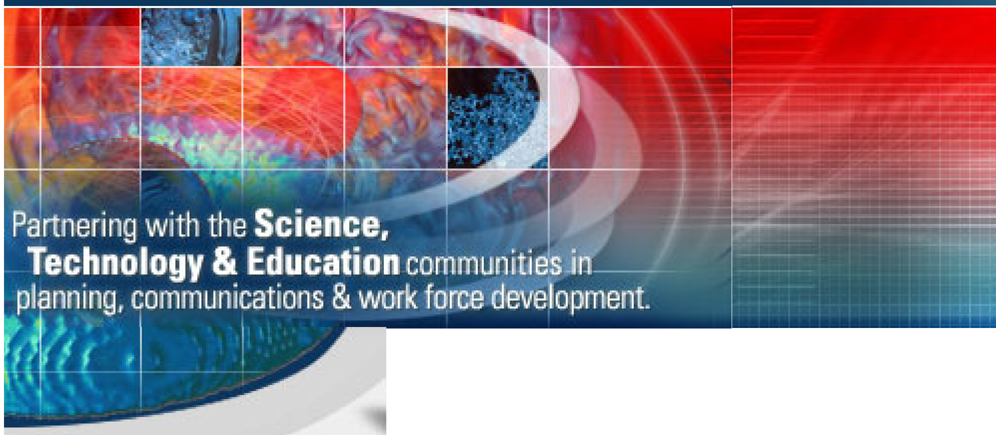


Discovering new science through HPC: An Alumna's Story

Mary Ann Leung, Ph.D.

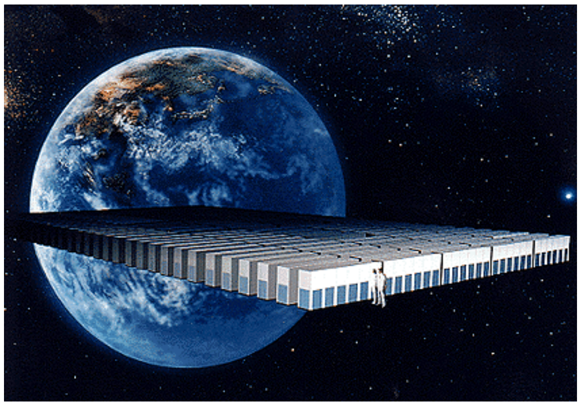
Krell Institute

CSGF Annual Meeting

June 18, 2008

Why HPC?

2002

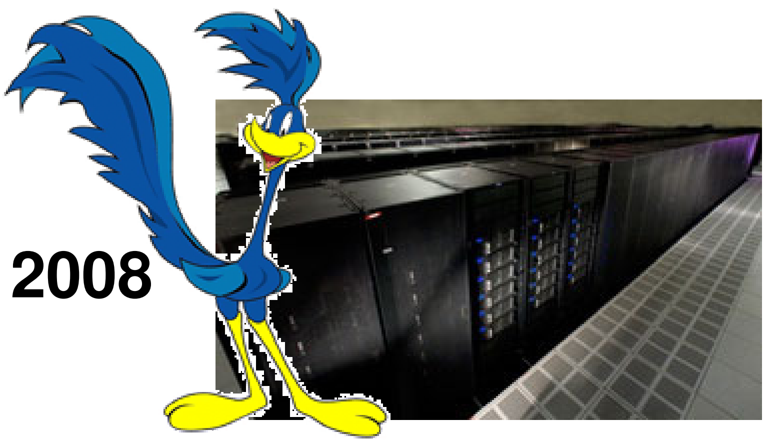


Earth Simulator 35.6 Teraflops

2006

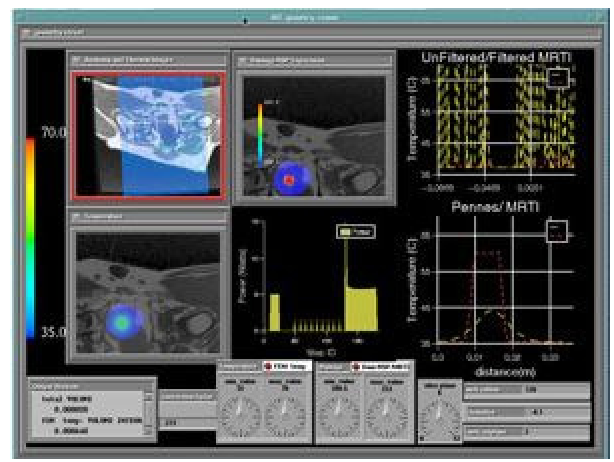
Jaguar ORNL 101.7 Teraflops

2008



Roadrunner LANL Petaflop

2008

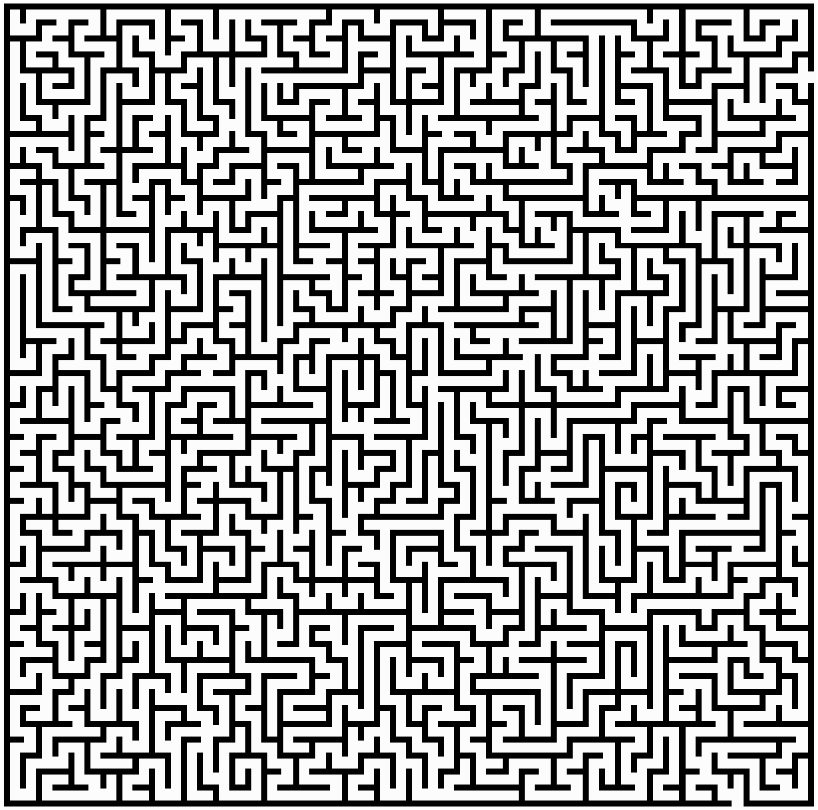


TACC Lonestar
canine cancer laser surgery

Outline

- Pathways to Ph.D.
- Overcoming the activation barrier
- How HPC impacted my research
- A short survey

