Add, Multiple, Divide...and Conquer:
Factorization Algorithms for Large-Scale Many-Body Problems

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THE KEY IDEAS

Basic problem: find extremal eigenvalues of very large, very sparse Hermitian matrix

Lanczos algorithm

fundamental operation is *matrix-vector multiply*

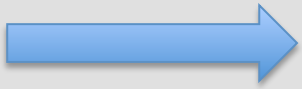
Despite sparsity, nonzero matrix elements can require TB of storage

Only a fraction of matrix elements are unique; **most are reused.**
Reuse of matrix elements understood through *spectator* particles.

Reuse can be **exploited using exact factorization**
enforced through *additive/multiplicative quantum numbers*

THE BASIC PROBLEM

Find extremal eigenvalues of very large, very sparse Hermitian matrix



Lanczos algorithm

fundamental operation is *matrix-vector multiply*

The basic *science question* is to model detailed quantum structure of many-body systems, such the electronic structure of an atom, or structure of an atomic nucleus.

THE BASIC PROBLEM

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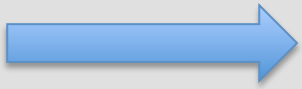


Lanczos algorithm

fundamental operation is *matrix-vector multiply*

To answer this, we attempt to solve *Schrödinger's equation*:

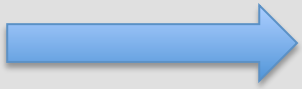
$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)\right)\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots) = E\Psi$$

or

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

THE BASIC PROBLEM

Find extremal eigenvalues of very large, very sparse Hermitian matrix



Lanczos algorithm

fundamental operation is *matrix-vector multiply*

This differential equation is too difficult to solve directly

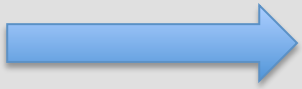
$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j) \right) \Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots) = E\Psi$$

so we use the matrix formalism

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

THE BASIC PROBLEM

Find extremal eigenvalues of very large, very sparse Hermitian matrix



Lanczos algorithm

fundamental operation is *matrix-vector multiply*

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha} |\alpha\rangle \qquad H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} | \beta \rangle$$

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha} \quad \text{if} \quad \langle \alpha | \beta \rangle = \delta_{\alpha\beta}$$

so we use the matrix formalism

$$\hat{\mathbf{H}} |\Psi\rangle = E |\Psi\rangle$$

THE BASIC PROBLEM

Find extremal eigenvalues of very large, very sparse Hermitian matrix

→ Lanczos algorithm

fundamental operation is *matrix-vector multiply*

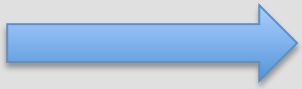
$$H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} | \beta \rangle$$

* **H** is generally a very large matrix – dimensions up to 10^{10} have been tackled.
* **H** is generally very sparse.
* We usually only want a few low-lying states

→ Lanczos algorithm!

THE BASIC PROBLEM

Find extremal eigenvalues of very large, very sparse Hermitian matrix



Lanczos algorithm

fundamental operation is *matrix-vector multiply*

Standard algorithm to obtain *all* eigenvalues of a real, symmetric matrix **A**: Householder

Find orthogonal matrix **U** such that $\mathbf{U}^T \mathbf{A} \mathbf{U} = \mathbf{B}$, a tridiagonal matrix

The Lanczos algorithm is similar, in that it also uses an orthogonal matrix to take **A** to a tridiagonal matrix **B**.....

Lanczos algorithm!

