Making Schrödinger cat states from Bose Einstein Condensates (BECs) with massively parallel processors

Computational Science Graduate Fellowship (CSGF) Conference

June 22, 2005

Mary Ann Leung

University of Washington

What is a Schrödinger Cat state?

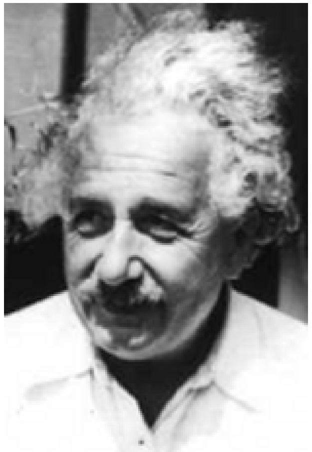
- Thought experiment to illustrate strange consequences of applying quantum mechanics to large objects:
  - cat in entangled state
  - simultaneously dead and alive
- Entangled states have been detected in lab:
  - Photons
  - Four ions
  - Cold atoms in optical lattices
  - Superconducting Josephson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

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

Brief intro to gaseous BEC

- 1924: New state of matter predicted by Bose & Einstein
- 1995: First realized in lab by Cornell & Weiman at CU Boulder & NIST and Ketterle at MIT
- 2001: Nobel prize awarded to Cornell, Ketterle, Wieman

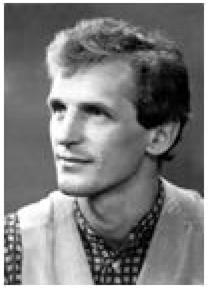
Satynathra Bose



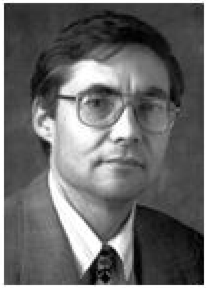
Albert Einstein

The Nobel Prize in Physics 2001

Eric A. Cornell



Wolfgang Ketterle

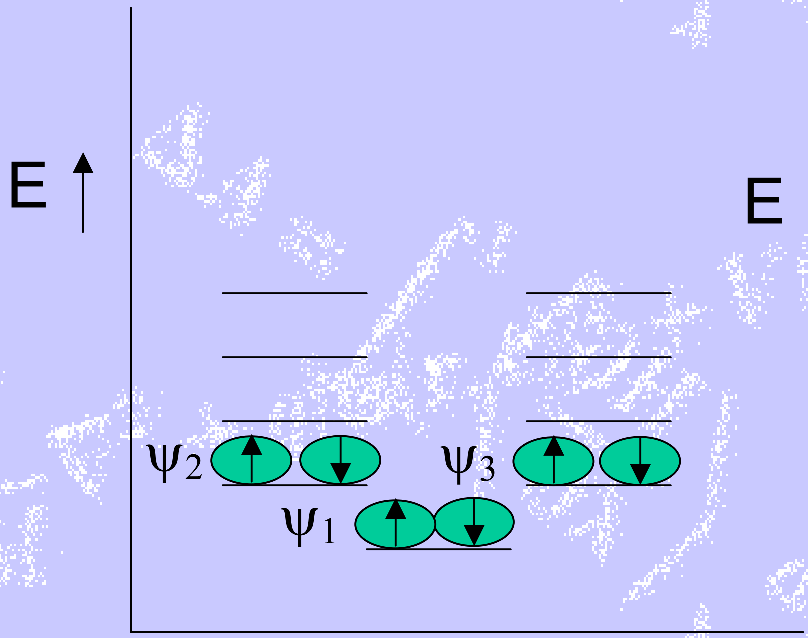


Carl E. Wieman

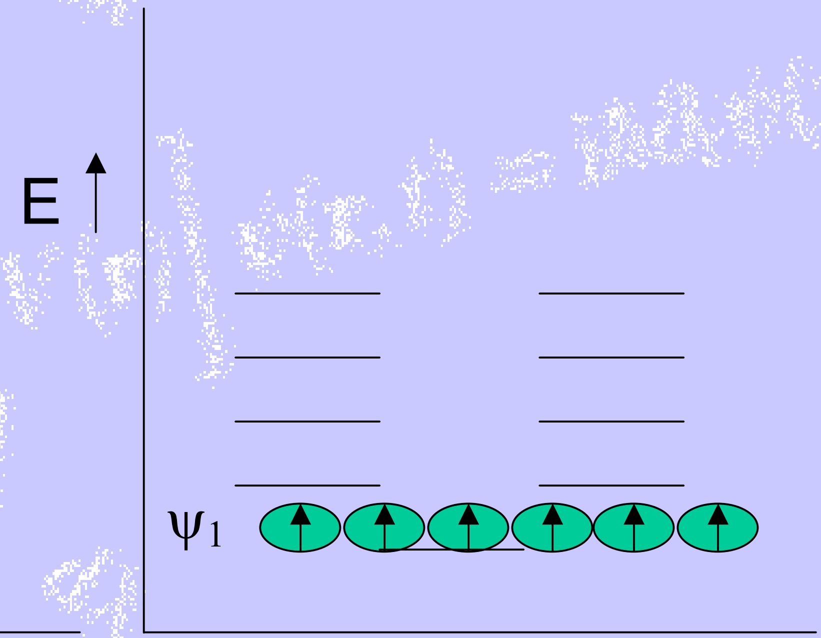
What is Bose-Einstein Condensation?

- Normally, when gases cooled undergo phase transition to liquid or solid
- However, when 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
- Condense into lowest energy state
- Described by single wavefunction
- Macroscopic quantum object

Fermions and bosons and the Pauli exclusion principle



Fermions



Bosons

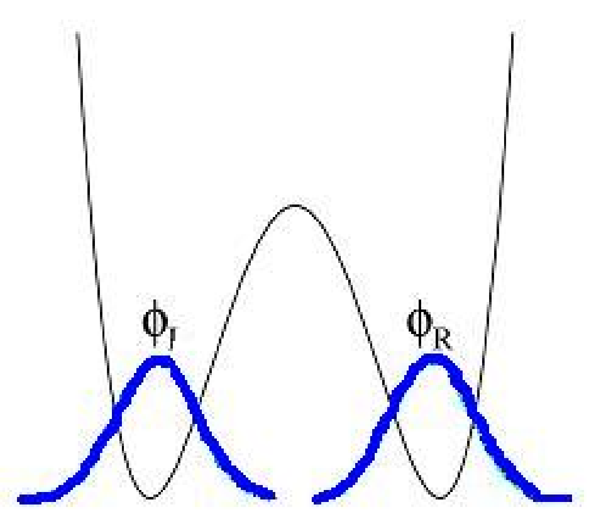
Why interesting?

- Macroscopic nature of BEC makes it ideal for exploring fundamental properties of quantum mechanics such as entangled states
- 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 cat states and 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?