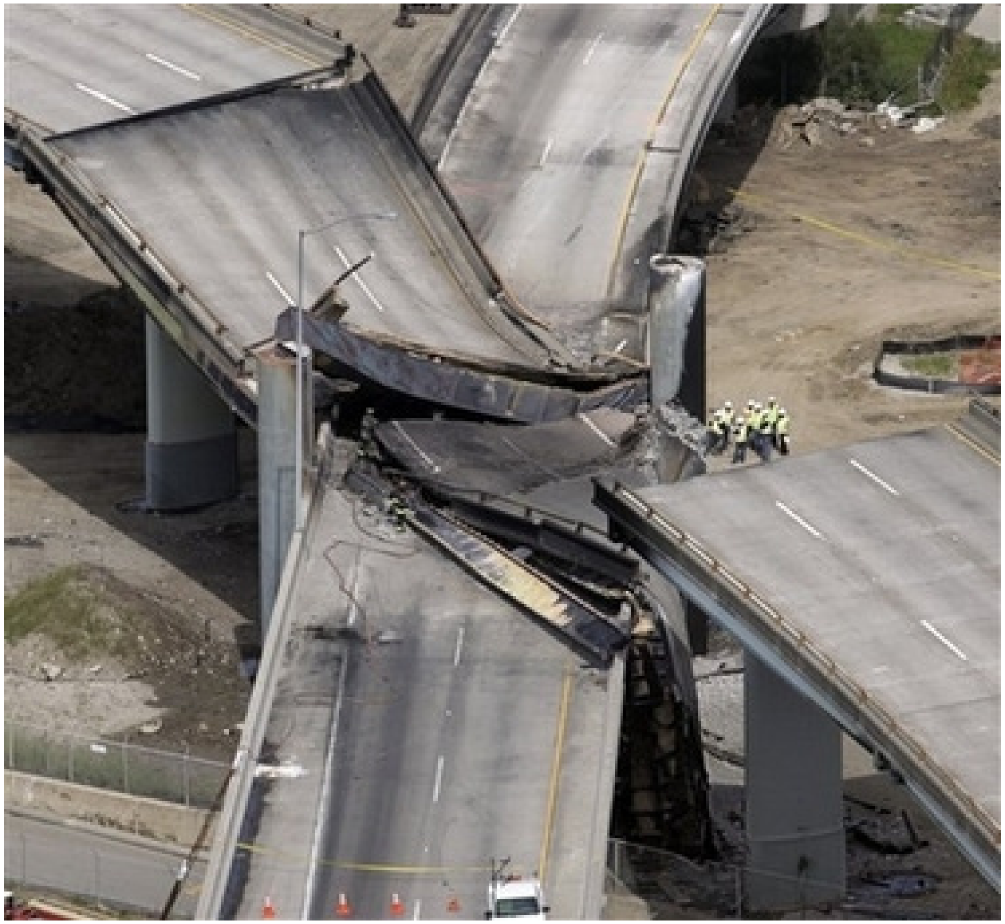
Pathways to Ph.D.



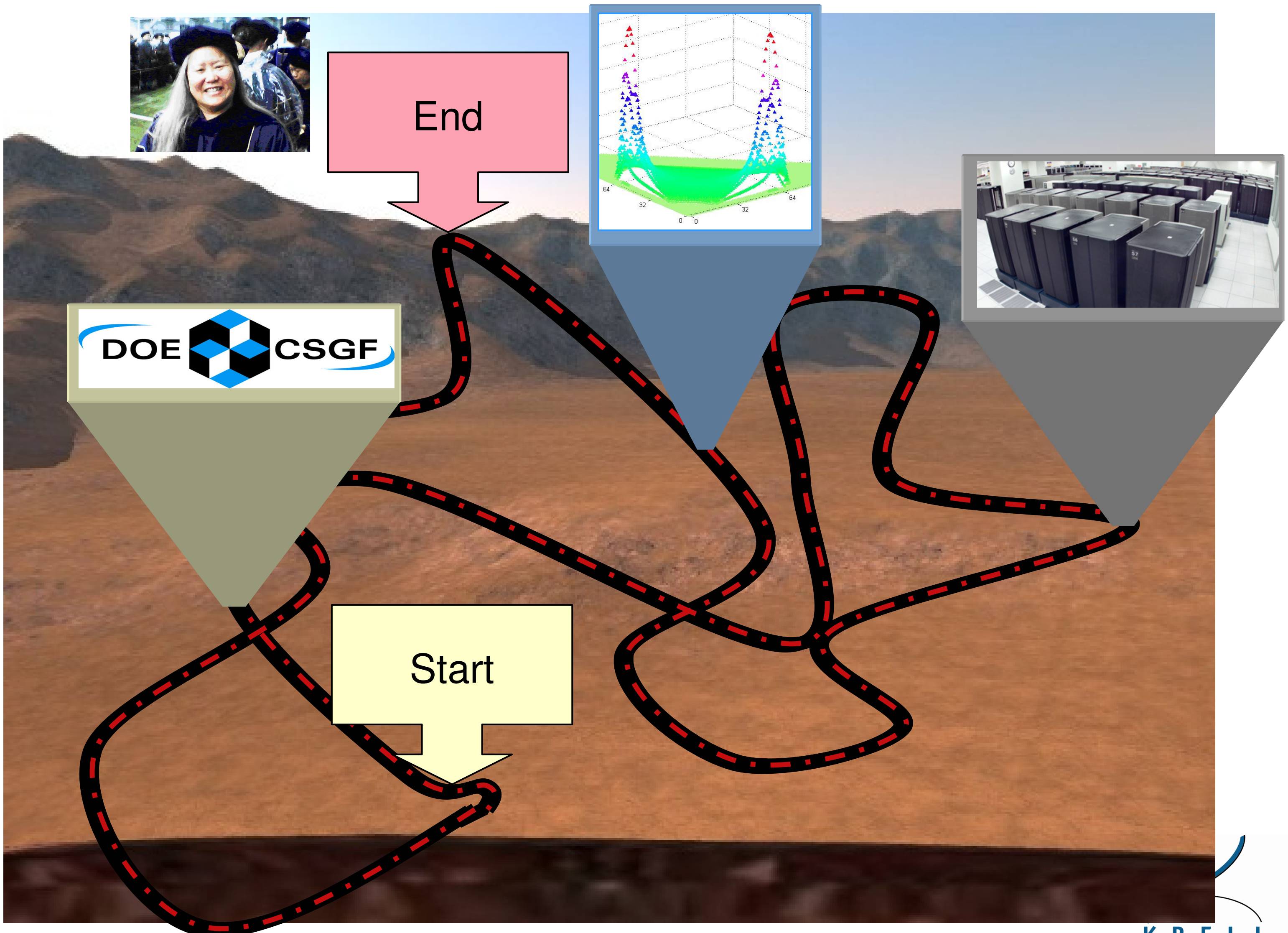
Pathways to Ph.D.

Pathways to Ph.D.

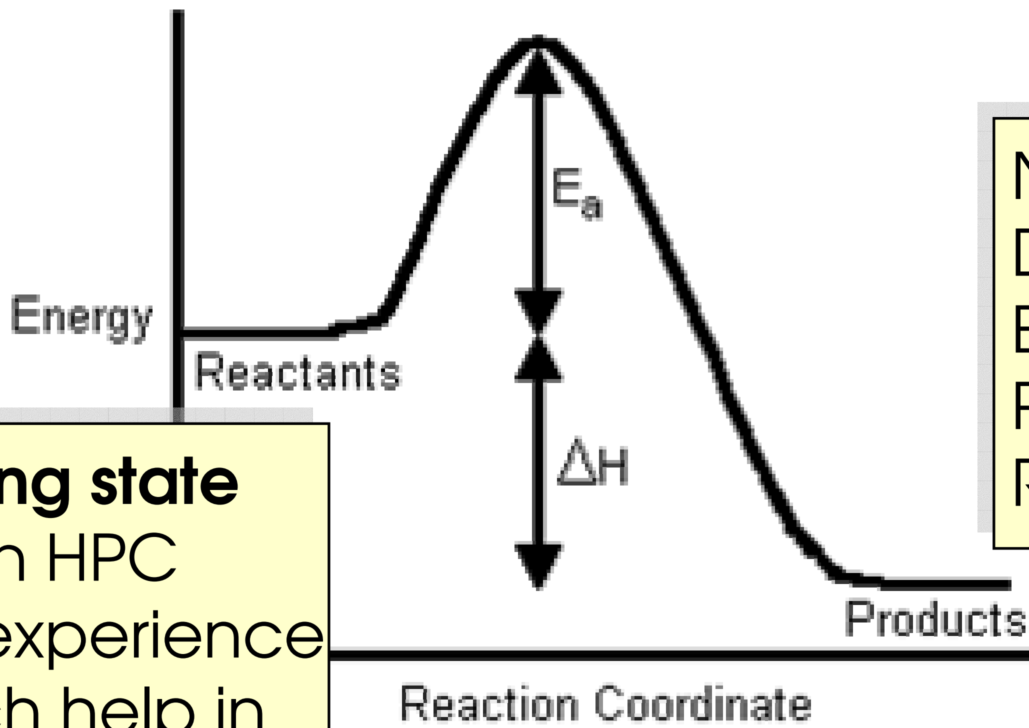
Pathways to Ph.D.