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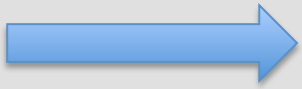


Lanczos algorithm

fundamental operation is *matrix-vector multiply*

$$\mathbf{A}\vec{v}_1 = \alpha_1\vec{v}_1 + \beta_1\vec{v}_2$$

$$\mathbf{A}\vec{v}_2 = \beta_1\vec{v}_1 + \alpha_2\vec{v}_2 + \beta_2\vec{v}_3$$

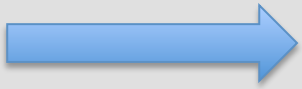
$$\mathbf{A}\vec{v}_3 = \beta_2\vec{v}_2 + \alpha_3\vec{v}_3 + \beta_3\vec{v}_4$$

$$\mathbf{A}\vec{v}_4 = \beta_3\vec{v}_3 + \alpha_4\vec{v}_4 + \beta_4\vec{v}_5$$

Lanczos algorithm!

THE BASIC PROBLEM

Find extremal eigenvalues of very large, very sparse Hermitian matrix



Lanczos algorithm

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$$\mathbf{A}\vec{v}_1 = \alpha_1\vec{v}_1 + \beta_1\vec{v}_2$$

$$\mathbf{A}\vec{v}_2 = \beta_1\vec{v}_1 + \alpha_2\vec{v}_2 + \beta_2\vec{v}_3$$

$$\mathbf{A}\vec{v}_3 = \beta_2\vec{v}_2 + \alpha_3\vec{v}_3 + \beta_3\vec{v}_4$$

$$\mathbf{A}\vec{v}_4 = \beta_3\vec{v}_3 + \alpha_4\vec{v}_4 + \beta_4\vec{v}_5$$

matrix-vector multiply

Lanczos algorithm!

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

I need to quickly cover:

- How the basis states are represented
- How the Hamiltonian operator is represented
- Why most matrix elements are zero
- Typical dimensions and sparsity

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- How the basis states are represented

This differential equation is too difficult to solve directly

$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)\right)\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots) = E\Psi$$

Can only really solve 1D differential equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + U(r)\right)\phi_i(r) = \varepsilon_i\phi_i(r)$$

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- How the basis states are represented

Can only really solve 1D differential equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+U(r)\right)\phi_i(r)=\varepsilon_i\phi_i(r) \quad \Rightarrow \quad \{\phi_i(\vec{r})\}$$

Single-particle wave functions labeled by, *e.g.*, n, j, l, m

Atomic case: 1s, 2s, 2p, 3s, 3p, 3d *etc*

Nuclear: $0s_{1/2}$, $0p_{3/2}$, $0p_{1/2}$, $0d_{5/2}$, $1s_{1/2}$, $0d_{3/2}$, *etc*

A Sparse Matrix, but....

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- How the basis states are represented

Can only really solve 1D differential equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+U(r)\right)\phi_i(r)=\varepsilon_i\phi_i(r) \Rightarrow \{\phi_i(\vec{r})\}$$

Product wavefunction ("Slater Determinant")

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots)=\phi_{n_1}(\vec{r}_1)\phi_{n_2}(\vec{r}_2)\phi_{n_3}(\vec{r}_3)\ldots\phi_{n_N}(\vec{r}_N)$$

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- How the basis states are represented

Product wavefunction ("Slater Determinant")

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots) = \phi_{n_1}(\vec{r}_1)\phi_{n_2}(\vec{r}_2)\phi_{n_3}(\vec{r}_3)\ldots\phi_{n_N}(\vec{r}_N)$$

Each many-body state can be *uniquely* determined by a list of "occupied" single-particle states = "occupation representation"

$$|\alpha\rangle = \hat{a}^+_{n_1}\hat{a}^+_{n_2}\hat{a}^+_{n_3}\ldots\hat{a}^+_{n_N}|0\rangle$$

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- How the Hamiltonian is represented

"occupation representation"

$$|\alpha\rangle = \hat{a}^+_{n_1} \hat{a}^+_{n_2} \hat{a}^+_{n_3} \ldots \hat{a}^+_{n_N} |0\rangle$$