Background theory: BEC in a double well

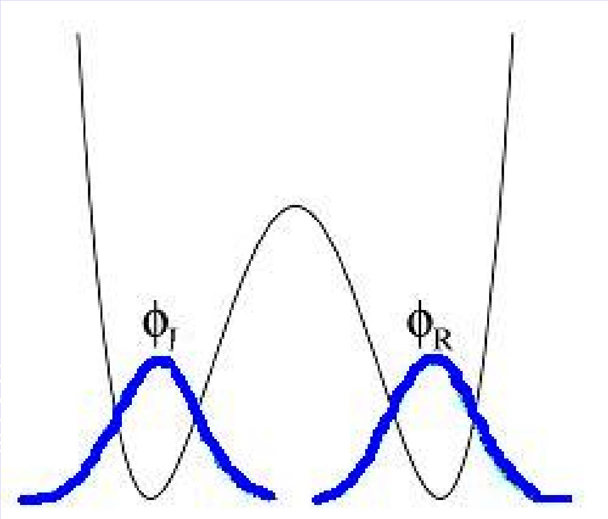


- Simplest lattice configuration
  - J. Phys B., 36, 2003, L265-L272, Mahmud, K., Perry,H., Reinhardt, W.P.
  - Phys. Rev. A.. 71, 23615, 2005, Mahmud, K., Perry,H., Reinhardt, W.P.

Schrödinger Equation

- Time Dependent:

$$\hat{H}\left|\Psi(t)\right\rangle = i\frac{d\left|\Psi(t)\right\rangle}{dt}$$



- Bose Hubbard Hamiltonian
  - tunneling
  - single particle energy
  - particle interaction energy

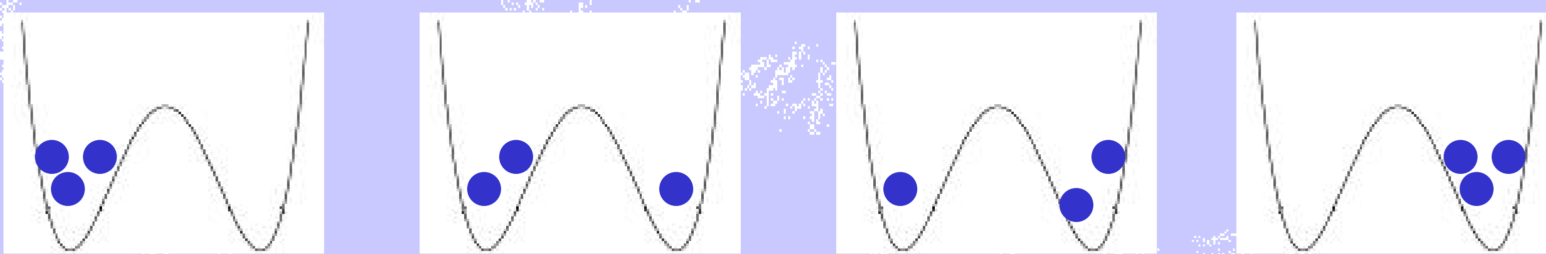
Fock basis states

- General form:

$$\left|\Psi(t)\right\rangle = \sum_{n_{L=0}}^{N} c_{n_L}(t)\left|n_L, N-n_L\right\rangle$$

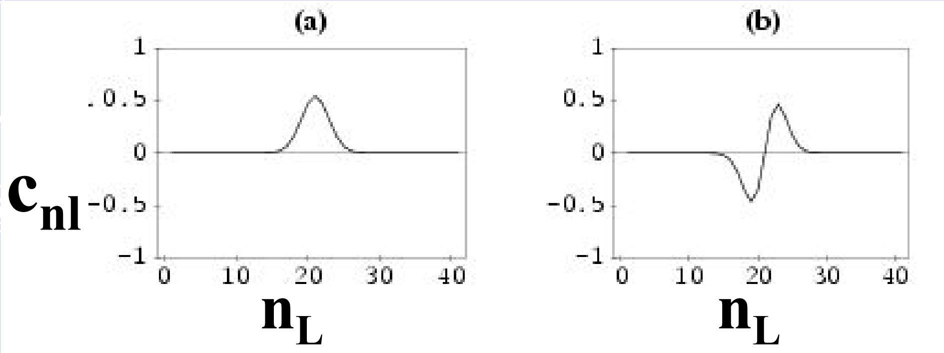
- For 3 particles in two wells

$$\left|\Psi\right\rangle = c_1\left|3,0\right\rangle + c_2\left|2,1\right\rangle + c_3\left|1,2\right\rangle + c_4\left|3,0\right\rangle$$



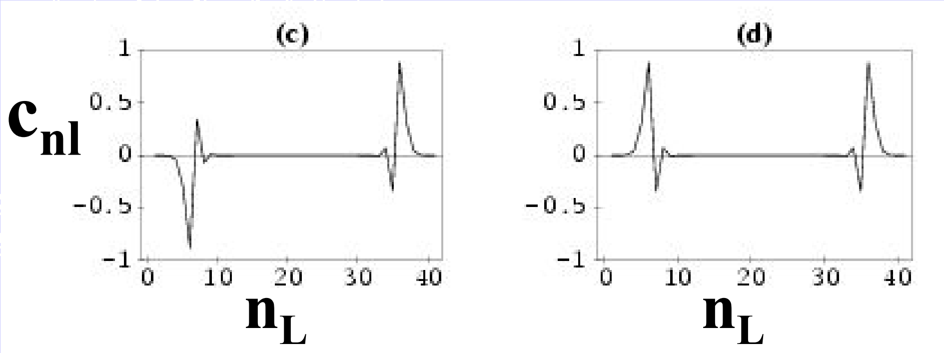
Finding the eigenvectors & eigenvalues

- Lowest states are Gaussian-like



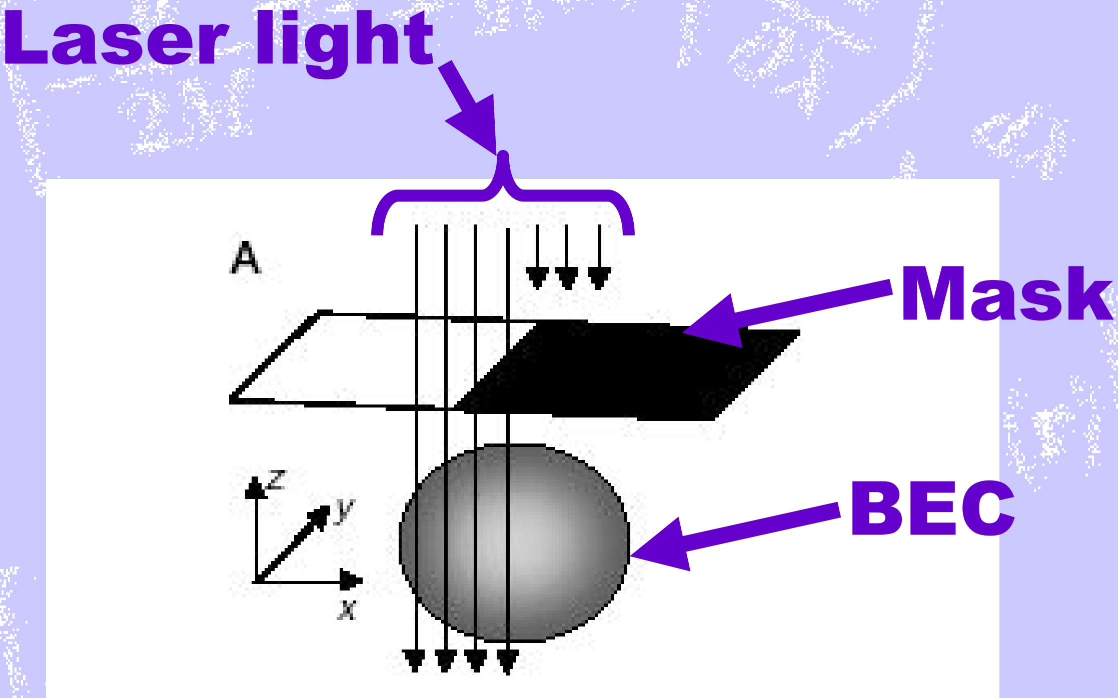
- Highest states are "cat-like"

