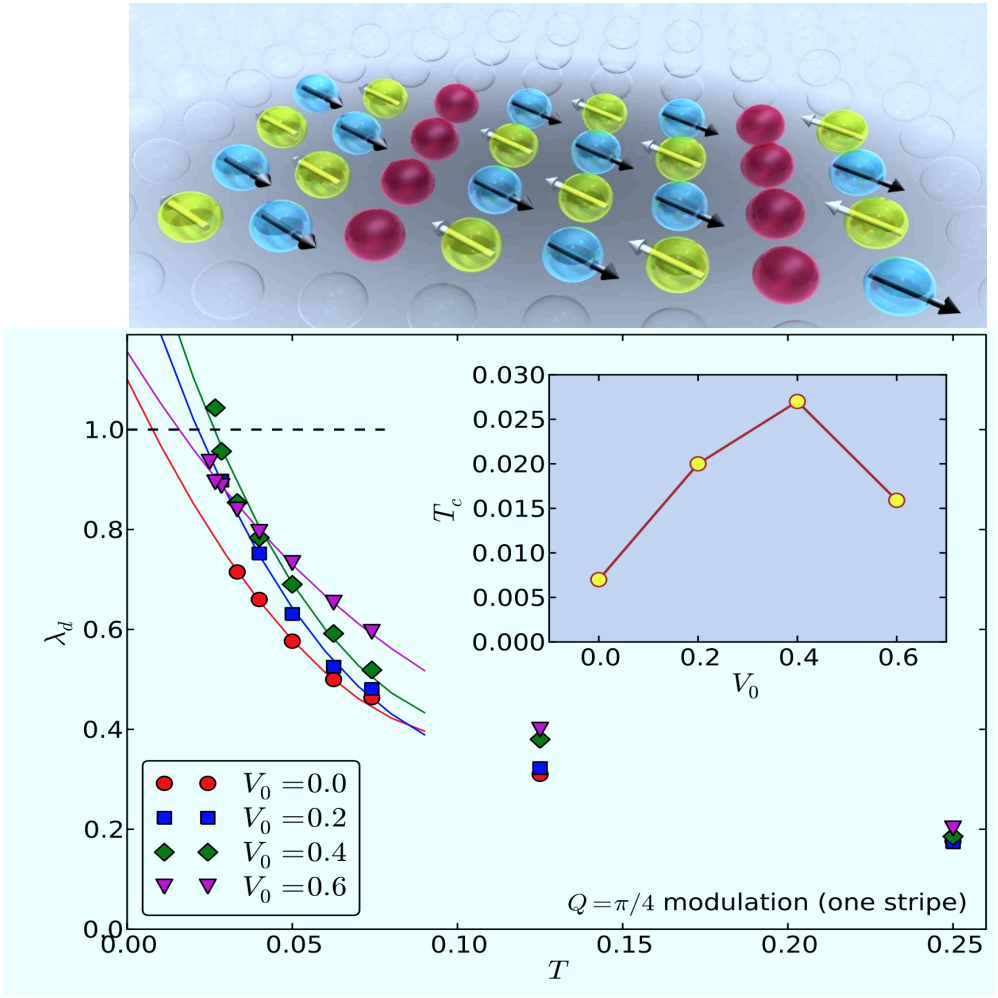
$U = 4$ Fermi function:



$U = 4$ Gradient of Fermi function:



