# Implementation of "A Center-of-Mass Principle"

Benigno Parra
&
Vittal Pai

Ohio University

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# Goal

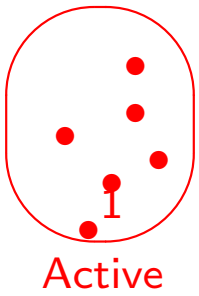
The main goal of the research is to **Implement and Test** the **"Center-of-Mass Principle for the Multiparticle Schrödinger Equation"**

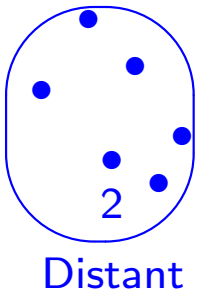
Also, to come up with ways to **IMPROVE** the **RUNNING TIME** of the equation.

This research has been carried out under the guidance of Dr. Martin Mohlenkamp.

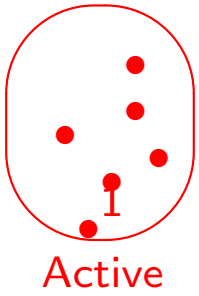
# The Classical Center-of-Mass Principle

Consider two subsets of $N$ particles each that are "far" apart. To compute the force of each particle in group 2 on the particles in group 1 costs $N^2$.




If we spend $\mathcal{O}(N)$ effort and replace group 2 with a single massive particle located at its center-of-mass then computing the forces on the particles in group 1 now costs only $N$, so the total cost is $\mathcal{O}(N)$.

