Analyzing Quantum Systems Using Cray MTA-2

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NRL’s CRAY MTA-2

40 200 MHz Processors
160 Gigabytes of Memory
128 hardware streams per processor
3 flops per cycle
1 terabyte scratch disk

Mathematical Formulation

$$\boxed{H = t \quad {}_{<ij>} \left(c_i^{+} c_j \ + h.c.\right) + U \quad {}_{i} \ n_{i\neq} n_i \ + V \quad {}_{<ij>} \ n_i n_j}$$

$$E = \quad {}_{m} \ E_m \,\mathbf{exp}(\quad E_m) \Big/ \quad {}_{m} \ \mathbf{exp}(\quad E_m)$$

$$= \frac{1}{N} \frac{\partial E}{\partial V}$$

Hamiltonian Matrix

$$M = S + V \cdot D; \qquad V = 0.2, \ldots, 6.0$$

$$M = \begin{matrix} M_1 & 0 & \cdots & 0 \\ 0 & M_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & M_{156} \end{matrix}$$

Manganite Topology

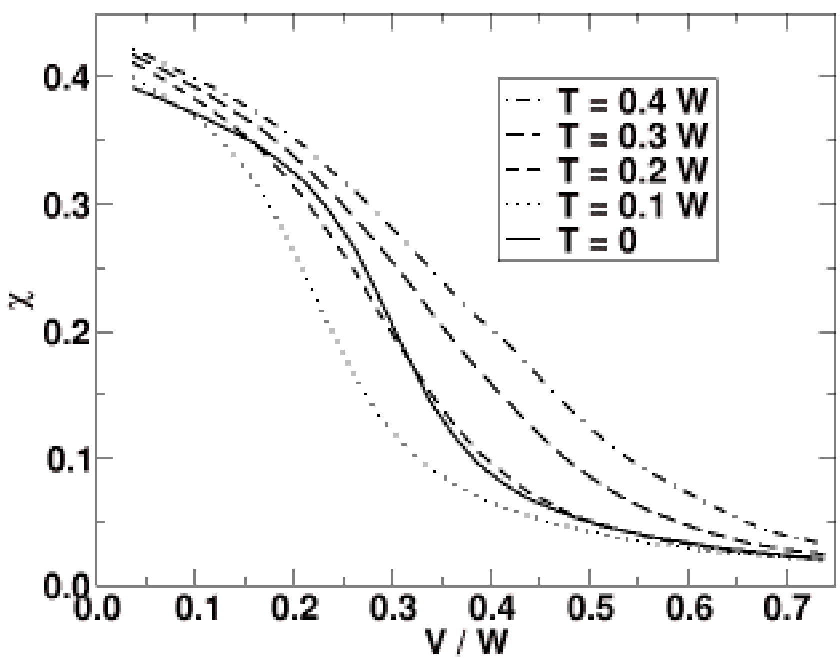
4x4 periodic cluster

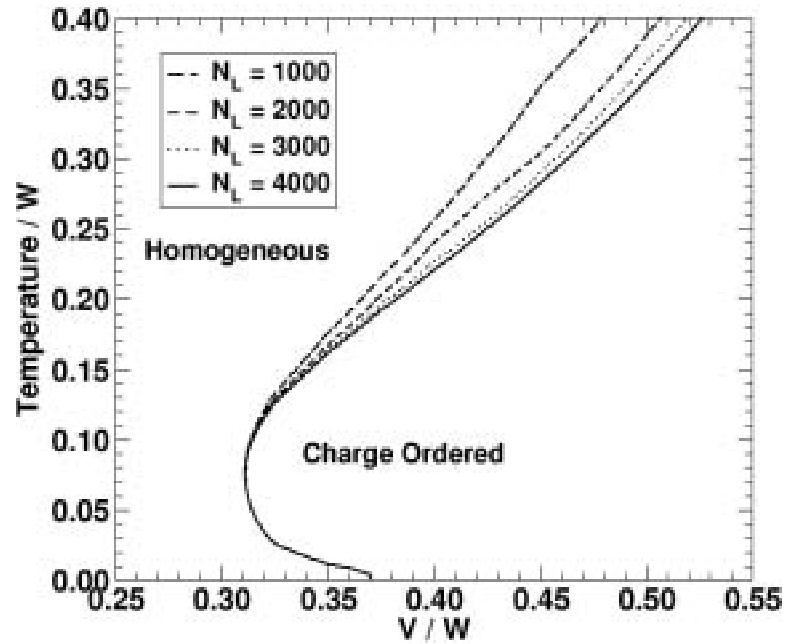
- Equivalent to 2x2x2x2 hypercube
- Up to 2×10^5 Hamiltonian