Dynamic Cluster Quantum Monte Carlo: pairing in the 2D Hubbard model

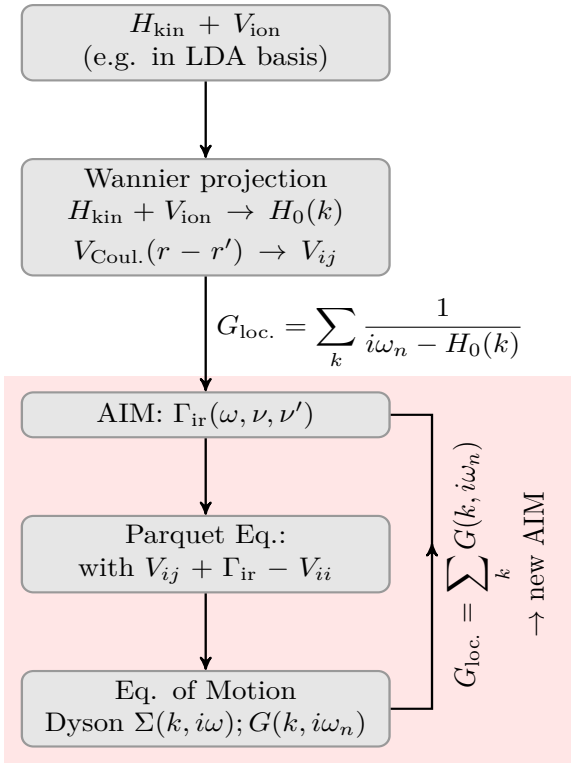


Superconducting T_c significantly enhanced by charge inhomogeneity.
Can do 100 site momentum space clusters.

Maier etal PRL 104, 247001 (2010)

Dynamical Vertex Approximation

Include vertex corrections in the merger of LDA with DMFT.



Tested extensively for Hubbard model (3D, 2D)

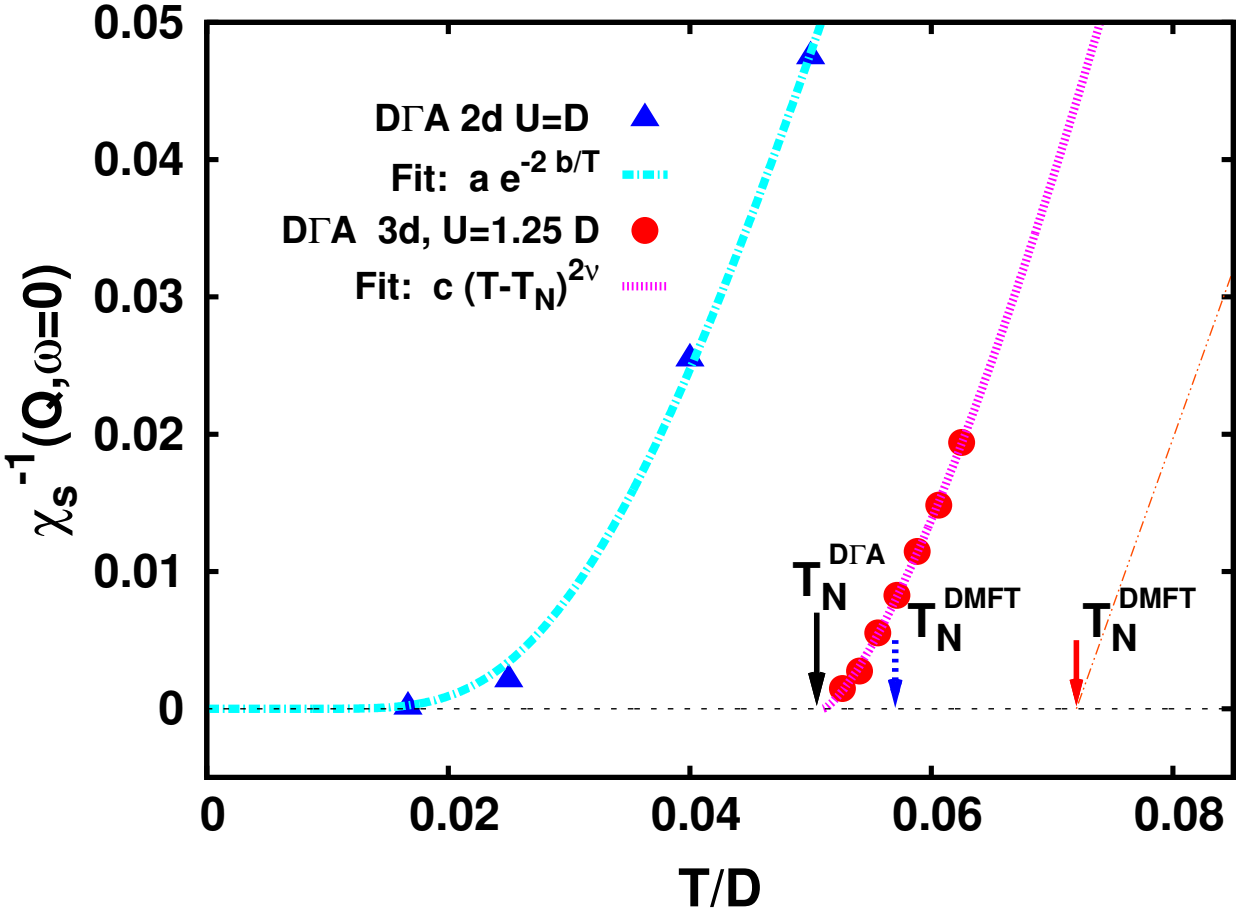
Future: Integrate with LDA codes.