$$c_1|5,35\rangle \pm c_2|35,5\rangle$$

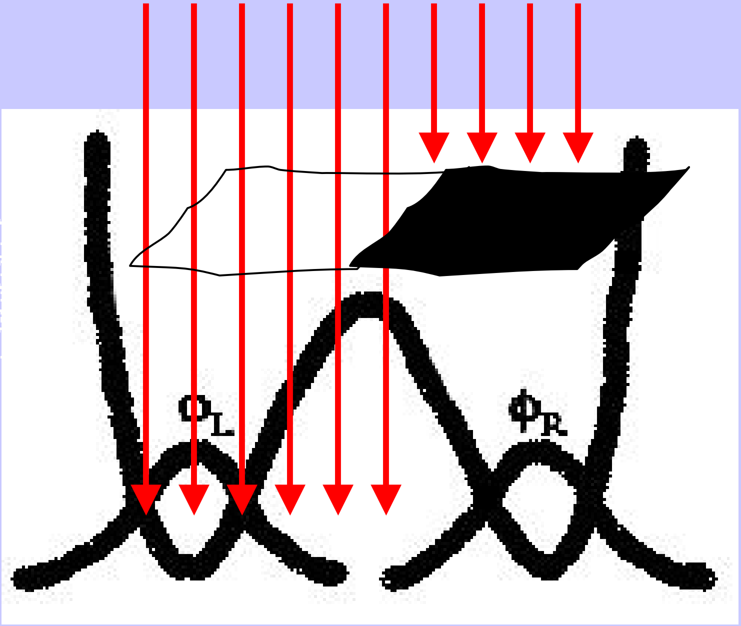


How can we generate these highly excited states?