Ph.D. Roadmap



Activation Energy



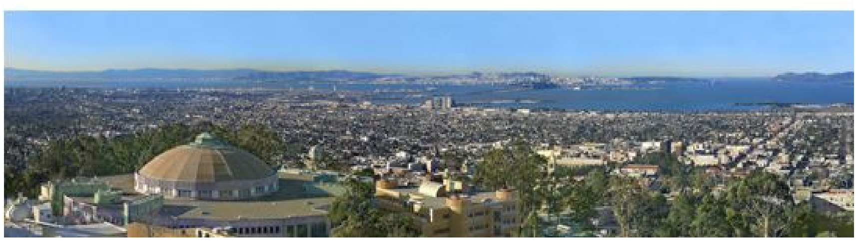
My starting state
Interest in HPC
but, no experience
Not much help in
Immediate sphere

New knowledge
Discovery
Employment
Prestige
Rewarding work

Overcoming activation barrier

- CSGF
  - ACTS (Advanced CompuTational Software)
  - Practicum: LBNL
  - Supercomputer time grant at LBNL
  - Scaling reimbursement program

Advanced CompuTational Software



- Tools for HPC development
  - Numerical
  - Code Development
  - Code Execution
  - Library development
- 9^{th} Annual Workshop
  - LBNL
  - Workshop Dates: August 19-22, 2008
  - Application deadline: June 20, 2008

http://acts.nersc.gov/events/Workshop2008/

ACTS Tools

Numerical Tools

- Aztec
- Hypre
- OPT++
- PETSc
- ScaLAPACK
- SLEPc
- SUNDIALS
- SuperLU
- TAO

Tools for Code Development

- Global Arrays
- Overture

Tools for Code Execution

- CUMULVS
- TAU

Tools for Library Development

- ATLAS

LBNL NERSC Center

- National Energy Research Scientific Computing Center (NERSC)
- ERCAP (Energy Research Computing Allocations Process) system for managing allocation requests
- Start up allocation grant 2004
- Renewals 2005, 2006, 2007

Year	Allocation Award (Hrs)
2004	20,000
2005	20,000
2006	20,000
2007	80,000

Summary of Usage

Year	Used (hrs)	Charged (hrs)
2004	466	466
2005	27,288	27,288
2006	307,265	175,427
2007	99,102	54,506

Note: 50% discount for 768+ processor jobs

Scaling Reimbursement Program

- 2.5 million MPP hours set aside
- New scaling projects
- 64 or more Seaborg nodes (1,024+ processors)

Outline

- Pathways to Ph.D..
- Overcoming the activation barrier
- **How HPC impacted my research**
- A short survey

A little background

- **Thesis:**

  "Computational studies of macroscopic superposition states in gaseous atomic Bose-Einstein Condensates in multiple wells"

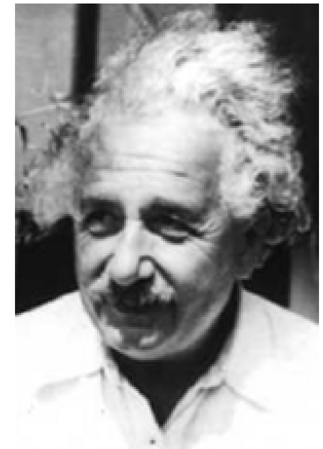
Brief intro to gaseous BEC

1924: predicted by
Bose & Einstein

1995: First realized in lab

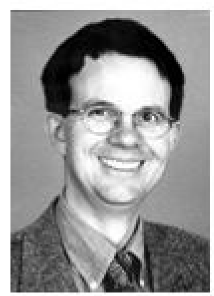
2001: Nobel prize to
Cornell, Ketterle,
Wieman

Satynathra Bose

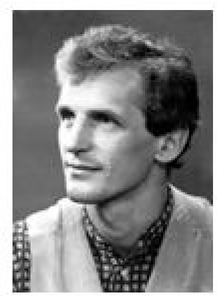


Albert Einstein

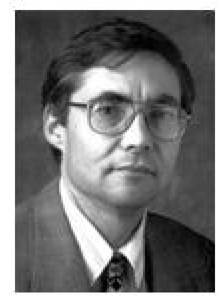
The Nobel Prize in Physics 2001



Eric A. Cornell



Wolfgang Ketterle



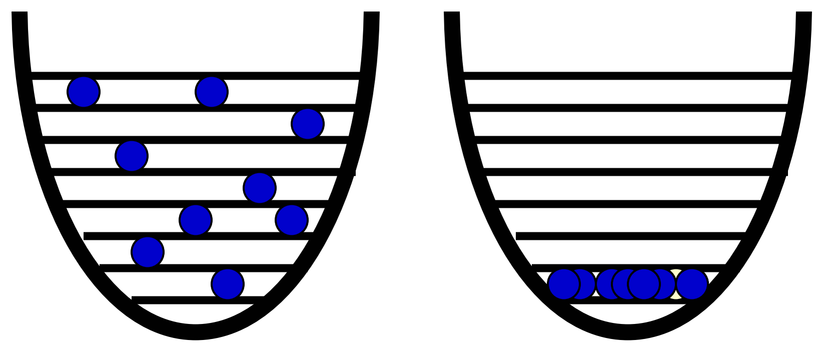
Carl E. Wieman

What is Bose-Einstein condensation?

- Normally, cooled gases undergo phase transition to liquid or solid
- However, when Bose gases are really cold and very dilute, undergo special phase transition called Bose-Einstein Condensation
  - BEC: 10^15 particles/cm^3 vs.
  - air: 10^19 particles/cm^3 air

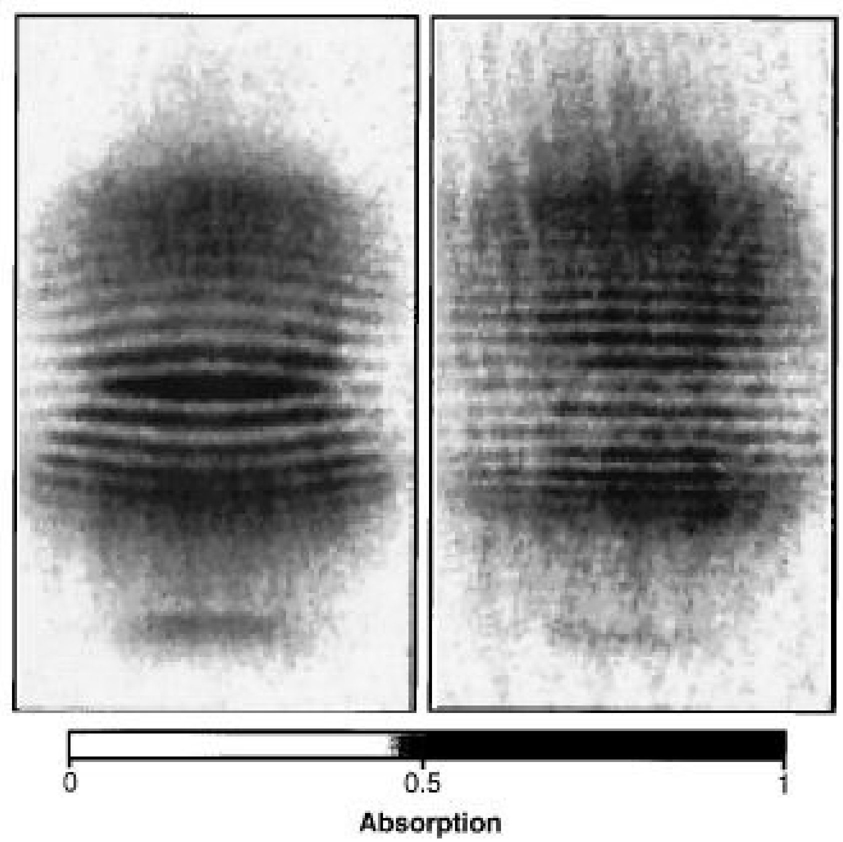
Bose-Einstein condensation

- Cooling dilute gaseous atoms causes Bose-Einstein condensation
- Condense into lowest energy state
- Described by single wave function
- Behave like a single macroscopic quantum object



Coherence: Interference experiment

- **Science, 275, 1997, Ketterle and co-workers**
- **Demonstrated BEC behaves as single macroscopic quantum object**
  - **Wave-like behavior of gaseous atoms**
  - **Coherence**



SCIENCE • VOL. 275 • 31 JANUARY 1997

What is a Schrödinger cat?