"creation operator"

$$\hat{H} = \sum_{ij} T_{ij} \hat{a}^+_i \hat{a}_j + \frac{1}{4} \sum_{ijkl} V_{ijkl} \hat{a}^+_i \hat{a}^+_j \hat{a}_l \hat{a}_k$$

motion of a single particle ("one-body operator")

interaction of two particles ("two-body operator")

$$V_{ijkl} = \iint \phi_i(\vec{r}) \phi_j(\vec{r}') V(\vec{r}, \vec{r}') \phi_k(\vec{r}) \phi_l(\vec{r}') d^3r d^3r'$$

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- How the Hamiltonian is represented

"occupation representation" $\left|\alpha\right\rangle = \hat{a}^{+}_{n_1}\hat{a}^{+}_{n_2}\hat{a}^{+}_{n_3}\ldots\hat{a}^{+}_{n_N}\left|0\right\rangle$

n_i	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0

$$\hat{H} = \sum_{ij} T_{ij}\hat{a}^{+}_{i}\hat{a}_{j} + \frac{1}{4}\sum_{ijkl} V_{ijkl}\hat{a}^{+}_{i}\hat{a}^{+}_{j}\hat{a}_{l}\hat{a}_{k}$$

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- How the Hamiltonian is represented

"occupation representation" $\left|\alpha\right\rangle = \hat{a}^{+}_{n_1}\hat{a}^{+}_{n_2}\hat{a}^{+}_{n_3}\ldots\hat{a}^{+}_{n_N}\left|0\right\rangle$

n_i	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0

$$\hat{a}^{+}_3\hat{a}^{+}_6\hat{a}_4\hat{a}_5\left|\alpha=1\right\rangle = \left|\alpha=2\right\rangle$$

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- How the Hamiltonian is represented

"occupation representation" $\left|\alpha\right\rangle = \hat{a}^{+}_{n_1}\hat{a}^{+}_{n_2}\hat{a}^{+}_{n_3}\ldots\hat{a}^{+}_{n_N}\left|0\right\rangle$

n_i	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0

$$\hat{a}_2^{+}\hat{a}_4^{+}\hat{a}_1\hat{a}_7\left|\alpha=2\right\rangle = \left|\alpha=3\right\rangle$$

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- Why most matrix elements are zero

"occupation representation" $\left|\alpha\right\rangle = \hat{a}^{+}_{n_1}\hat{a}^{+}_{n_2}\hat{a}^{+}_{n_3}\ldots\hat{a}^{+}_{n_N}\left|0\right\rangle$

n_i	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0

$$\hat{a}_2^{+}\hat{a}_4^{+}\hat{a}_6^{+}\hat{a}_1\hat{a}_5\hat{a}_7\left|\alpha=1\right\rangle = \left|\alpha=3\right\rangle$$

need 3 particles to interact simultaneously!

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

- Typical dimensions and sparsity

Nuclide	valence space	valence Z	valence N	basis dim	sparsity (%)
^{20}Ne	"sd"	2	2	640	10
^{25}Mg	"sd"	4	5	44,133	0.5
^{49}Cr	"pf"	4	5	6M	0.01
^{56}Fe	"pf"	6	10	500M	2×10^{-4}

This corresponds to 2 Tb of data!

Recycled Matrix Elements

Only a fraction of matrix elements are unique; **most are reused.**

Reuse of matrix elements understood through *spectator* particles.

n_i	1	2	3	4	5	6	7	8
α=1	1	1	1	0	0	0	0	1
α=2	1	1	0	1	1	0	0	0
α=3	0	1	1	0	0	1	0	1
α=4	0	1	0	1	1	1	0	0
α=5	0	0	1	0	0	1	1	1
α=6	0	0	0	1	1	1	1	0

$$\hat{a}_4^+\hat{a}_5^+\hat{a}_3\hat{a}_8|\alpha=1\rangle = |\alpha=2\rangle$$

$$\hat{a}_4^+\hat{a}_5^+\hat{a}_3\hat{a}_8|\alpha=3\rangle = |\alpha=4\rangle$$

$$\hat{a}_4^+\hat{a}_5^+\hat{a}_3\hat{a}_8|\alpha=5\rangle = |\alpha=6\rangle$$

All of these have the same matrix element: V_{4538}

Recycled Matrix Elements

Only a fraction of matrix elements are unique; **most are reused.**

Reuse of matrix elements understood through *spectator* particles.