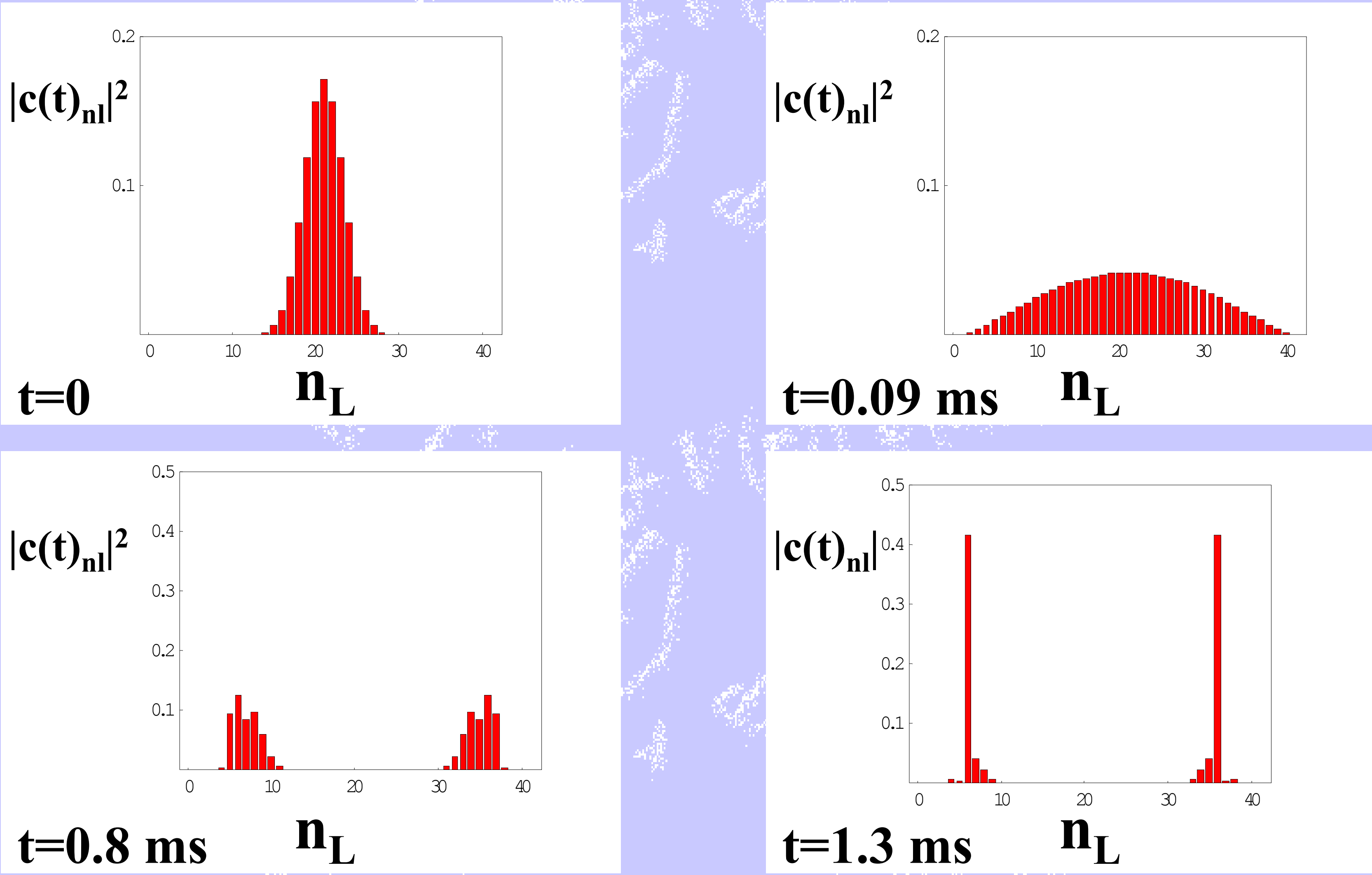
Phase imprinting



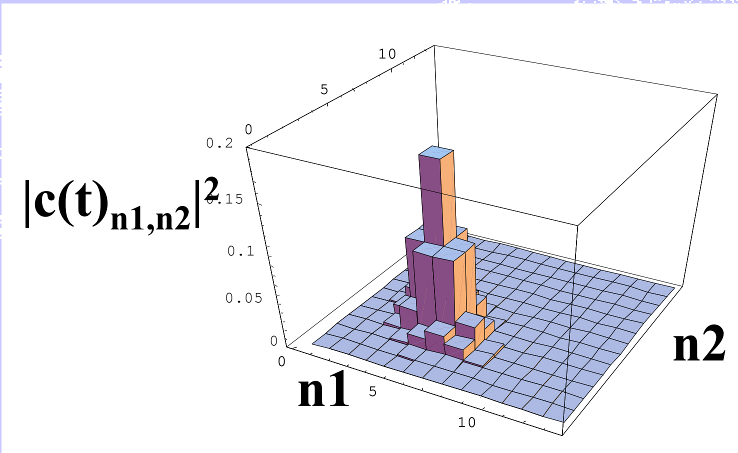
Source: Science 287, 2000, 97



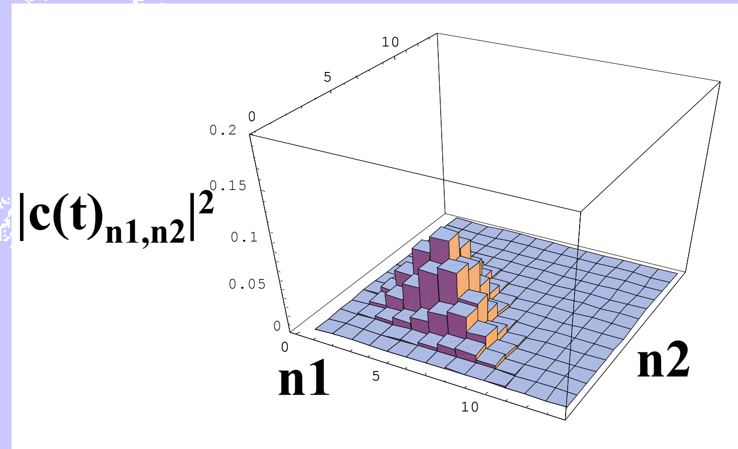
Time Evolve into cat state



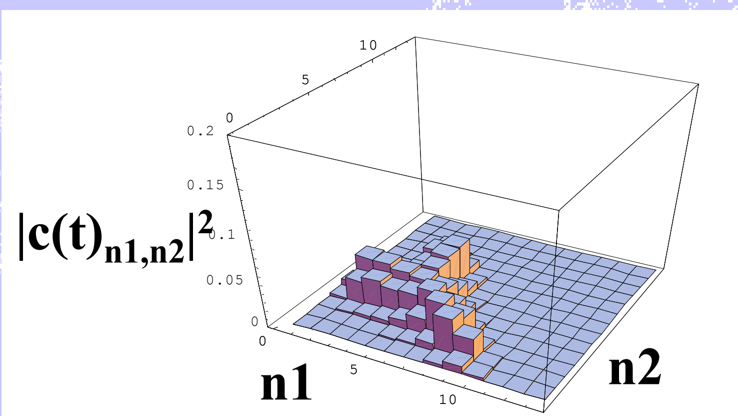
Evolution of three well system



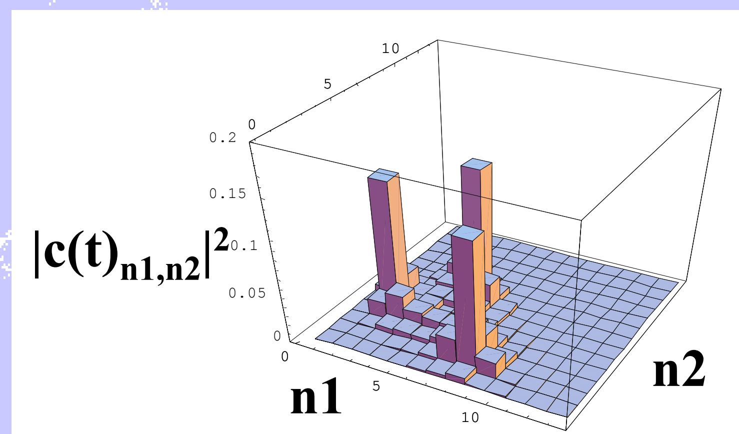
t=0



t=0.22 ms



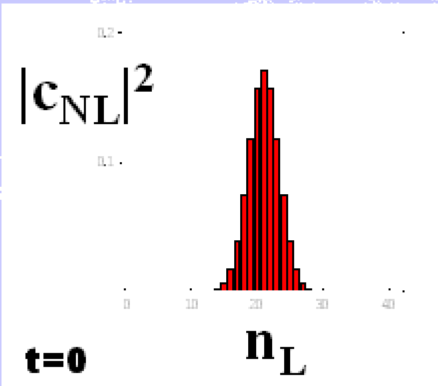
t=0.37 ms

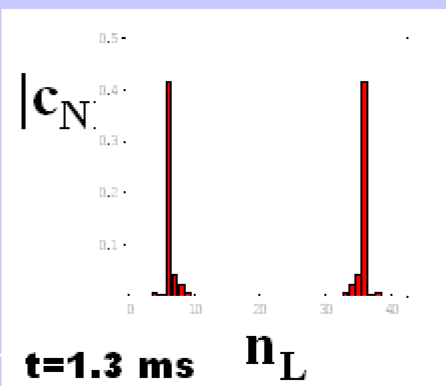


t=0.68 ms

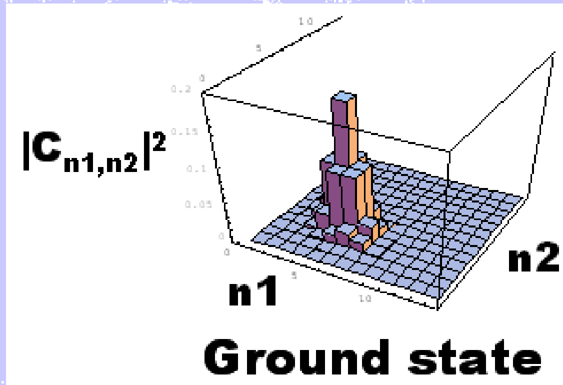
Evolution of 4-well system

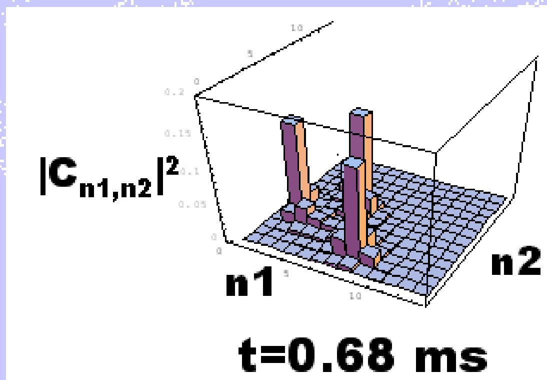
Two well



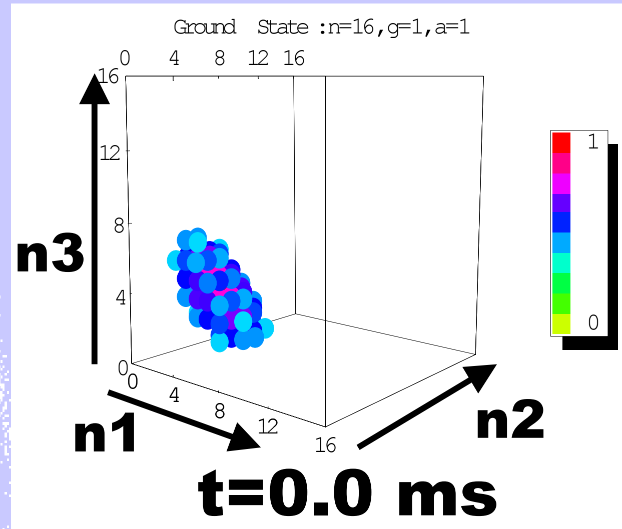


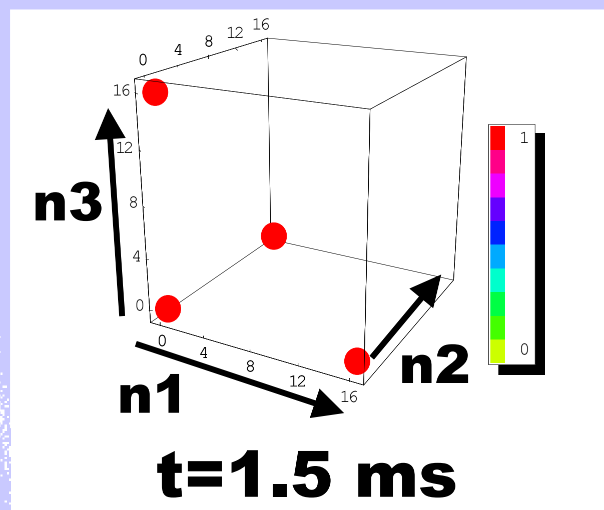
Three well





Four well





Extension to supercomputers

Submitted to Phys Rev A., Mahmud, K., Leung,M., Reinhardt, W.P.

Environment:
- LBNL, seaborg

Development platform:
- PETSc

NERSC's IBM SP, *Seaborg*, has 6,080 CPUs