- **Thought experiment to illustrate strange consequences of applying quantum mechanics to large objects:**
  - — cat in entangled state
  - — simultaneously dead and alive
- **Entangled states have been detected in lab:**
  - — Photons
  - — Four ions
  - — Cold atoms in optical lattices

Source: In Search of Schrodinger's Cat, John Gribbin

Why interesting?

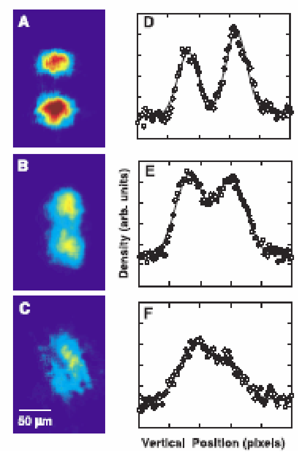
- **Entangled states are essential resource for quantum computing:**
  - —**Classical bits are on OR off**
  - —**Quantum bits are on AND off**
- **Still a long way to go but…**

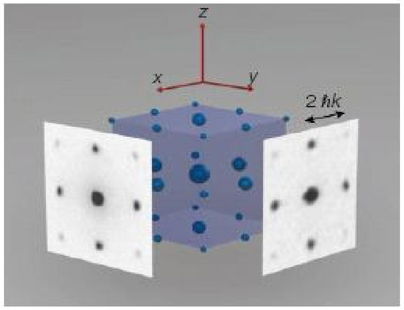
Schrödinger cats & BEC

- Why try to make Schrödinger cat states with a BEC?
  - Added stability?
    - coherence properties
    - macroscopic nature
- How can we generate Schrödinger cat states with a BEC?
- How large of a Schrödinger cat state can we generate?

Experiments

- **Two experimental regimes**
  - **Large $\mathcal{N}$/M regime:**
    - **Kasevich: 1 dimensional multiwell array**
    - **~125-2000 particles in 12 sites**
  - **Small $\mathcal{N}$/M regime**
    - **Hänsch: 3 dimensional optical lattice**
    - **~1-3 atoms in 150,000 sites**





With **$\mathcal{N}$ = number particles**
M = number wells

Novel approach

- **HPC allowed:**
  - Use of more rigorous techniques
  - Investigation of large systems

Time propagation

$$\sum_k [H]_{jk} c_k(t) = i \frac{dc_j(t)}{dt}$$

- **Computational challenge:**
  - **—Matrix-vector multiplication**

Scaling issues

$$\sum_k [H]_{jk} c_k(t) = i \frac{dc_j(t)}{dt}$$

where H is an N by N matrix with

$$N = \frac{(\mathcal{N} + M - 1)!}{\mathcal{N}!(M-1)!}$$

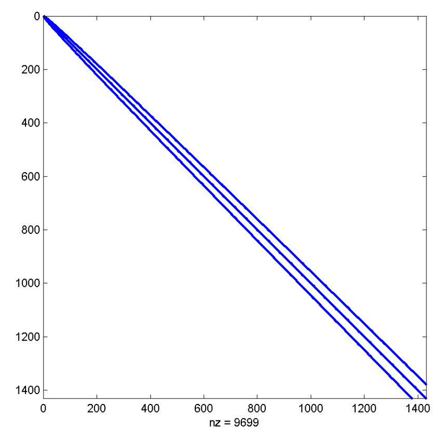
$$\text{where}: \mathcal{N} = \text{number of particles},$$
$$M = \text{number wells}$$

4-Well System

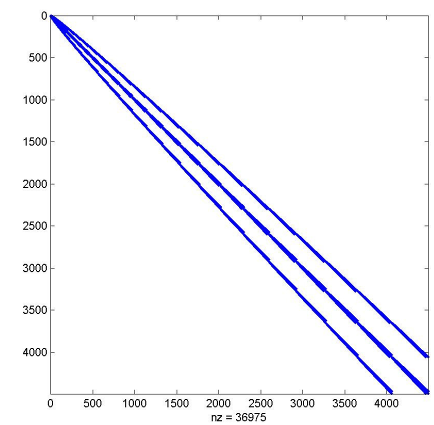
$\mathcal{N}$	N
16	969
32	6,545
64	47,905
128	366,145
256	2,862,209
512	22,632,705

Hamiltonian matrix sparsity pattern

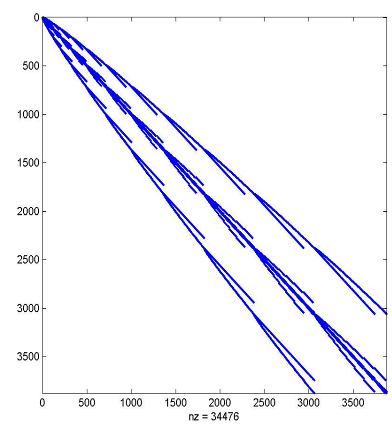
Sparsity pattern
- 52 particles in 3 wells
- 1431x1431 matrix
- 9,699 non-zero entries



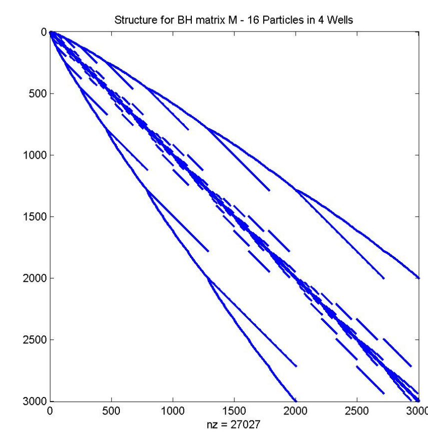
Sparsity pattern
- 28 particles in 4 wells
- 4495x4495 matrix
- 36,975 non-zero entries



Sparsity pattern
- 15 particles in 5 wells
- 3876x3876 matrix
- 34,476 non-zero entries