Held, Ann. Phys. (2011)

Critical exponents

Toschi, Katanin, KH '09

Antiferromagnetic phase transition in half-filled Hubbard model

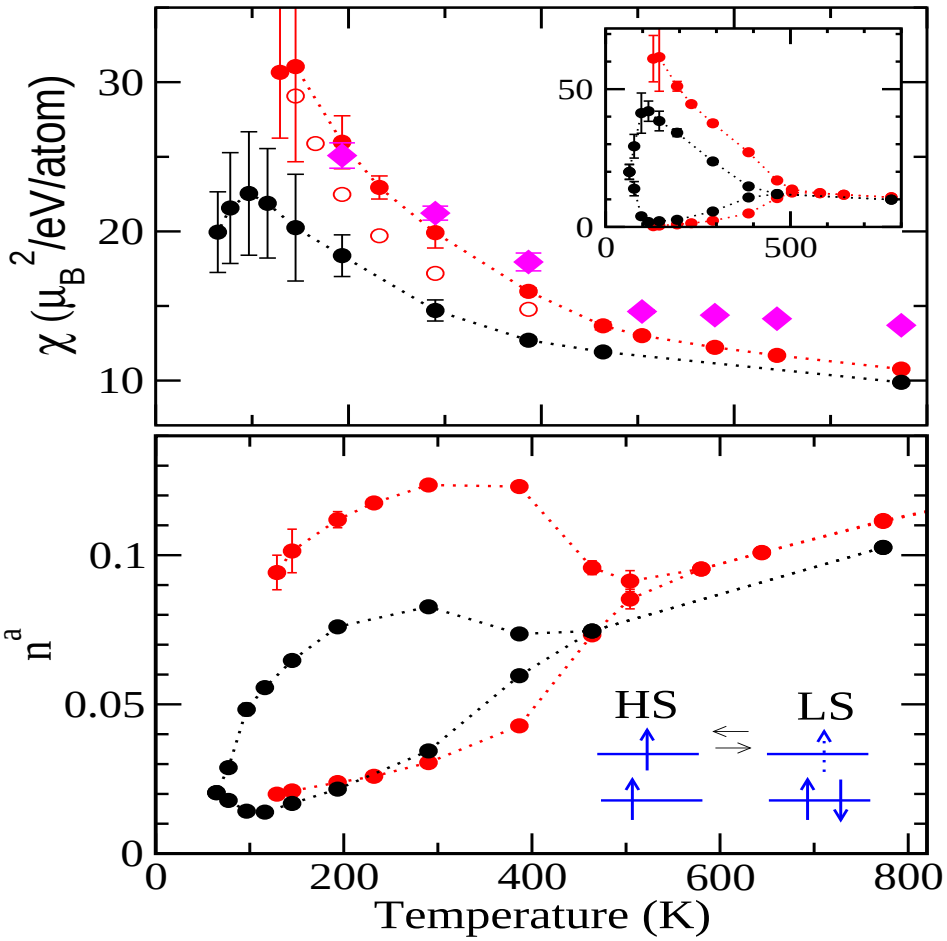


2D: Mermin-Wagner theorem fulfilled!
3D: critical exponent $\nu = 0.67 \pm 0.05$ agrees with Heisenberg model $\nu = 0.707...$

DMFT Revealing Unexpected Physics in Multi-Orbital/Band Models

Two band Hubbard model with crystal field splitting (appropriate to $LaCoO_3$)

"Spin Disproportionation": Alternation of high spin (magnetic) and low spin (nonmagnetic) sites at intermediate temperature.



Susceptibility (inset: site resolved)

Difference in site occupations.

$\Delta_{cf} = 3.40, (3.42)$ for red(black)

Kunes etal, arXiv:1103.2249

Generalizing LDA+DMFT towards improved cluster solvers

Strong correlation physics (eg Mott gap) difficult to achieve in LDA.

But LDA + U is too much of a good thing (overestimates Mott).