Computational tasks

1. Determine non-zero matrix entries
2. Find lowest engery eignestate by complex time evolution
3. Phase imprint lowest energy states
4. Time propagate phase imprinted states to follow dynamics

Scaling issues

$$\sum_j [H]_{ij} c_j(t) = i \frac{dc_i(t)}{dt}$$

where H is an N by N matrix with

$$N = \frac{(n+w-1)!}{n!(w-1)!}$$

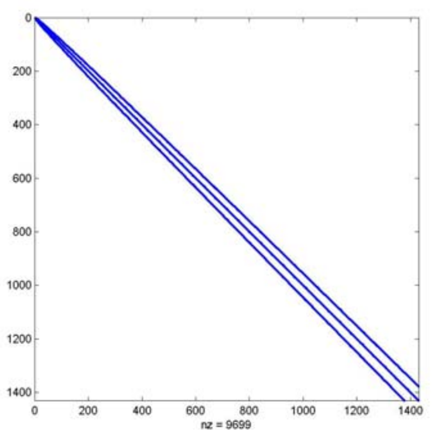
$$where: n = number\ of\ particles,$$
$$w = number\ wells$$

4-Well System

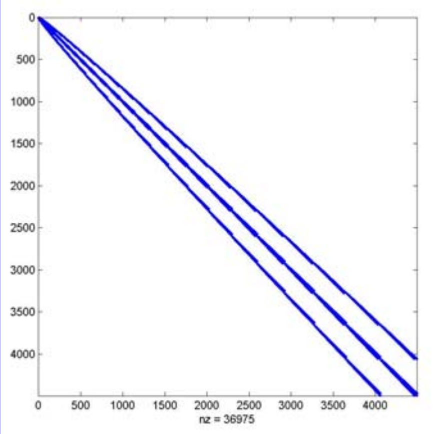
n	N
16	969
32	6,545
64	47,905
128	366,145
256	2,862,209

Hamiltonian matrix sparsity pattern

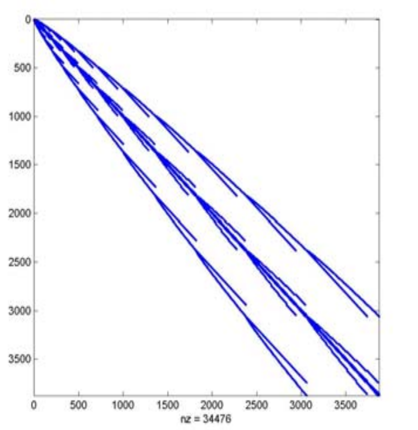
Sparsity pattern
- 52 particles in 3 wells
- 1431x1431 matrix
- 9,699 non-zero entries



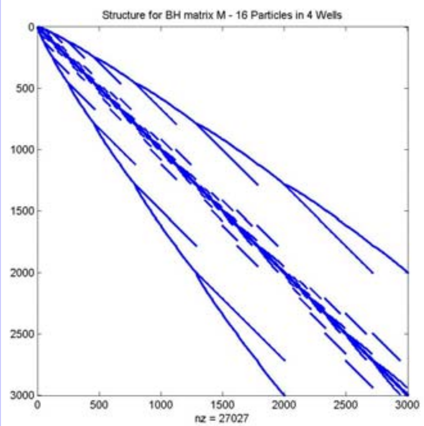
Sparsity pattern
- 28 particles in 4 wells
- 4495x4495 matrix
- 36,975 non-zero entries