# of nonzero matrix elements vs. # unique matrix elements

Nuclide	valence space	valence Z	valence N	# nonzero	# unique
^{28}Si	"sd"	6	6	26 x 10^6	3600
^{52}Fe	"pf"	6	6	90 x 10^9	21,500

FACTORIZATION

Reuse can be **exploited using exact factorization**
enforced through *additive/multiplicative quantum numbers*

A quantum number is the eigenvalue of an operator

generally a operator that exactly commutes with the Hamiltonian

e.g. angular momentum $\mathbf{J}^2$ and z-component $\mathbf{J}_z$

$$\hat{J}^2|\Psi\rangle = J(J+1)|\Psi\rangle \qquad \hat{J}_z|\Psi\rangle = M|\Psi\rangle$$

FACTORIZATION

Reuse can be **exploited using exact factorization**
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A quantum number is the eigenvalue of an operator

For composite systems, one can apply the operator to each component separately:

$$\hat{O}|\Psi\rangle = \left(\hat{O}_1 + \hat{O}_2 + \hat{O}_3 + \ldots\right)\left(|\Psi_1\rangle \otimes |\Psi_2\rangle \otimes |\Psi_3\rangle \otimes \ldots\right)$$

Sometimes the total quantum number is a simple sum/product as is the case for $\mathbf{J}_z$ or parity....

$$\hat{J}_z|\Psi\rangle = M|\Psi\rangle = (m_1 + m_2 + m_3 + \ldots)|\Psi\rangle$$

...but in other cases the addition is complicated (e.g. for $\mathbf{J}^2$)

FACTORIZATION

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I consider composite many-fermion systems,
in particular those with 2 major components
protons and *neutrons*
or
spin-up and *spin-down* electrons

$$\left|\Psi\right\rangle = \left|\Psi_1\right\rangle \otimes \left|\Psi_2\right\rangle$$

Each component itself is a Slater determinant which is composed of many particles

$$\hat{J}_z\left|\Psi\right\rangle = M\left|\Psi\right\rangle \qquad M = M_1 + M_2$$

$$M_1 = m_1^{(1)} + m_1^{(2)} + m_1^{(2)} + \ldots$$

FACTORIZATION

Reuse can be **exploited using exact factorization**
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Because the M values are discrete integers or half-integers
(-3, -2, -1, 0, 1, 2, … or -3/2, -1/2, +1/2, +3/2….)
we can organize the basis states in discrete *sectors*

Example: 2 protons, 4 neutrons, total M = 0

$M_z(\pi) = -4$	$M_z(\upsilon) = +4$
$M_z(\pi) = -3$	$M_z(\upsilon) = +3$
$M_z(\pi) = -2$	$M_z(\upsilon) = +2$

FACTORIZATION

Reuse can be **exploited using exact factorization**
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In fact, we can see an example of factorization here because all proton Slater determinants in one M-sector *must* combine with all the conjugate neutron Slater determinants

Example: 2 protons, 4 neutrons, total M = 0

$M_z(\pi) = -4$: 2 SDs	$M_z(\upsilon) = +4$: 24 SDs	48 combined
$M_z(\pi) = -3$: 4 SDs	$M_z(\upsilon) = +3$: 39 SDs	156 combined
$M_z(\pi) = -2$: 9 SDs	$M_z(\upsilon) = +2$: 60 SDs	540 combined

FACTORIZATION

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In fact, we can see an example of factorization here because all proton Slater determinants in one M-sector *must* combine with all the conjugate neutron Slater determinants