Past decade: LDA + DMFT (dynamical mean field theory)

Proper balance: Kondo resonance/quasiparticle renormalization

Now being integrated into standard LDA programs

Two big problems

- Double counting of interaction energy
- Effect of "non-local" corrections not included (DMFT is "single site")

Solution Arriving in Form of improved impurity solvers

- Dynamic Vertex Approximation, Dynamic Cluster Approximation (Kotliar, Jarrell)
- Better QMC methods (continuous time methods) (Rubtsov, Werner, Troyer, Haule)

Even more open (and very important) issue:

- Self-consistency (feedback of DMFT/DCA/DΓA into LDA band structure)

Dynamics

QMC methods mostly focus on equilibrium phase diagrams: $e^{-\beta \hat{H}}$.

E.g. magnetic, charge density wave, superconducting transitions.

A frontier of QMC is to dynamics: $e^{-i\hat{H}t}$.

For exactly soluble models: Thermalization (Rigol).

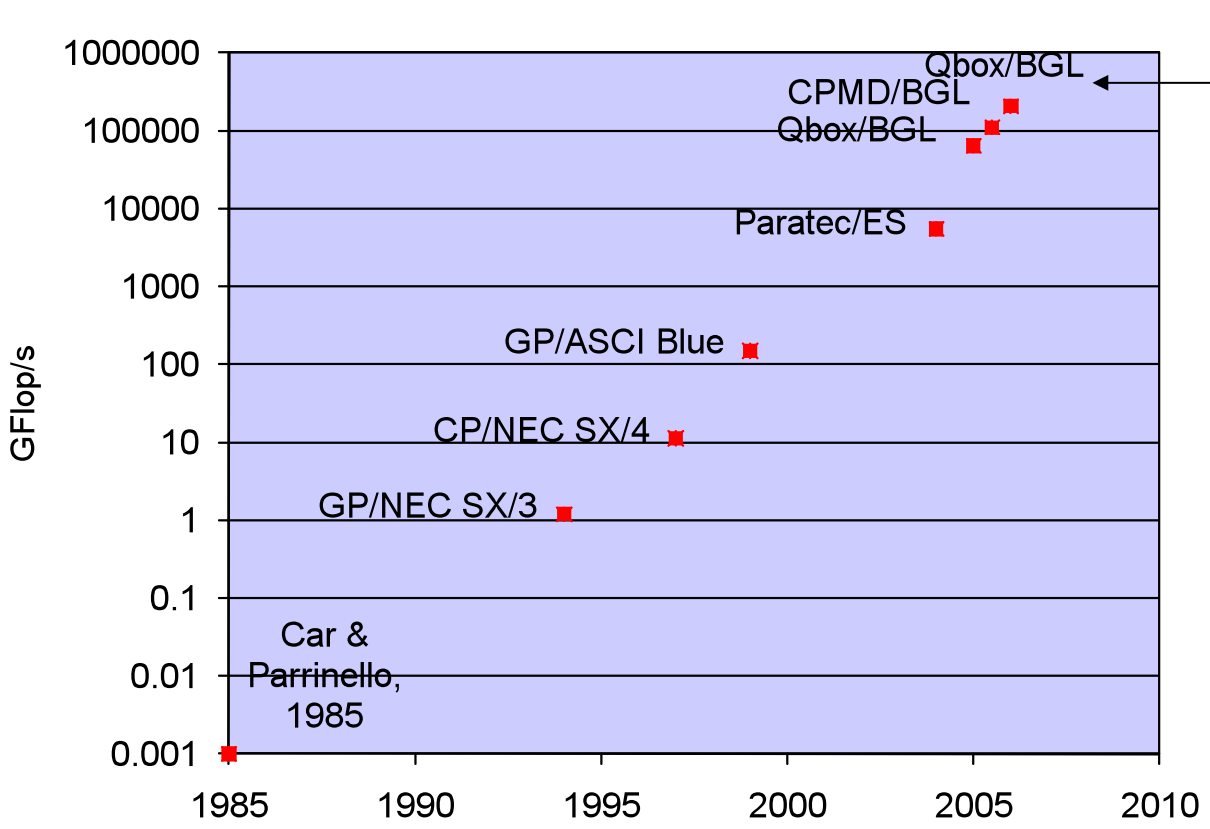
Computational electronic structure methods:

Dynamics is increasingly well developed, and important.