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

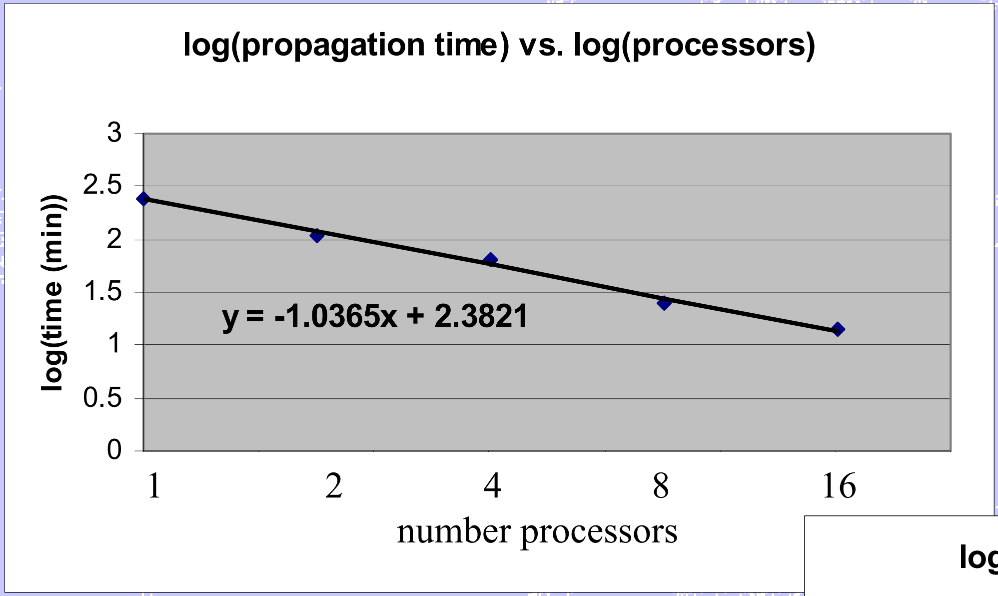


Time propagation

$$\sum_j [H]_{ij} c_j(t) = i \frac{dc_i(t)}{dt}$$

- Computational challenge:
  - Sparse matrix-vector multiplication

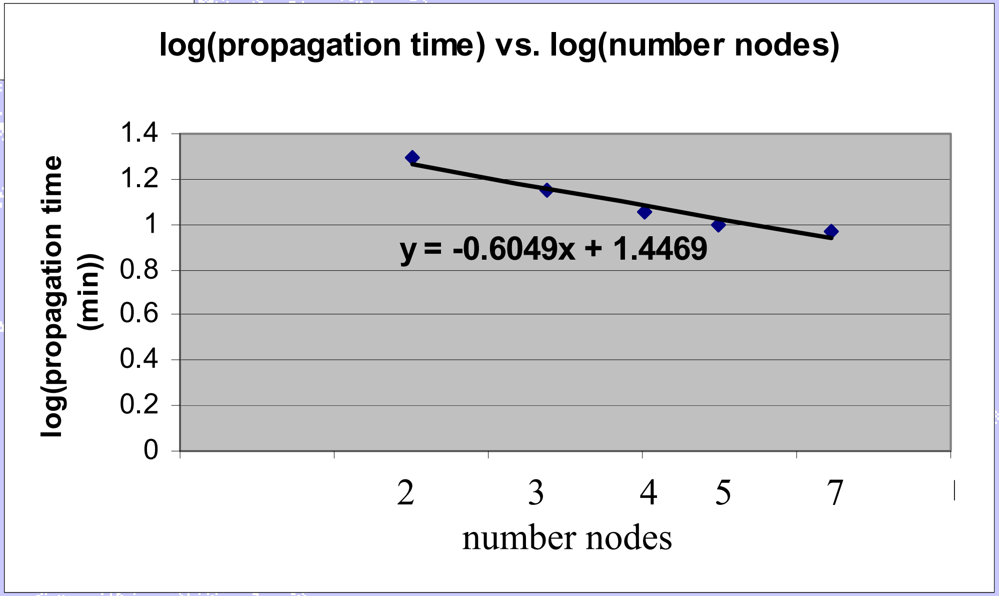
Speed up: time propagation



84 particles in 4 wells, 105,995 x 105,995

128 particles in 4 wells, 366145 x 366145

2-7 nodes with 16 proc/node



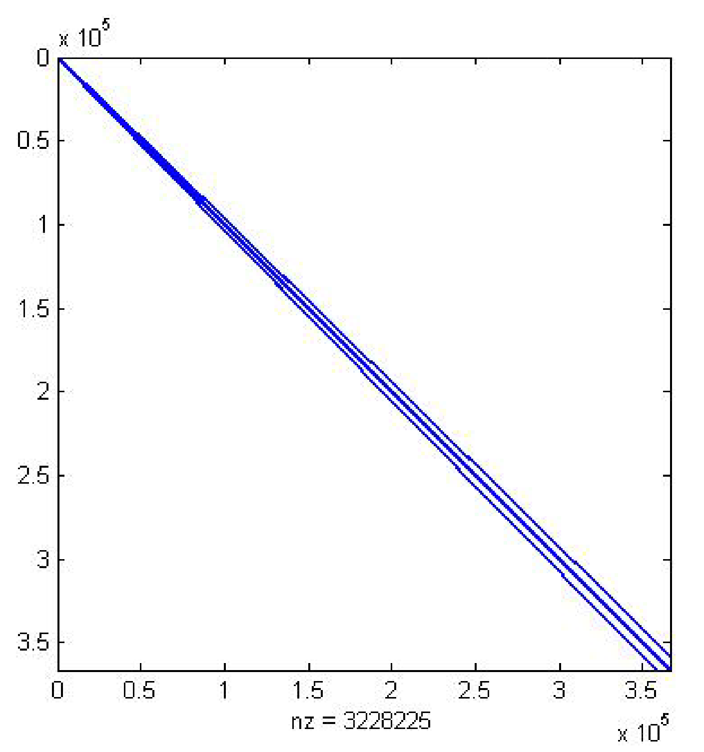
Unexpected computational challenge

- Computing matrix requires:
  - Determining all non-zero matrix entries
    - a single particle moving from one well to another well
    - number of particles in well