$M_z(\pi) = -4$: 2 SDs | $M_z(\upsilon) = +4$: 24 SDs | 48 combined

$$\begin{matrix} |\pi_1\rangle \\ |\pi_2\rangle \end{matrix} \quad \times \quad \begin{matrix} |\nu_1\rangle \\ |\nu_2\rangle \\ |\nu_3\rangle \\ |\nu_4\rangle \\ \vdots \\ |\nu_{24}\rangle \end{matrix} \quad = \quad \begin{matrix} |\pi_1\rangle|\nu_1\rangle \\ |\pi_2\rangle|\nu_1\rangle \\ |\pi_1\rangle|\nu_2\rangle \\ |\pi_2\rangle|\nu_2\rangle \\ \vdots \\ |\pi_1\rangle|\nu_{24}\rangle \\ |\pi_2\rangle|\nu_{24}\rangle \end{matrix}$$

FACTORIZATION

Reuse can be **exploited using exact factorization**
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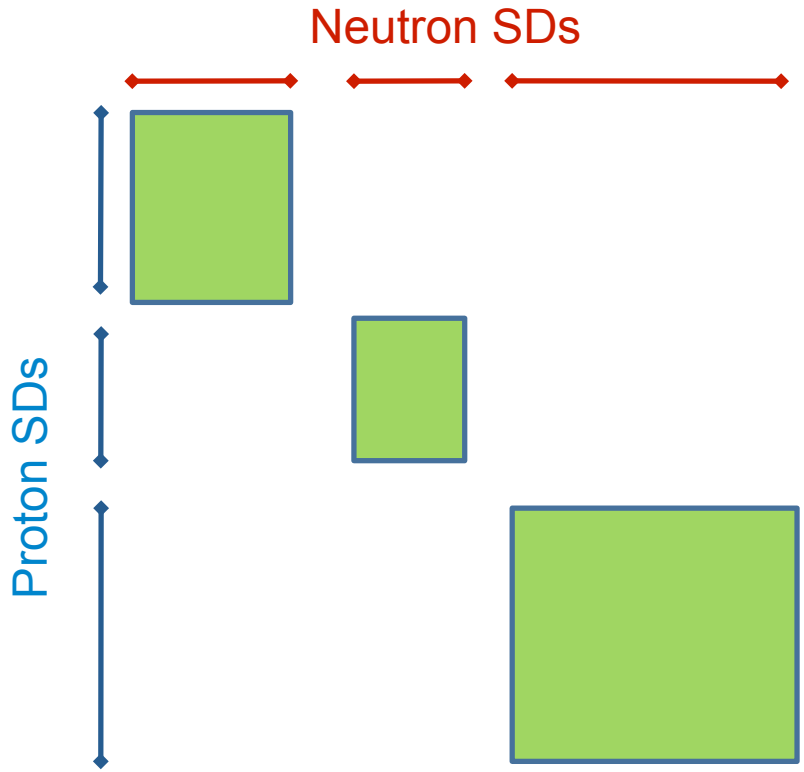
$$|\alpha\rangle = |\alpha_p\rangle \times |\alpha_n\rangle$$



Example N = Z nuclei

Nuclide	Basis dim	# pSDs (=#nSDs)
^{20}Ne	640	66
^{24}Mg	28,503	495
^{28}Si	93,710	924
^{48}Cr	1,963,461	4895
^{52}Fe	109,954,620	38,760
^{56}Ni	1,087,455,228	125,970

FACTORIZATION

Reuse can be **exploited using exact factorization**
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Factorization allows us to keep track of all basis states
without writing out every one explicitly
-- we only need to write down the proton/neutron components