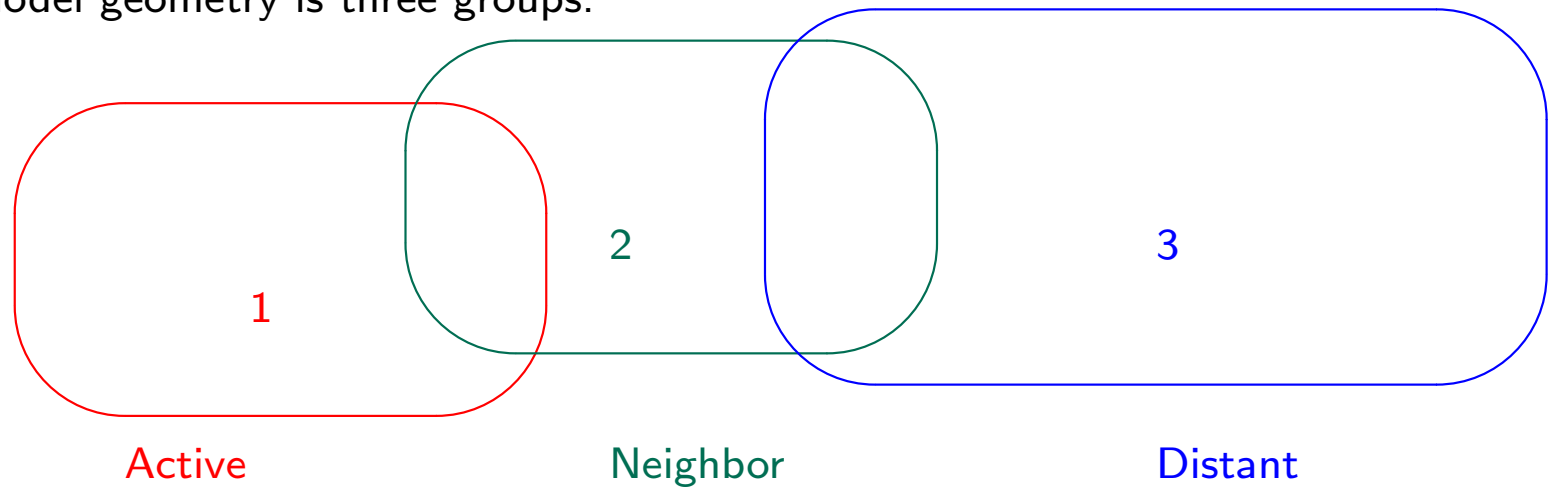




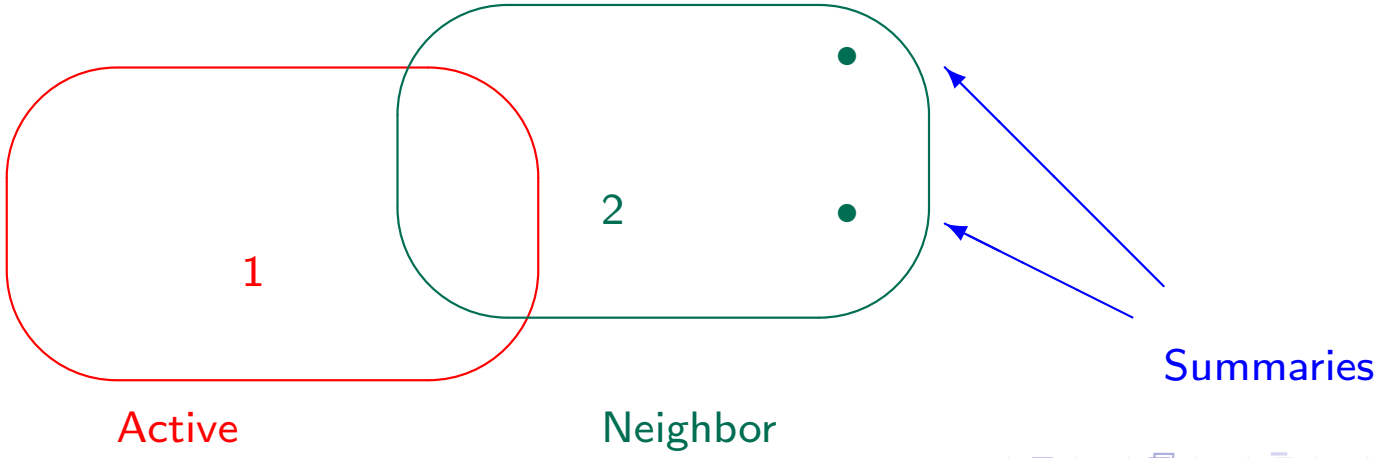
The Fast Multipole Method (Greengard and Rokhlin) exploits this principle to compute approximate forces rapidly, and has been extended to other types of interactions.

# A Quantum Center-of-Mass Principle

The model geometry is three groups:




Due to the antisymmetry constraint, the interaction of group 3 with group 1 is effected by the presence of group 2. The interaction is nonlinear and nonlocal. We show that it is still possible to summarize, and that these summaries become embedded in group 2.



# Determinant Properties

For all our work we use the following determinant Propositions:

Let $\mathbb{A}$ and $\mathbb{B}$ be the two **n x n** matrices. Let $\alpha_0 = \beta_0 =$ ordered set {1, 2,...,n}.

Then we have:

$\sigma(\alpha \subset \alpha_0) =$ Sum of indices of the set $\alpha$ within the set $\alpha_0$.

Example, $\sigma(\{2,4,7\} \subset \{2,3,4,7,8\}) = 1+3+4 = 8$.

$\alpha_0 \setminus \alpha =$ Complement of $\alpha$ in $\alpha_0$.

Example, $\{2,3,4,7,8\}\setminus\{2,4,7\} = \{3,8\}$.

$|\alpha| =$ number of elements in the set $\alpha$.

$\mathbb{A}[\alpha;\beta] =$ Matrix $\mathbb{A}$ with rows in $\alpha$ and columns in $\beta$.

Determinant of the sum of two matrices:

$$|\mathbb{A}+\mathbb{B}| = \sum_{k=0}^{|\alpha_0|} \sum_{\substack{\alpha\subset\alpha_0,\ \beta\subset\alpha_0,\\ |\alpha|=|\beta|=k}} (-1)^{\sigma(\alpha\subset\alpha_0)+\sigma(\beta\subset\alpha_0)} \, |\mathbb{A}[\alpha_0\setminus\alpha;\alpha_0\setminus\beta]| \cdot |\mathbb{B}[\alpha;\beta]|$$