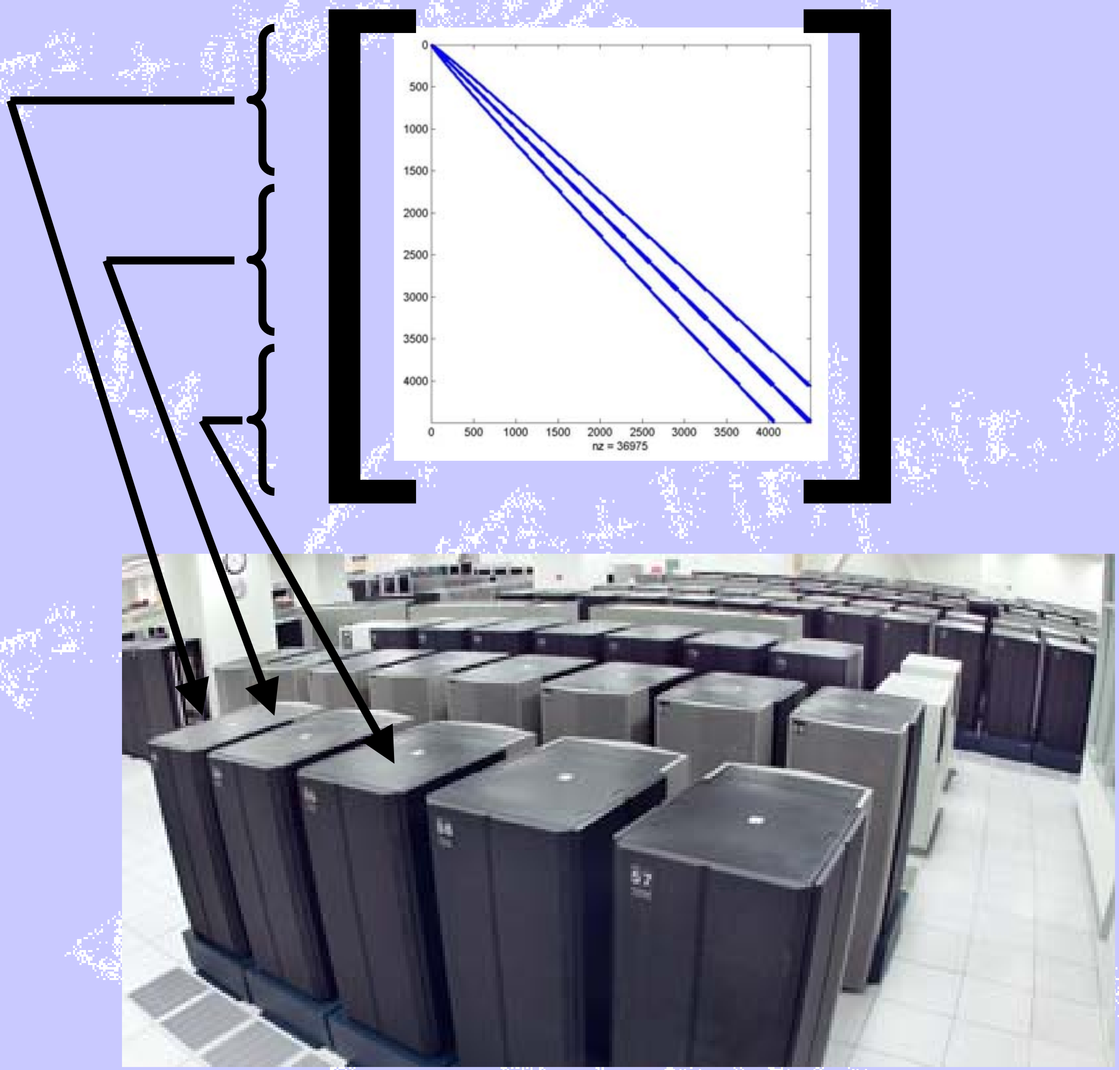
$$N = \frac{(n+w-1)!}{n!(w-1)!}$$

128 particles in 4 wells

- Matrix dimensions: 366,145 x 366,145
- ~ 2 x 10^{12} IF statements
- ~ 5 x 10^{11} assignments
- Rough estimate for sequential algorithm: 33 days

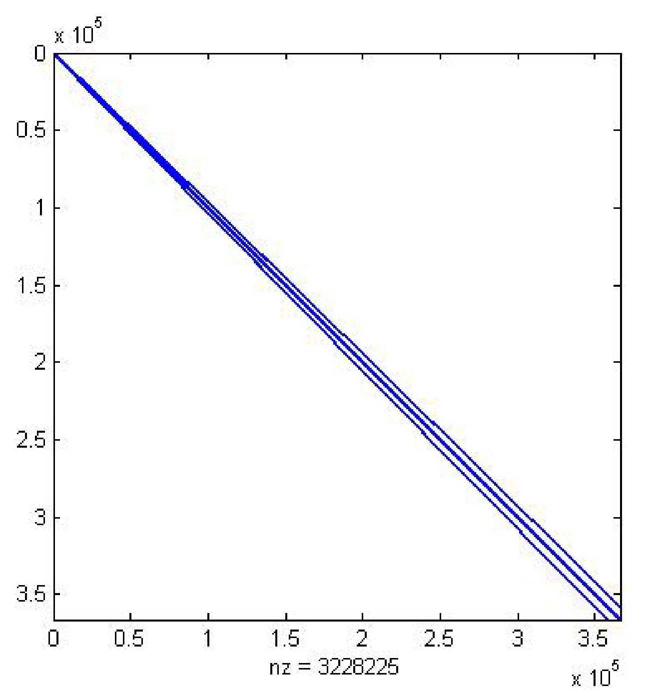


Parallel algorithm for matrix generation



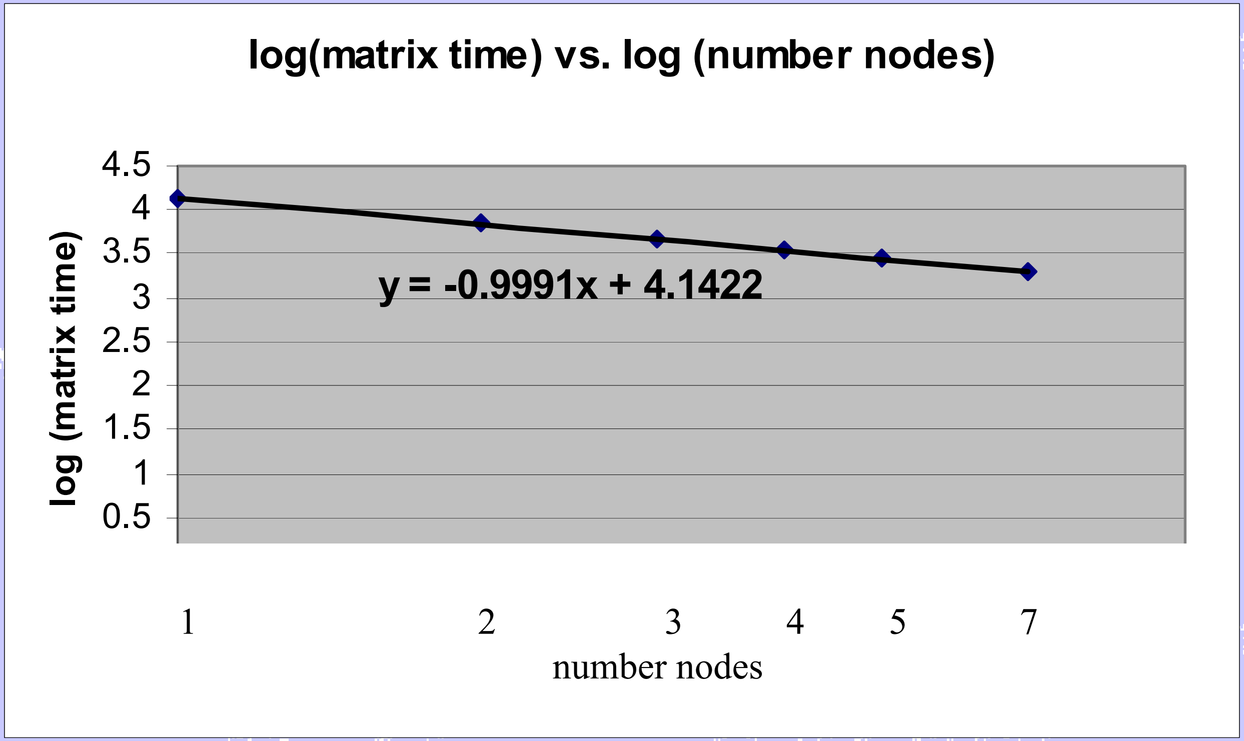
Parallel algorithm: 128 particles in 4 wells