The same trick can be applied to matrix-vector multiply

$$\hat{H} = \hat{H}_{pp} + \hat{H}_{nn} + \hat{H}_{pn}$$

Move 2 protons; *neutrons are spectators*

Move 2 neutrons; *protons are spectators*

Move 1 proton + 1 neutron; *rest are spectators*

FACTORIZATION

Reuse can be **exploited using exact factorization**
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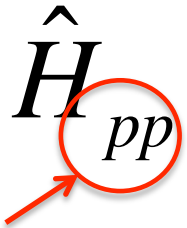

Move 2 protons;
neutrons are spectators

Example: 2 protons, 4 neutrons, total M = 0

$M_z(\pi) = -4$: 2 SDs	$M_z(\upsilon) = +4$: 24 SDs	48 combined

There are potentially 48 × 48 matrix elements
But for H_{pp} at most 4 × 24 are nonzero
and we only have to look up 4 matrix elements

Advantage: **we can store 98 matrix elements as 4 matrix elements** and avoid 2000+ zero matrix elements.

FACTORIZATION

Reuse can be **exploited using exact factorization**
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$M_z(\pi) = -4$: 2 SDs	$M_z(\upsilon) = +4$: 24 SDs	48 combined

$$\begin{matrix} |\pi_1\rangle \\ |\pi_2\rangle \end{matrix} \qquad H_{pp} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \qquad \begin{matrix} |\nu_1\rangle \\ |\nu_2\rangle \\ |\nu_3\rangle \\ |\nu_4\rangle \\ \vdots \\ |\nu_{24}\rangle \end{matrix}$$

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FACTORIZATION

Reuse can be **exploited using exact factorization**
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$M_z(\pi) = -4$: 2 SDs

$M_z(\upsilon) = +4$: 24 SDs

48 combined

$$|\pi_1\rangle \quad |\pi_2\rangle \qquad H_{pp} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

$$\begin{aligned}
|\nu_1\rangle \quad & H_{pp}|\pi_1\rangle|\nu_1\rangle = H_{11}|\pi_1\rangle|\nu_1\rangle + H_{12}|\pi_2\rangle|\nu_1\rangle \\
|\nu_2\rangle \quad & H_{pp}|\pi_2\rangle|\nu_1\rangle = H_{12}|\pi_1\rangle|\nu_1\rangle + H_{22}|\pi_2\rangle|\nu_1\rangle \\
|\nu_3\rangle \quad & H_{pp}|\pi_1\rangle|\nu_2\rangle = H_{11}|\pi_1\rangle|\nu_2\rangle + H_{12}|\pi_2\rangle|\nu_2\rangle \\
|\nu_4\rangle \quad & H_{pp}|\pi_2\rangle|\nu_2\rangle = H_{12}|\pi_1\rangle|\nu_2\rangle + H_{22}|\pi_2\rangle|\nu_2\rangle \\
\vdots \quad & \vdots \\
|\nu_{24}\rangle \quad & H_{pp}|\pi_1\rangle|\nu_{24}\rangle = H_{11}|\pi_1\rangle|\nu_{24}\rangle + H_{12}|\pi_2\rangle|\nu_{24}\rangle \\
& H_{pp}|\pi_2\rangle|\nu_{24}\rangle = H_{12}|\pi_1\rangle|\nu_{24}\rangle + H_{22}|\pi_2\rangle|\nu_{24}\rangle
\end{aligned}$$

Advantage: **we can store 98 matrix elements as 4 matrix elements** and avoid 2000+ zero matrix elements.

FACTORIZATION

Reuse can be **exploited using exact factorization**
enforced through *additive/multiplicative quantum numbers*