# Determinant Properties Cont...

If we extend the previous formula to three matrices with one of them is the identity we obtain the formula:

$$|\mathbb{I}+\mathbb{A}+\mathbb{B}| = \sum_{k_1=0}^{|\alpha_0|} \sum_{\substack{\alpha_1\subset\alpha_0,\\ |\alpha_1|=k_1}} \sum_{k_2=0}^{|\alpha_1|} \sum_{\substack{\alpha\subset\alpha_1,\ \beta\subset\alpha_1,\\ |\alpha|=|\beta|=k_2}} (-1)^{\sigma(\alpha\subset\alpha_1)+\sigma(\beta\subset\alpha_1)} |\mathbb{A}[\alpha_1\setminus\alpha;\alpha_1\setminus\beta]|\cdot|\mathbb{B}[\alpha;\beta]|$$

When $k=0$ or $k=n$, the sub-matrix is considered to have determinant one.

**REFERENCE**

Determinants of Sums' by Marcus Marvin (The College Math J., Vol 21, No. 2. March 1990)

# Three Groups

Now we will consider the case of Interaction between the particles in Three Groups. These three groups overlap as in figure above. Therefore, from earlier research we have the antisymmetric inner product:

$$\left\langle (\sum_{l_1} \mathbf{\Phi}_1^{l_1})(\sum_{l_2} \mathbf{\Phi}_2^{l_2})(\sum_{l_3} \mathbf{\Phi}_3^{l_3}),(\sum_{l_1'} \tilde{\mathbf{\Phi}}_1^{l_1'})(\sum_{l_2'} \tilde{\mathbf{\Phi}}_2^{l_2'})(\sum_{l_3'} \tilde{\mathbf{\Phi}}_3^{l_3'}) \right\rangle_{\mathcal{A}}$$

Using Löwdin's rules, and further simplifying we have:

$$\sum_{p_1=1}^{t_1} \sum_{p_2=1}^{t_2} \sum_{p_3=3}^{t_3} |\mathbb{L}_{11}||\mathbb{L}_{22}||\mathbb{L}_{33}| \begin{vmatrix} \mathbb{I}_{n1} & \mathbb{L}^{-1}{}_{11}\mathbb{L}_{12} & O \\ \mathbb{L}^{-1}{}_{22}\mathbb{L}_{21} & \mathbb{I}_{n2} & \mathbb{L}^{-1}{}_{22}\mathbb{L}_{23} \\ O & \mathbb{L}^{-1}{}_{33}\mathbb{L}_{32} & \mathbb{I}_{n3} \end{vmatrix} \quad (1)$$

where n1, n2 and n3 are the sizes of Indentity matrices in the diagonal position of the overall matrix above.

# Cont...

Splitting the inner matrix and applying the proposition of sum of three matrices we have:

$$\sum_{p_1=1}^{t_1}\sum_{p_2=1}^{t_2}|\mathbb{L}_{p_1p_1}|\,|\mathbb{L}_{p_2p_2}|\sum_{k_1=0}^{|\alpha_0|}\sum_{\substack{\alpha_1\subset\alpha_0,\\|\alpha_1|=k_1}}\sum_{k_2=0}^{|\alpha_1|}\sum_{\substack{\alpha\subset\alpha_1,\ \beta\subset\alpha_1,\\|\alpha|=|\beta|=k_2}}(-1)^{\sigma(\alpha\subset\alpha_1)+\sigma(\beta\subset\alpha_1)}$$

$$|\mathbb{M}_{p_1p_2}[\alpha_1\setminus\alpha;\alpha_1\setminus\beta]|\cdot S_{p_2}(\alpha;\beta) \tag{2}$$

where

$$S_{p_2}(\alpha;\beta)=\sum_{p_3=1}^{t_3}|\mathbb{L}_{p_3p_3}||\mathbb{M}_{p_2p_3}[\alpha;\beta]|$$

This "Three Group Interaction" has been Implemented and tested in Python for its working. But there is an **ISSUE!!!**, it takes long time to compute.