- 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

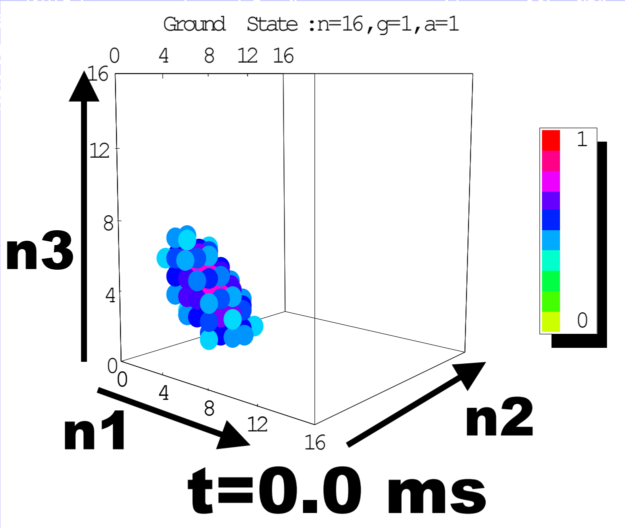


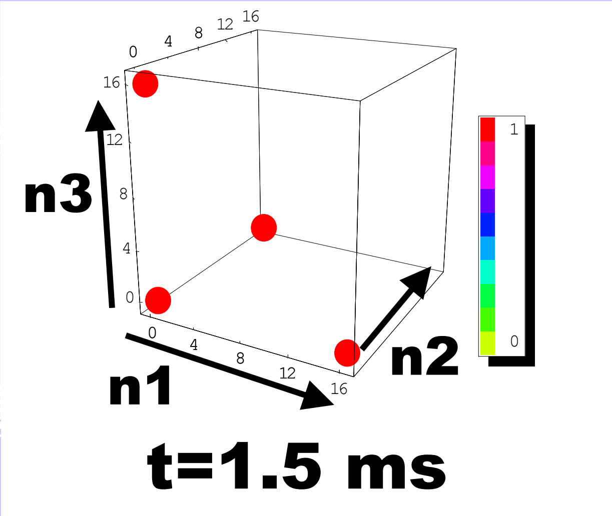
Speed up: parallel algorithm

- 128 particles in 4 wells, 366,145 x 366,145
  1-7 nodes, 16 proc/node

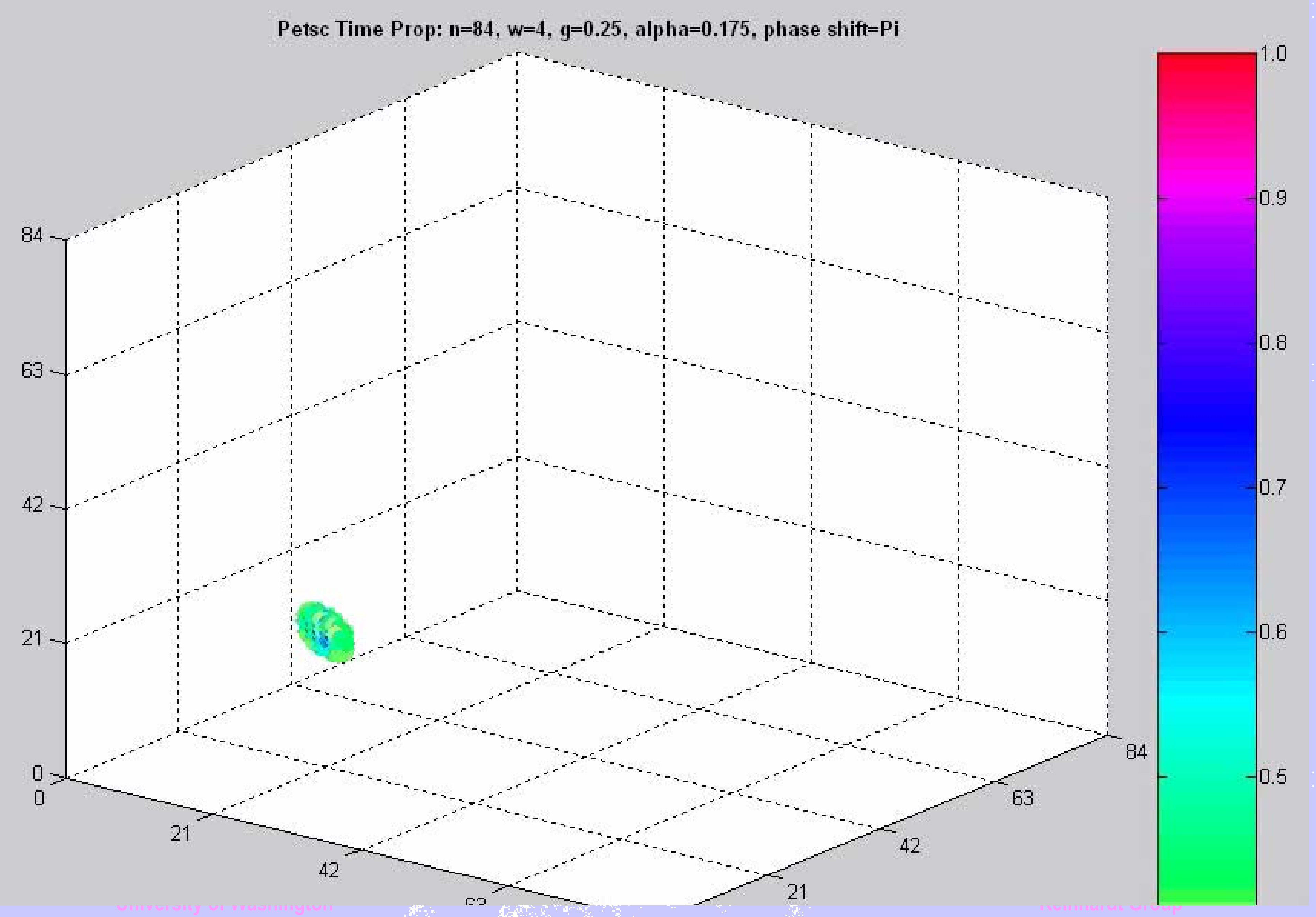


Evolution of 4-well system





Workstation: 16-32 particles


Petsc Time Prop: n=84, w=4, g=0.25, alpha=0.175, phase shift=Pi
84
63
42
21
0
0
21
42
63
21
42
63
84
1.0
0.9
0.8
0.7
0.6
0.5

Summary

- We are using high performance computing to investigate Schrödinger cat states in the BEC,
- may some day be useful in developing new high performance computing techniques (quantum computing)

Acknowledgements

- Reinhardt Group:
  William P. Reinhardt

  Present members:
  - David Masiello

  Past members:
  - Lincoln Carr
  - Kahn Mahmud
  - Sarah McKinney
  - Dorothy Caplow
  - Heidi Perry (undergraduate)

- Funding:
  - Department of Energy
  - Krell Institute

- A little help from my friends:
  - Andri Arnaldsson
  - Colleen Craig
  - August Depner
  - Kim Gunnerson
  - William Stier