Compute forces from energy changes when ions displaced.

Use in $F = ma$.

History of *ab-initio* MD performance



207.3 TFlops sustained

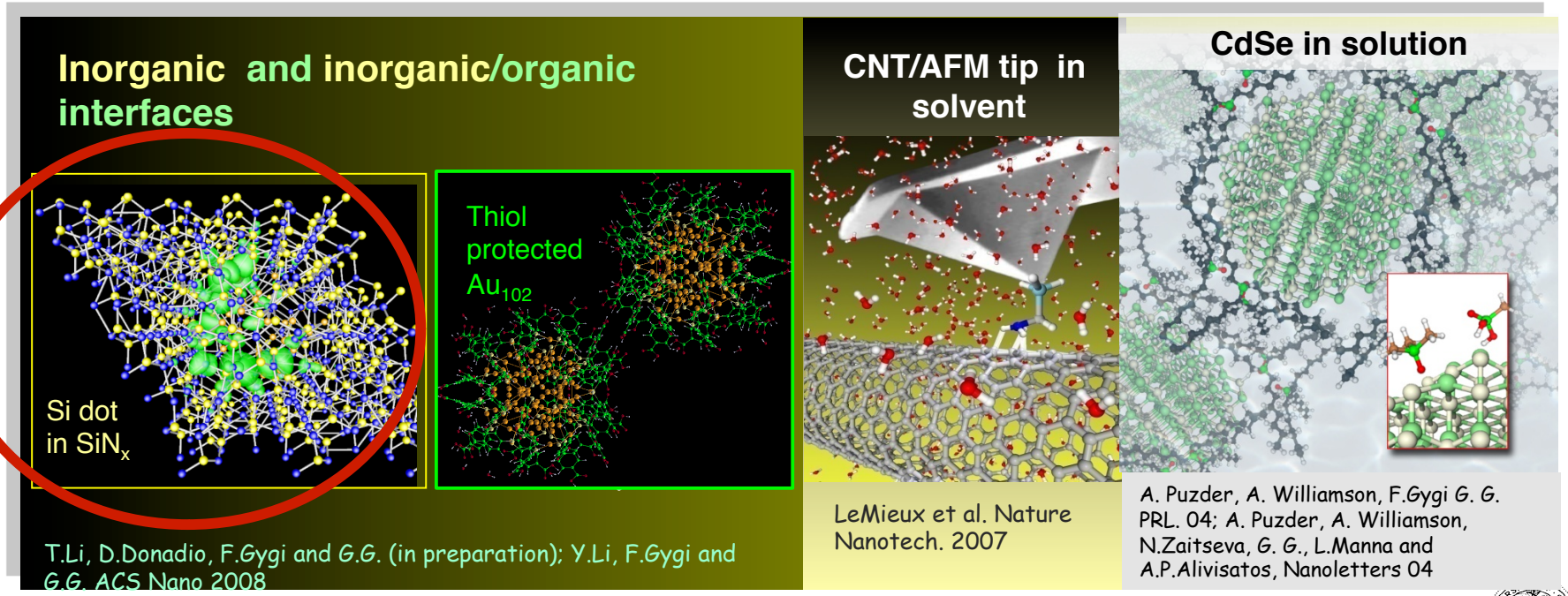
The performance of *ab-initio* molecular dynamics codes has doubled every 8 months

Parallelization `beats` Moore's Law: until when?

I/O and analysis of large data sets have become very challenging problems

Nanostructures in realistic environments

- Nanoparticles embedded in solid matrices
- Nanoparticles in solutions
- Nanostructures in external fields



"Linear Scaling Algorithms"

Many computational problems involve linear algebra

Dense Matrix Multiplication, Matrix inversion $o(N^3)$

Can algorithms be formulated as $o(N)$?

(Electronic Structure and Quantum Monte Carlo, for example)

General Argument that such algorithms might exist in principle:

"Nearsightedness principle" (Kohn 1996)

Influence of degrees of freedom in problem fall off sufficiently rapidly:

Partition problem into local spatial domains.

Issues in Practical Implementation:

How is domain size determined? Done for each separate problem?

How robust? Do small errors associated with partitioning blow up in "time"?