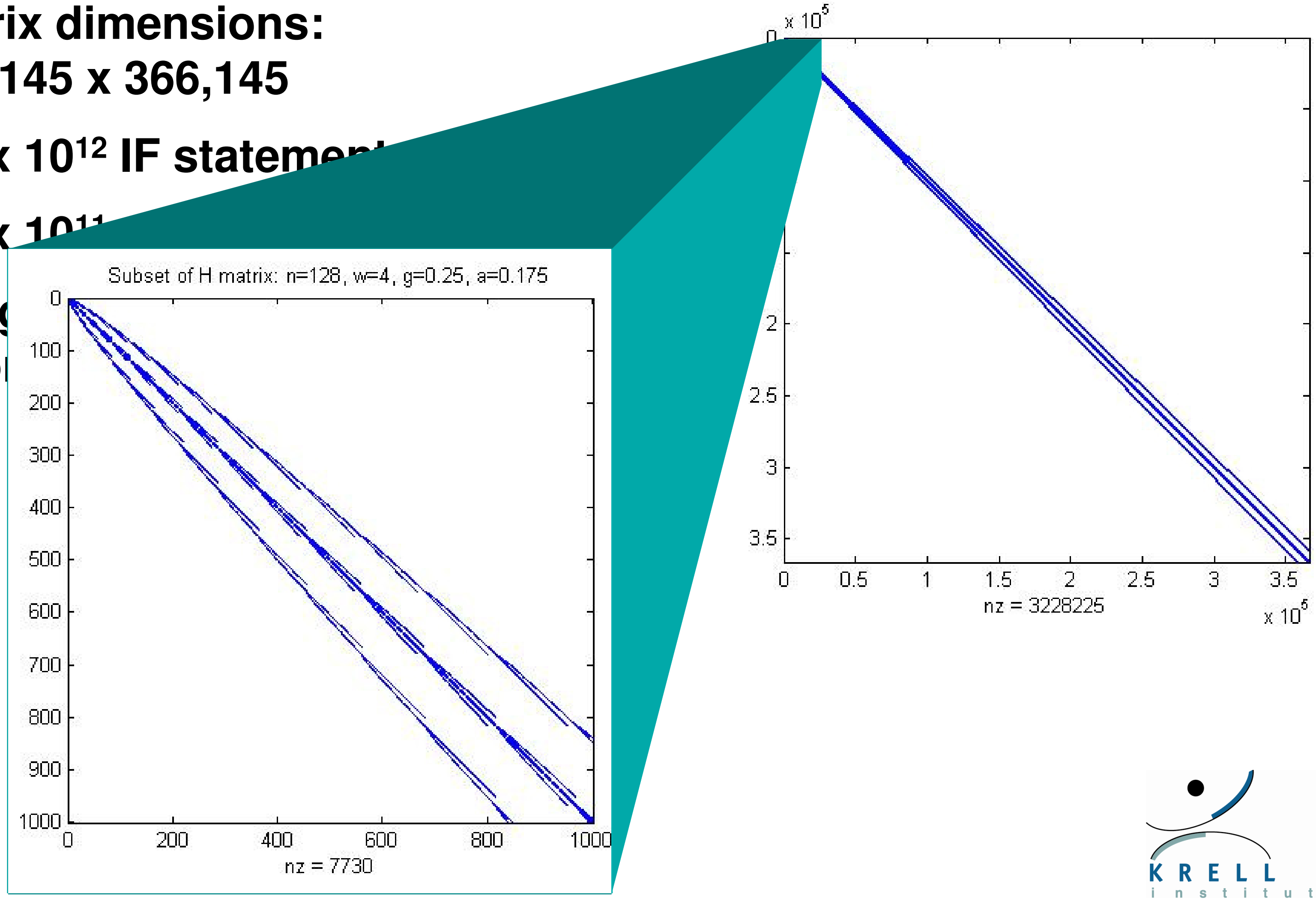
Sparsity pattern
- 10 particles in 6 wells
- 3003x3003 matrix
- 27,027 non-zero entries



DOE CSGF

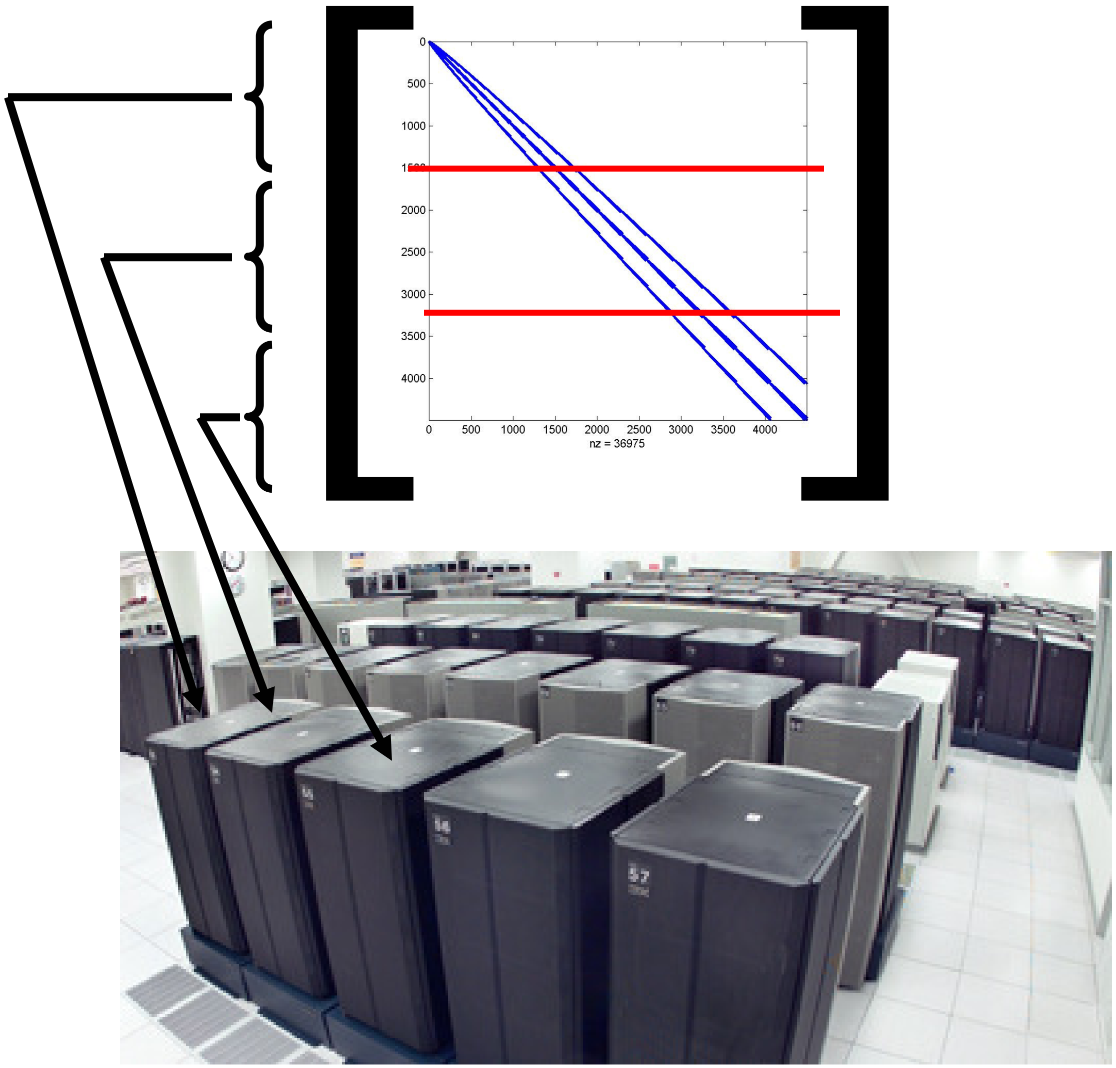
128 particles in 4 wells

- **Matrix dimensions: 366,145 x 366,145**
- **~ 2 x 10^{12} IF statemen**
- **~ 5 x 10**
- **Roug algo**