2D 20-site cluster

- No higher dimensional equivalent
- Up to 2.4×10^8 Hamiltonian

Re-entrant Behavior





Lanczos Algorithm

$$\boldsymbol{v}_{n+1} = \boldsymbol{M}\boldsymbol{v}_n - \boldsymbol{a}_n\boldsymbol{v}_n - \boldsymbol{b}_n\boldsymbol{v}_{n-1}$$

$$\boldsymbol{a}_n = \frac{\langle \boldsymbol{v}_n | \boldsymbol{M} | \boldsymbol{v}_n \rangle}{\langle \boldsymbol{v}_n | \boldsymbol{v}_n \rangle}, \qquad \boldsymbol{b}_n^2 = \frac{\langle \boldsymbol{v}_n | \boldsymbol{v}_n \rangle}{\langle \boldsymbol{v}_{n-1} | \boldsymbol{v}_{n-1} \rangle}$$

$$\boldsymbol{M} = \begin{matrix} \boldsymbol{a}_0 & \boldsymbol{b}_1 & \boldsymbol{0} & \boldsymbol{0} & \cdots \\ \boldsymbol{b}_1 & \boldsymbol{a}_1 & \boldsymbol{b}_2 & \boldsymbol{0} & \cdots \\ \boldsymbol{0} & \boldsymbol{b}_2 & \boldsymbol{a}_2 & \boldsymbol{b}_3 & \cdots \\ \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{b}_3 & \boldsymbol{a}_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{matrix}$$

Operation Counts

Q_{M_k} **Number of elements**

N_{M_k} **Number of rows / columns**

Type	Hardware Ops	Memory Ops
Real	$9N_{M_k} + Q_{M_k}$	$14N_{M_k} + 3Q_{M_k}$
Complex	$16N_{M_k} + 4Q_{M_k}$	$24N_{M_k} + 5Q_{M_k}$

Computer Codes

Original C++, MPI on N processors

- M_k/N rows in each processor
- Entire vector in each

MTA - F90

- Matrix spread across all 40 processors
- 1 copy of vectors.

Modified Compressed Row Format

$$M = \begin{matrix} 2.0 & 1.1 & 3.1 \\ 1.1 & 0.0 & 0.0 \\ 3.1 & 0.0 & 0.0 \end{matrix}, \quad D = \begin{matrix} 1.8 & 0.0 & 0.0 \\ 0.0 & 2.5 & 0.0 \\ 0.0 & 0.0. & 0.0 \end{matrix}$$

R	2.0	1.8	1.1	3.1	0.0	2.5	1.1	0.0	0.0	3.1

J	1	1	2	3	2	2	1	3	3	1

I	O	4	7	10

Sparse Matrix Vector Multiply

```
Do index= 1, Imax
  y(Index)=0
  DO index2 = I(Index+1),I(Index+1)
   Y(index)=Y(Index)+R(Index2)*Vvec(J(index2))
   ENDDO
  ENDDO
```

5 memory ops, 4 multiply-adds

7 instructions, 56 streams

Lanczos Coefficients

```
aval(iteration) = DOT_PRODUCT(Y,Vvec)
Uvec=Y+aval(iteration)*Vvec+Uvec
bval(iteration)=sqrt(DOT_PRODUCT(Uvec,Uvec))
Do index = 1, Imax
   Tmp = Vvec(index)
   Vvec(index)=Uvec(index)/bval(iteration)
   Uvec(index)=-Tmp*bval(iteration)
 ENDDO
```

Timing Results

Platform	Speed MHZ	16P	32P	Speed up
IBM P3	375	142.9	111.6	1.28
COMPAQ	1000	90.1	63.5	1.42
SGI 3800	400	158.4	160.6	0.99
MTA-2	200	28.2	16.6	1.73

MTA-2 Scalability