(eg as Molecular Dynamics or Monte Carlo simulation progresses)

Example from Quantum Monte Carlo for fermions:

$$Z = \int \mathcal{D}\mathbf{x}\ \det\mathcal{M}(\mathbf{x}) \Rightarrow \int \mathcal{D}\mathbf{x} \int \mathcal{D}\Phi\ \exp\Big[-\Phi(\mathcal{M}(\mathbf{x})^T\mathcal{M}(\mathbf{x}))^{-1}\Phi\Big]$$

$\mathbf{x}$: Field coupled to fermions, eg phonons, gluons, Hubbard-Stratonovich.

$\mathcal{M}$ is a sparse matrix.

Φ update is trivial: $\Phi = \mathcal{M}^T R$ where $P(R) \propto \exp\big[-R^T R\big]$

$\mathbf{x}$ update requires computation of $(M^T M)^{-1}\Phi$.

Do iteratively. Involves sparse matrix multiplication: $\rightarrow o(N)$!

Works well in Lattice Gauge Theory.

Works poorly in simulations of the Hubbard Hamiltonian.

Number of iterations grows slowly with linear lattice size.

Grows very rapidly (even becoming unstable) in imaginary time.

Molecular Dynamics in LGT!

$$\frac{d\mathbf{x}}{dt} = \mathbf{p} \qquad\qquad \frac{d\mathbf{p}}{dt} = \frac{d}{d\mathbf{x}}\Big[-\Phi(\mathcal{M}(\mathbf{x})^T\mathcal{M}(\mathbf{x}))^{-1}\Phi\Big]$$

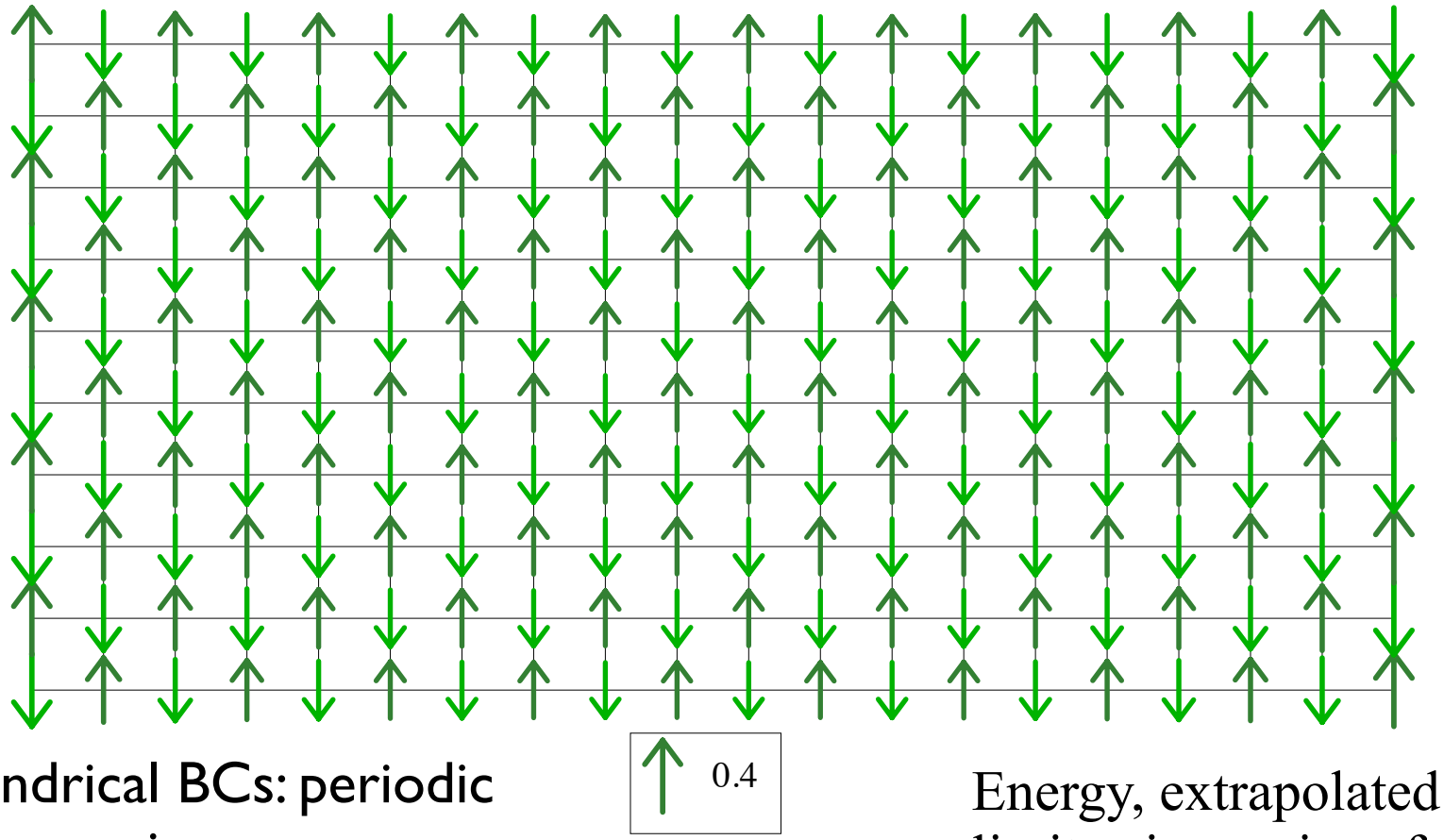
What happens at zero eigenvalues of $\mathcal{M}$?