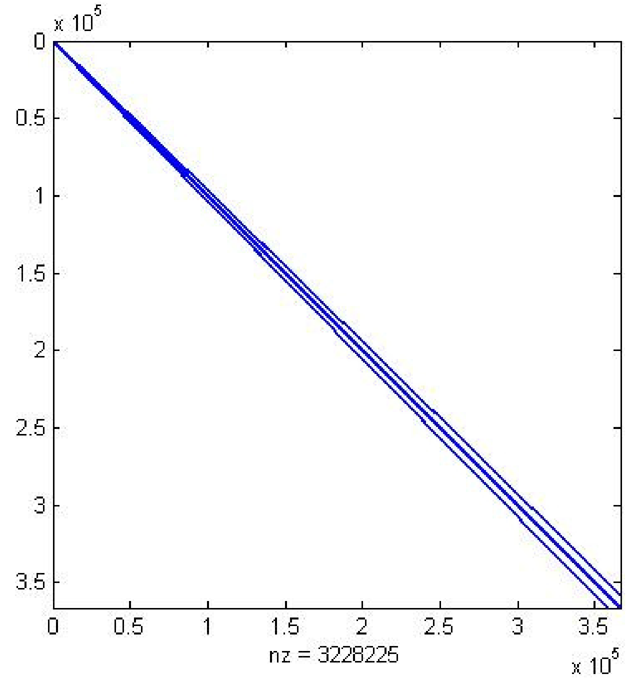
KRELL institute

Parallel algorithm for matrix generation



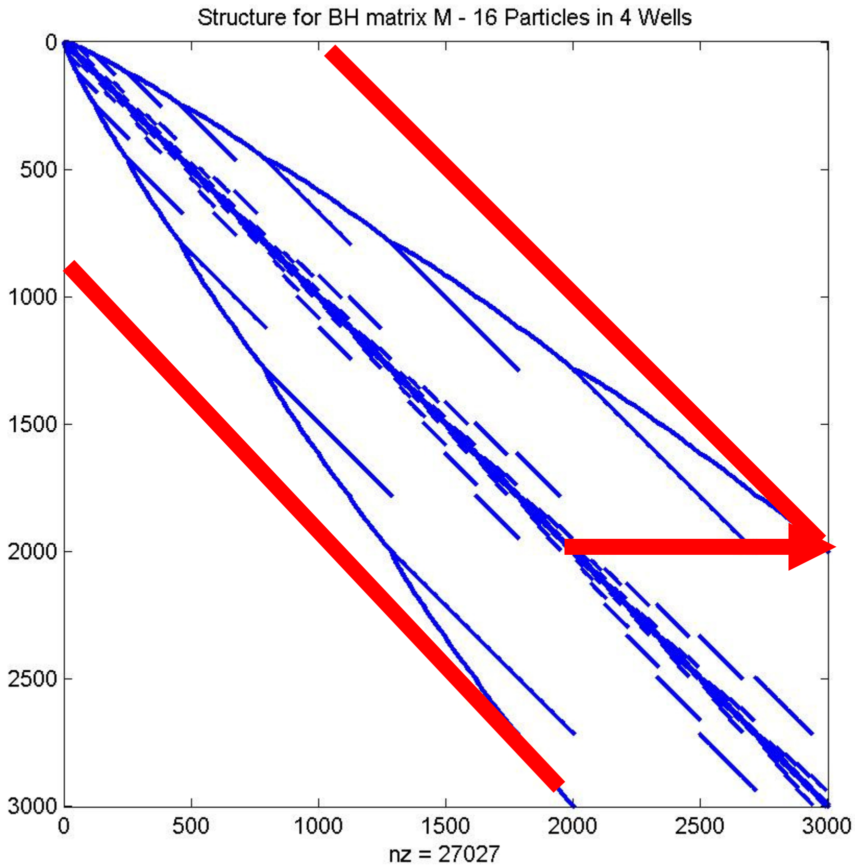
Parallel algorithm

- 128 particles in 4 wells
- Matrix dimensions: 366,145 x 366,145
- ~ 2 x 10^{12} IF statements
- ~ 5 x 10^{11} assignment statements
- Rough estimate for sequential algorithm: 33 days



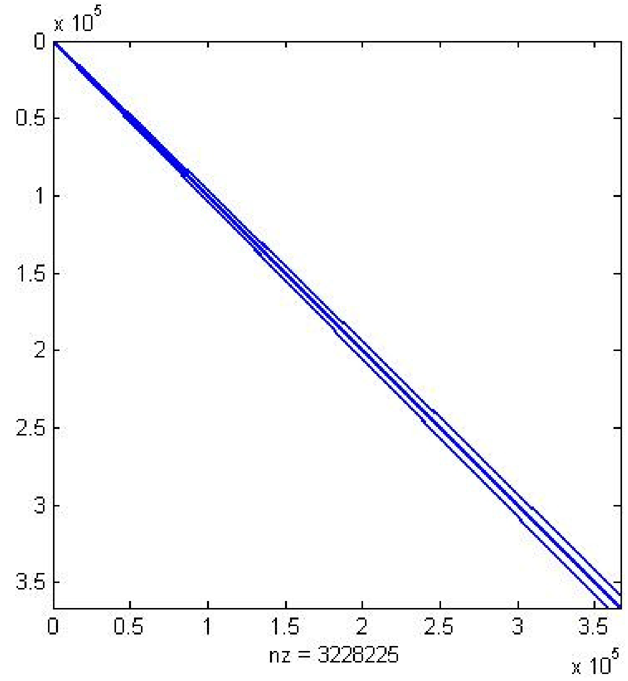
- Actual time for parallel algorithm on 112 processors: 33 min

Further speed up for matrix generation

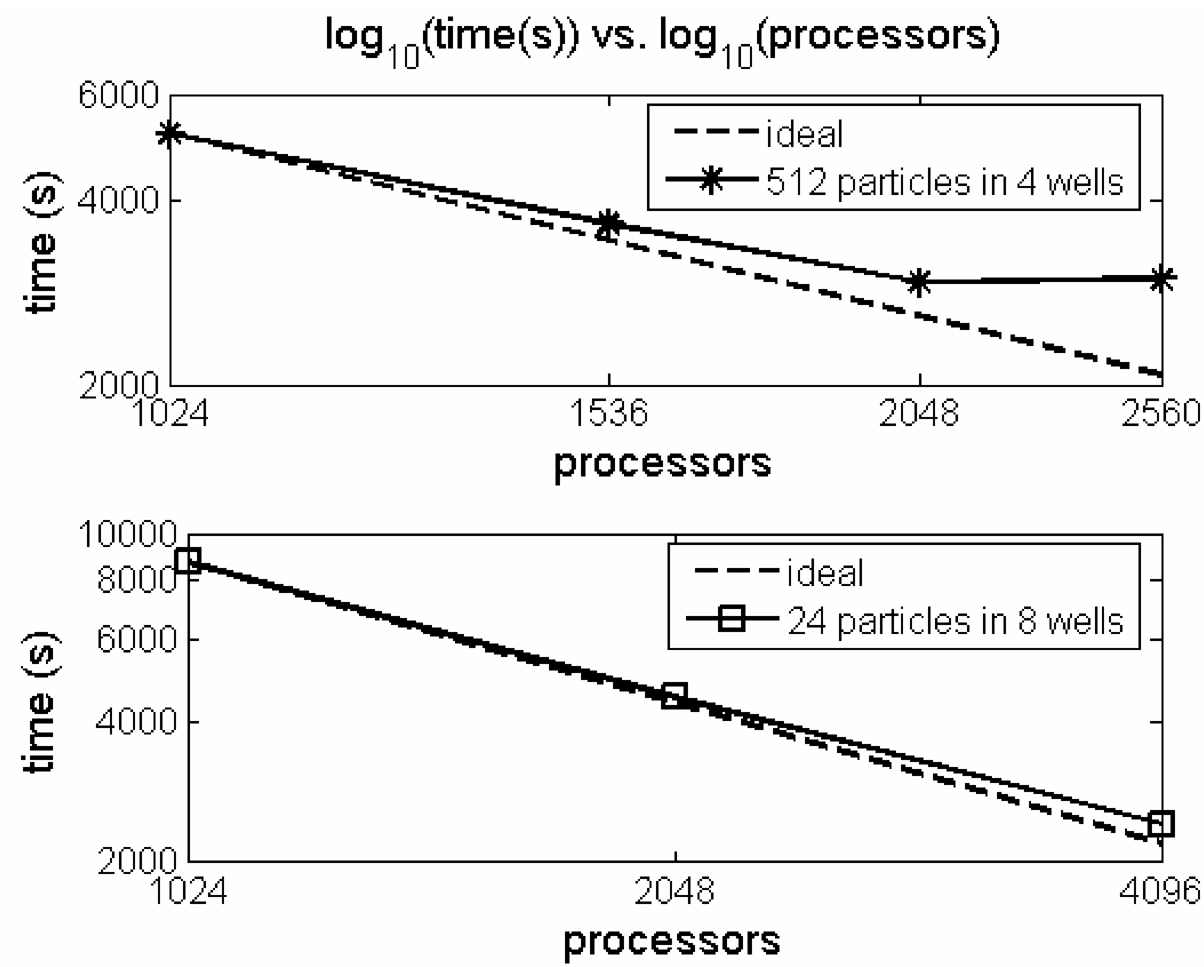


Parallel algorithm

- 128 particles in 4 wells
- Matrix dimensions: 366,145 x 366,145
- ~ 2 x 10^{12} IF statements
- ~ 5 x 10^{11} assignment statements
- Rough estimate for sequential algorithm: 33 days
- Simple embarrassingly parallel: 33 min.
- *Actual time after all enhancements on 112 processors: 53 seconds*