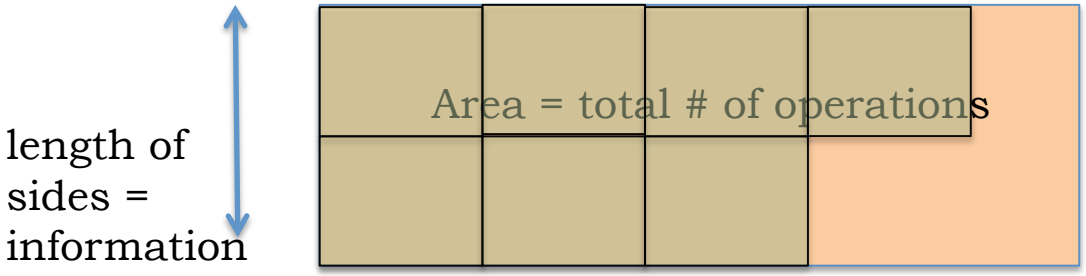
Comparison of nonzero matrix storage with factorization

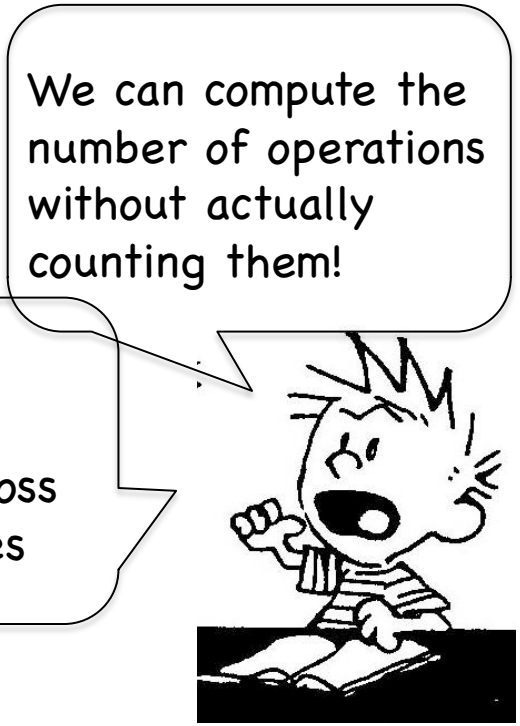
Nuclide	Space	Basis dim	matrix store	factorization
^{56}Fe	*pf*	501 M	290 Gb	0.72 Gb
^{7}Li	N_{max}=12	252 M	3600 Gb	96 Gb
^{7}Li	N_{max}=14	1200 M	23 Tb	624 Gb
^{12}C	N_{max}=6	32M	196 Gb	3.3 Gb
^{12}C	N_{max}=8	590M	5000 Gb	65 Gb
^{12}C	N_{max}=10	7800M	111 Tb	1.4 Tb
^{16}O	N_{max}=6	26 M	142 Gb	3.0 Gb
^{16}O	N_{max}=8	990 M	9700 Gb	130 Gb

PARALLEL IMPLEMENTATION

Factorization makes it easier to compute workload and distribute across multiple nodes