Numerical Approaches

- The key weakness in the theoretical approaches has been the "sign problem"--the lack of a reliable, accurate 2D approach.

Method	Approach	Variational	2D?	Sign problem	Biased	Computational Effort
Pure quantum Monte Carlo	Statistical sampling	No	Yes	Yes	No	N or N^3
Variational QMC	Statistical sampling	Yes	Yes	Fixed by guessed wavefunction	Yes	N^3
Series Expansion	Extrapolated Taylor Series	~No	Yes	No	Yes*	<10 or 20 terms
Density Matrix Renormalization Group(DMRG)	Low Entanglement	Yes	Width < 12	No	~No	m^3
PEPS, MERA	Low Entanglement	Yes	Yes	No	Slight	D^{10}

Square lattice: benchmark against QMC



20 x 10

- Cylindrical BCs: periodic in y, open in x
- 21 sweeps, up to m=3200 states, 80 hours
- See White&Chernyshev, PRL 99, 127004 (2007)

Energy, extrapolated to thermo limit using series of cylinders
-0.669444(5)

Sandvik, QMC (1997):
-0.669437(5)

Challenges to Algorithm Development I. Use of Sophisticated Machines

Old paradigm:

Invent algorithm

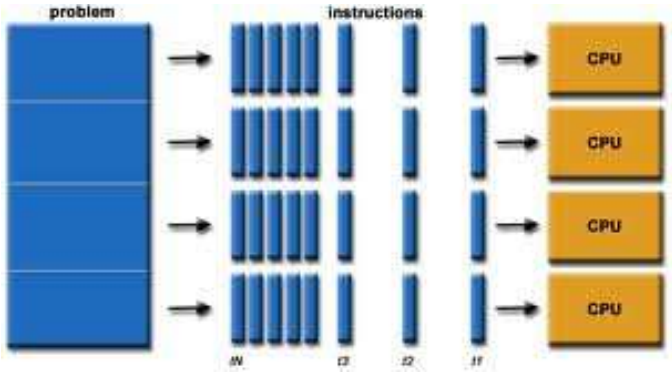
Write 'simple' (non-parallel) code. (Compiler does all the work.)

Compare with existing algorithms.

New paradigm:

Invent algorithm

Must compete with codes optimized on parallel architectures.



Much bigger effort needed to test ideas.

Concern to young scientists: method development is low yield in publications.

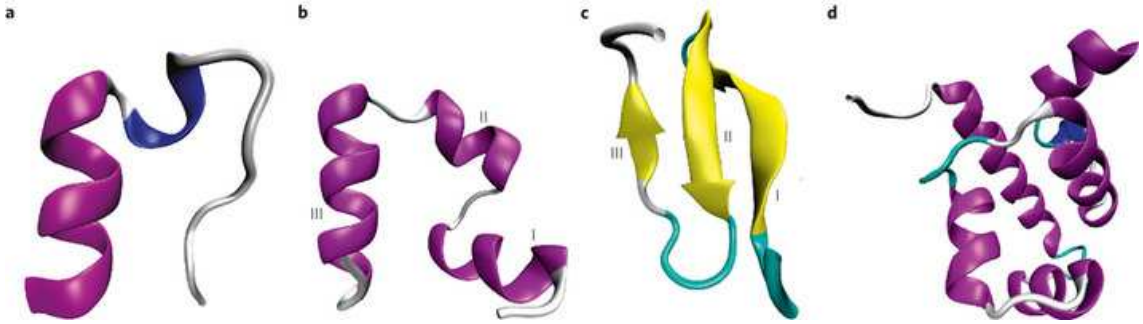
Of course, this sort of challenge common to all mature scientific fields.