Speed up curve parallel algorithm



Scaled codes to 1000's of processors

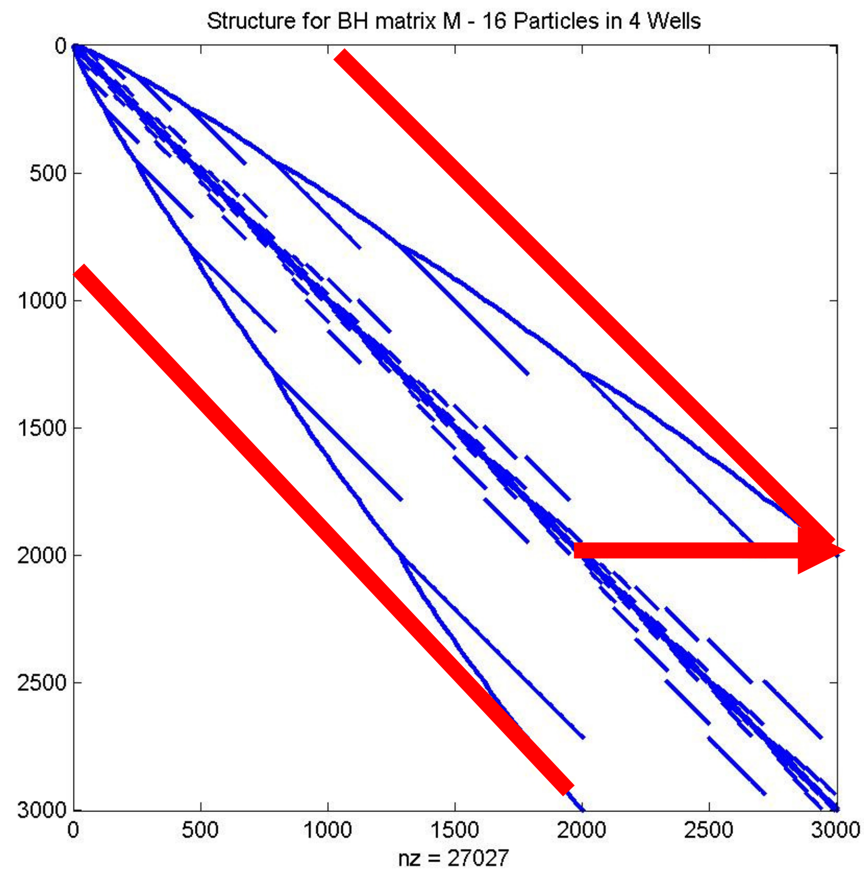
- **Leung, M.A., Reinhardt, W.P.**

  "Efficient parallel implementation of the Bose-Hubbard model: Exact numerical ground states and dynamics of gaseous Bose-Einstein Condensates"

  Comp. Phys. Comm., 177 (4), (2007), 348-356

Cool problems to solve

- **Brute force solution → insights for more elegant & efficient solution to problem**



Obtained results for big systems

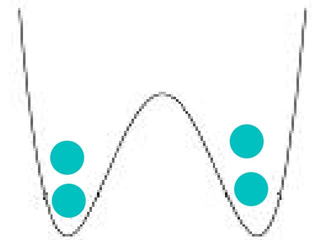
- **Provided evidence of cat states in these systems two experimental regimes:**

$\mathcal{N}$ Particles	M wells	N dimension
512	4	22,632,705
24	8	2,629,575

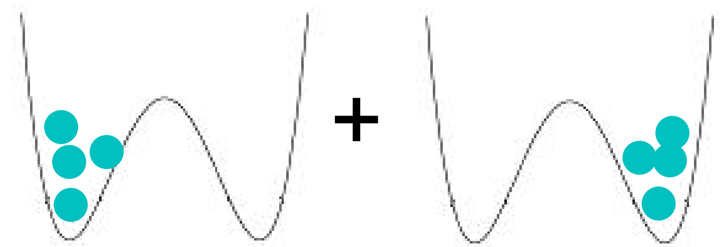
Cat states in two wells

Double Well - 4 particles:

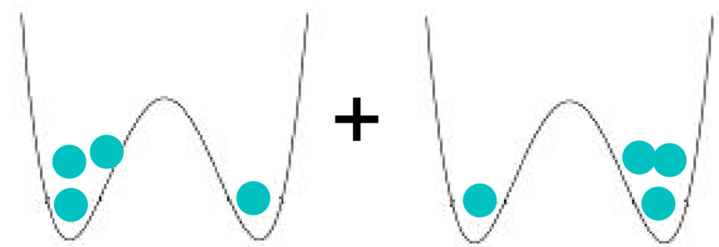
$$\left|\Psi\right\rangle_{inital} = \frac{1}{\sqrt{2}}\left[\left|\frac{\mathcal{N}}{2},\frac{\mathcal{N}}{2}\right\rangle\right]$$



$$\left|\Psi\right\rangle_{extreme} = \frac{1}{\sqrt{2}}\left[\left|\mathcal{N},0\right\rangle + \left|0,\mathcal{N}\right\rangle\right]$$



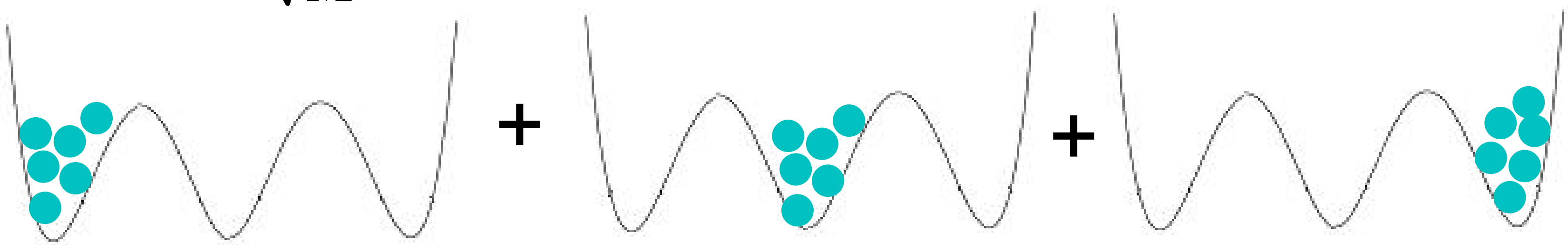
$$\left|\Psi\right\rangle_{squeezed} = \frac{1}{\sqrt{2}}\left[\left|\mathcal{N}-n,n\right\rangle + \left|n,\mathcal{N}-n\right\rangle\right]$$



Cat states in multiple wells

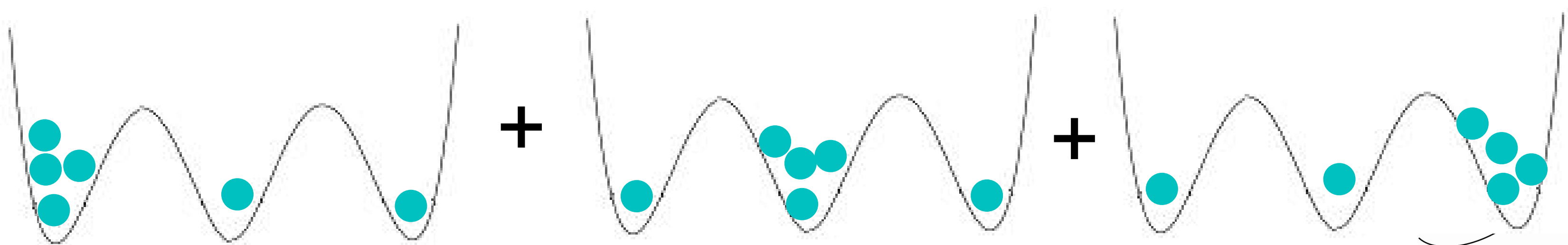
Multi Well:

$$|\Psi\rangle_{extreme} = \frac{1}{\sqrt{M}}\left[|\mathcal{N},0,\ldots,0\rangle + |0,\mathcal{N},0,\ldots,0\rangle + \ldots + |0,\ldots,0,\mathcal{N}\rangle\right]$$



$$|\Psi\rangle_{squeezed} = \frac{1}{\sqrt{M}}\left[|\mathcal{N}-jn,n,\ldots,n\rangle + |n,\mathcal{N}-jn,n,\ldots,n\rangle + \ldots + |n,\ldots,n,\mathcal{N}-jn\rangle\right]$$