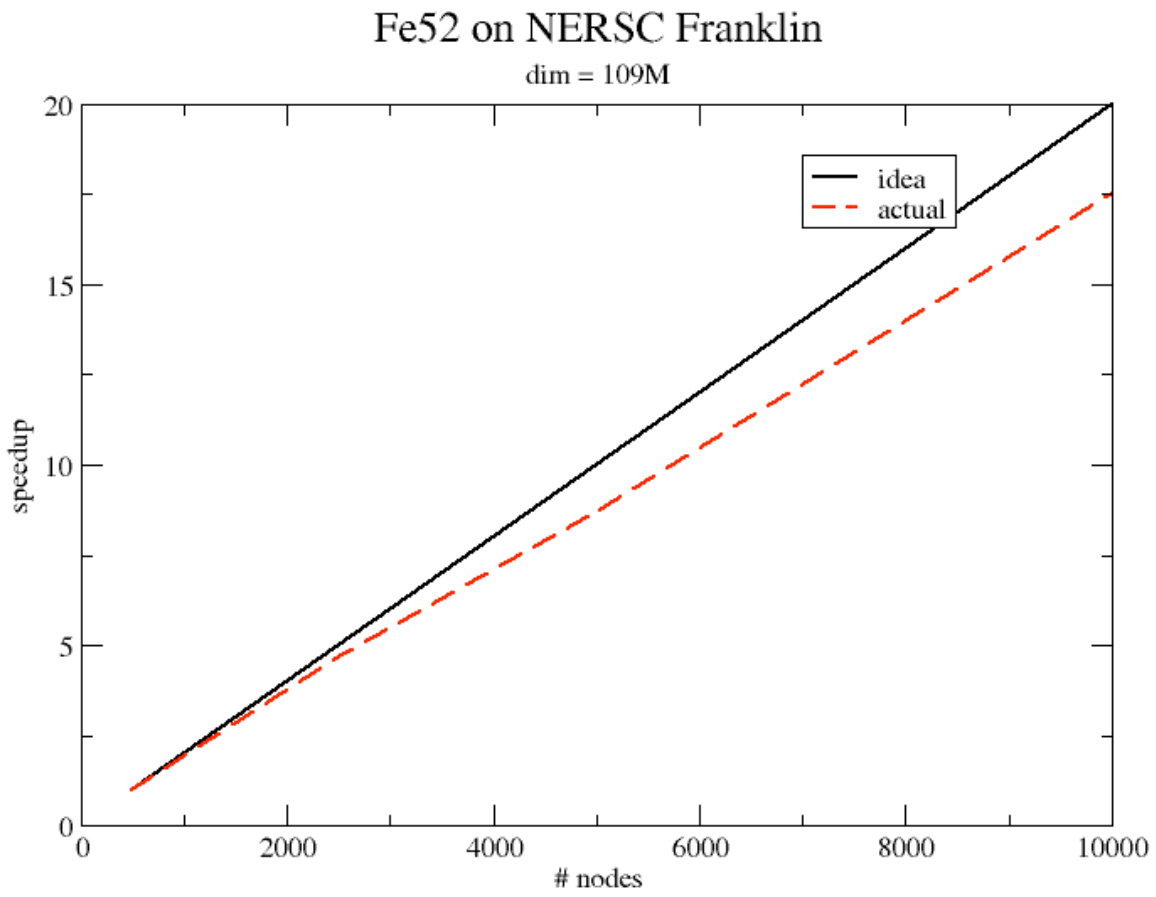
length of sides = information to be stored





PARALLEL IMPLEMENTATION

Factorization makes it easier to compute workload and distribute across multiple nodes



THE BIGSTICK CODE

Many-fermion code: 2nd generation after REDSTICK code
(started in *Baton Rouge, La.*)

Arbitrary single-particle radial waveforms
Allows local or nonlocal two-body interaction
Applies to both nuclear and atomic cases

Runs on both desktop and parallel machines
--can run at least dimension 100M+ on desktop
(20 Lanczos iterations in 300 CPU minutes)

20-30k lines of codes
Fortran 90 + MPI + OpenMP
Partially funded by SciDAC
Plans to run on 50,000-100,000 compute nodes
Plans to publish code late 2011

SCIENCE APPLICATIONS

Comparison of "exact" results versus approximations
-- *e.g.* mean-field, density-functional, time-dependent mean-field, projection of mean-field onto exact symmetries, *etc.*

How "unique" in the nucleon-nucleon interaction?
--*i.e.*, the input V_{ijkl} look like random numbers; what happens if we actually use random numbers?
-- can we use ambiguity in the interaction to our advantage?

Looking for and using broken symmetries
--isospin breaking and the unitarity of the CKM matrix

CONCLUSIONS

Basic problem: find extremal eigenvalues of very large, very sparse Hermitian matrix

Lanczos algorithm

fundamental operation is *matrix-vector multiply*

Despite sparsity, nonzero matrix elements can require TB of storage

Only a fraction of matrix elements are unique; **most are reused.**
Reuse of matrix elements understood through *spectator* particles.

Reuse can be **exploited using exact factorization**
enforced through *additive/multiplicative quantum numbers*