Challenges to Algorithm Development II. Long time vs big size

Parallel computers help if problem involves more degrees of freedom.

What if you confront a "small" problem that you want to run for a long time?

Molecular dynamics simulation of biomolecules



Protein folding time scale micro- to milli-second.

Time step is femto-second!

Thermalization in Monte Carlo

2000 equilibration sweeps + 20000 measurement sweeps.

Measurement sweeps can be trivially parallelized.

10 cpus: each does 2000 equilibration sweeps + 2000 measurement sweeps

Speed-up is $22000/4000 = 5.5$

100 cpus: each does 2000 equilibration sweeps + 200 measurement sweeps

Speed-up is $22000/2200 = 10.0$

Can thermalization/equilibration be parallelized?

Challenges to Algorithm Development III. Robustness to node failure

Parallel codes need to survive failure of node during course of computation.

What to do if (small) subset of data missing?

What to do if a query is sent and there is no response?

Will future computational physics codes have a stochastic element?

Algorithm robust to small amount of missing data.

Mimic robustness of physical phenomena codes are simulating.

Is missing data from one node like, for example, a non-magnetic impurity?

Challenges to Algorithm Development IV.

Old paradigm:

Student wrote/knew own code.

(Has drawbacks too: Student graduate and code abandonned)

New paradigm:

Codes and students increasingly have separate lives.

Student is "user" (sometimes even the PI unfamiliar with code details).

To what extent should users know algorithm details?

Again, this problem common to mature fields.

Who will maintain codes? Are NSF repositories as widely used as they could be?

ALPS (Algorithms and Libraries for Physics Simulations)

open source simulation codes for strongly correlated QM systems

Computational Physics Education

NSF, NAS emphasize the need for K-12 computing education:

"It's one of the most vexing paradoxes facing the U.S. today, even if most people are not aware of it. American IT and software companies dominate the world market place and the vast majority of colleges and universities have excellent computer science programs, yet at the K-12 level, computer science education is almost nonexistent."

http://www.nsf.gov/news/news_summ.jsp?cntn_id=116059

Yet, computer programming classes remain absent from secondary schools, or moving in the wrong direction.

Percentages of high schools offering:

	2005	2010
Introductory Programming Course	78%	65%
AP Programming Course	40%	27%

Meanwhile, other countries have implemented a comprehensive (required) secondary school computer science curriculum.

Undergraduate and graduate level:

- 5-6 undergraduate programs in computational physics
- 25 minors/concentrations/tracks

But, in many cases, computational physics is not being emphasized in university physics curriculum despite its increasing pervasiveness in research and in industry.

"we are teaching the same things we taught 50 years ago".

"Report of the Joint AAPT-APS Task Force of Graduate Education in Physics", June 2006.

Rubin Landau/Steven Gottlieb
(editors of new series of textbooks incorporating computational physics)

DCOMP Conference on Computational Physics

Trondheim, Norway 23 - 26 June 2010.

- Electronic Structure Theory: Yesterday, Today and Tomorrow
- Multiscale science of biological protein materials in extreme conditions
- Quantum Mechanics in a Glass of Water
- Tensor product states for strongly correlated electron systems
- Robustness of Networks
- Simulations of the growth of structure in our Universe
- Building a National Digital Library for Computational Physics Education
- Understanding the Human Genome: Excitement, Challenges and Opportunities
- Preparing for Discovery with the Large Hadron Collider
- Simulating Core-Collapse Supernova Explosions
- Car-Parrinello Investigation of Electronic Properties of Oxide-Water Interfaces
- Monte Carlo simulations of the HP model (the "Ising model of protein folding")
- Coloring the noise or cheating ones way to quantum effects

Outlook

Computational Physics is at the same time:

A Mature Field: Can solve very difficult and important problems.

Developing Rapidly: Many algorithm and physics challenges remain.

Need to consider how better to bring into classrooms.