$where\ n < \mathcal{N},\ j = M-1$



A new kind of cat state

8 Well Example 24 particles:

Expected:

$$\left|\varphi\right\rangle_{t=2.79} = \frac{1}{8}c(t)(\left|24,0,0,0,0,0,0,0\right\rangle + \left|0,24,0,0,0,0,0,0\right\rangle + \left|0,0,24,0,0,0,0,0\right\rangle + \left|0,0,0,24,0,0,0,0\right\rangle + \left|0,0,0,0,24,0,0,0\right\rangle + \left|0,0,0,0,0,24,0,0\right\rangle + \left|0,0,0,0,0,0,24,0\right\rangle + \left|0,0,0,0,0,0,0,24\right\rangle)$$

Found:

$$\left|\varphi\right\rangle_{t=2.79} = \frac{1}{8}c(t)(\left|6,0,6,0,6,0,6,0\right\rangle + \left|0,6,0,6,0,6,0,6\right\rangle)$$

General form:

$$\left|\Psi\right\rangle_{squeezed} = \frac{1}{\sqrt{M}}\left[\left|\frac{2\mathcal{N}}{M} - n, n, \frac{2\mathcal{N}}{M} - n, \ldots, n\right\rangle + \left|n, \frac{2\mathcal{N}}{M} - n, n, \ldots, \frac{2\mathcal{N}}{M} - n\right\rangle\right]$$

$$\text{where } n < \mathcal{N}$$

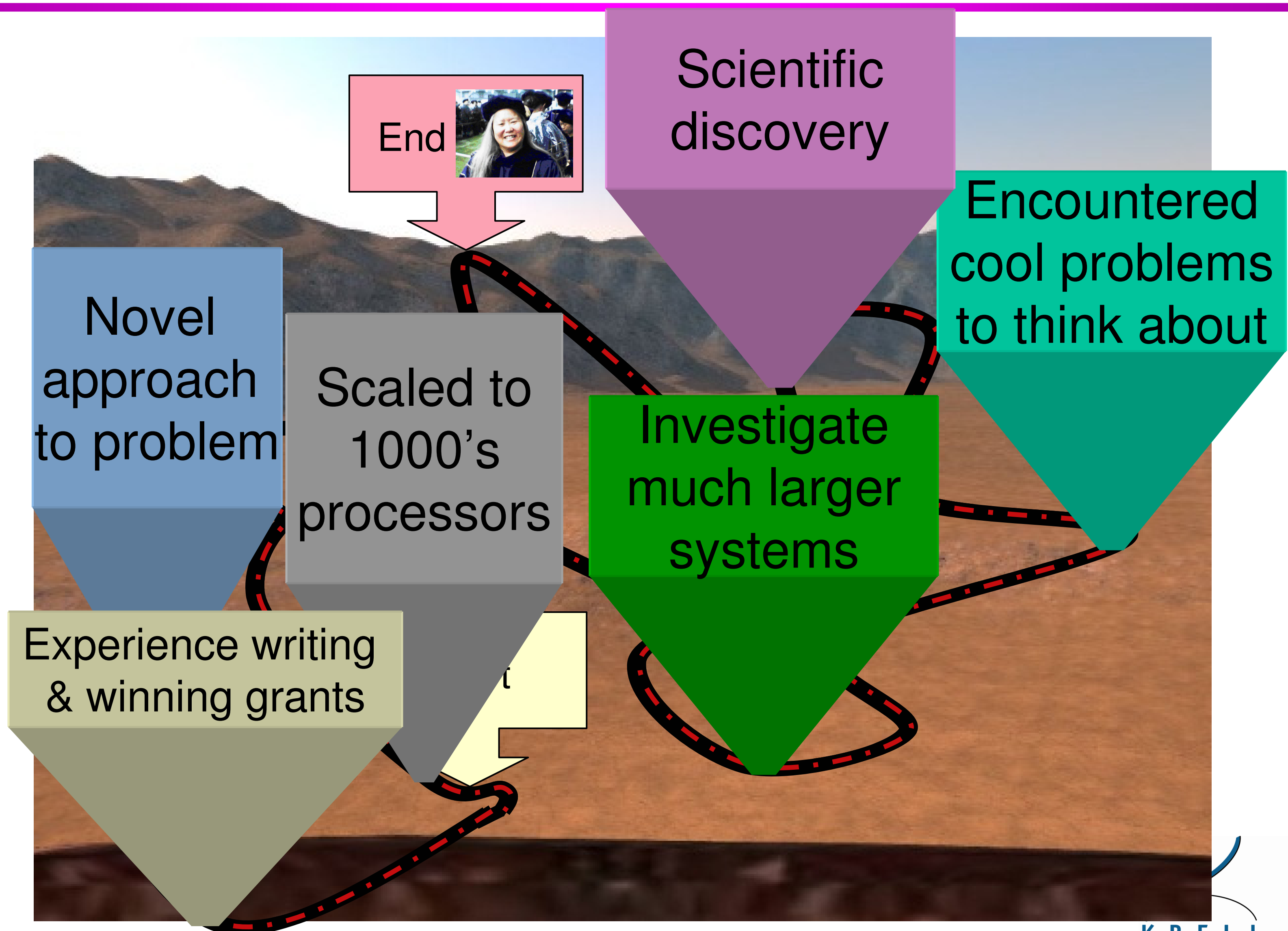
Excitement of discovery

- **Leung, M.A., Reinhardt, W.P.**

  "Dynamical studies of entangled number states of the gaseous Bose-Einstein condensate and a new kind of macroscopic superposition state",

  in progress, to be submitted to Phys. Rev. A

HPC & my research

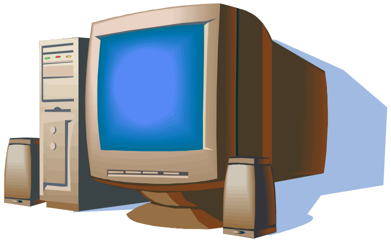


Informal survey

- Fellows:
  - How many have some level of interest in HPC?
  - How many interested in exploring HPC projects?
  - How many might want help?
- Alumnus
  - How many interested in exploring HPC?
- Alumnus, faculty, staff
  - How many working with HPC now?
  - How many interested in working with fellows?

Where are you computing now?

- **Goals of CSGF**
  - **Broaden vision of what machine you use to compute**
  - **Engage fellows, alumni, advisors in HPC**
  - **Stretching to most powerful platforms**



Interested?

- Focus group/information gathering session:
  - Wednesday 3:00, Monticello Room
- Special Session on HPC - Thursday

Moderator: Daniel Hitchcock, Office of Science, DOE

9:00-9:30	Barbara Helland, DOE Office of Science	DOE facilities for HPC
9:30-10:00	Robert Harrison, ORNL	Scientific Discovery Advanced by HPC
10:00-10:30	David Skinner, NERSC	SciDAC Outreach Center
10:30 - 11:00		Open discussion on HPC

Acknowledgements

- William P. R
- Thesis com
  - Loyce A
  - D. Mich
  - Xioaso
  - Bruce
  - Oleg
- DOE C
- NERS