# Making it FAST !!!
## Non-Zero Minors...

Formula (1) can be expressed as:

$$\left|\begin{bmatrix} \mathbb{I}_{n1} & 0 & 0 \\ 0 & \mathbb{I}_{n2} & 0 \\ 0 & 0 & \mathbb{I}_{n3} \end{bmatrix} + \begin{bmatrix} 0 & \mathbb{L}^{-1}{}_{11}\mathbb{L}_{12} & 0 \\ \mathbb{L}^{-1}{}_{22}\mathbb{L}_{21} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathbb{L}^{-1}{}_{22}\mathbb{L}_{23} \\ 0 & \mathbb{L}^{-1}{}_{33}\mathbb{L}_{32} & 0 \end{bmatrix}\right|$$

Let us denote last two matrices above as $\mathbb{M}_{12}$ and $\mathbb{M}_{23}$ (shorthand notations for $\mathbb{M}_{p_1 p_2}$ and $\mathbb{M}_{p_2 p_3}$) respectively. Both these matrices have lot of **ZERO MINORS** which would not add anything to the determinant value. So, it would make sense to **PRE-DISCARD** these instead of including them in the calculation.

**How to find them ???**

# Indentifying Non-Zero Minors

$$\text{Let } \mathbb{A} = \begin{bmatrix} \mathbb{O}_{11} & \mathbb{O}_{12} & \mathbb{O}_{13} \\ \mathbb{O}_{21} & \mathbb{O}_{22} & \mathbb{A}_{23} \\ \mathbb{O}_{31} & \mathbb{A}_{32} & \mathbb{O}_{33} \end{bmatrix}.$$

The blocks $\mathbb{O}_{11}$, $\mathbb{O}_{22}$, and $\mathbb{O}_{33}$ are square matrices of dimensions $n_1^2$, $n_2^2$, and $n_3^2$ respectively, and all of the matrices $\mathbb{O}_{ij}$ are zero matrices.

Let $I = \{1, \ldots, n_1\}$, $J = \{n_1 + 1, \ldots, n_1 + n_2\}$, and $K = \{n_1 + n_2 + 1, \ldots, n_1 + n_2 + n_3\}$. Let $\alpha$, and $\beta$ be ordered subsets of the ordered set $\{1, 2, ..., n_1 + n_2 + n_3\}$.

Following same notation as above we have,

$$\text{If } |\mathbb{A}[\alpha; \beta]| \neq 0 \text{ then}$$
$$|\alpha \cap J| + |\alpha \cap K| = |\alpha| = |\beta| = |\beta \cap J| + |\beta \cap K|,$$
$$\text{and } |\alpha \cap J| = |\beta \cap K|, \text{ and } |\alpha \cap K| = |\beta \cap J|.$$

# Indentifying Non-Zero Minors (cont...)

Let $\alpha^I = \alpha \cap I$, $\alpha^J = \alpha \cap J$, and so on.

Therefore, the formula (2) after dropping all the Zero-Minors as identified above becomes:

$$\sum_{p_1=1}^{t_1} \sum_{p_2=1}^{t_2} \sum_{p_3=1}^{t_3} |\mathbb{L}_{p_1 p_1}|\,|\mathbb{L}_{p_2 p_2}|\,|\mathbb{L}_{p_3 p_3}| \sum_{k_1=0}^{|\alpha_0|} \sum_{\substack{\alpha_1 \subset \alpha_0, \\ |\alpha_1| = k_1}} \sum_{k_2=0}^{|\alpha_1|} \sum_{\substack{\alpha^J \subset \alpha_1 \cap J, \\ \left|\alpha^J\right| = k_2 - |\alpha_1 \cap K|}}$$

$$\sum_{\substack{\beta^J \subset \alpha_1 \cap J, \\ \left|\beta^J\right| = k_2 - |\alpha_1 \cap K|}} (-1)^{\sigma(\alpha \subset \alpha_1) + \sigma(\beta \subset \alpha_1)} \, |\mathbb{M}_{12}[\alpha_1 \setminus \alpha; \alpha_1 \setminus \beta]| \cdot |\mathbb{M}_{23}[\alpha; \beta]|$$

# Making it fast (Cont...)

## Low Rank of matrices...

Exploiting the special **LOW RANK** properties of $\mathbb{M}_{p_2 p_3}$ and its components $\mathbb{L}^{-1}{}_{22}\mathbb{L}_{23}$ and $\mathbb{L}^{-1}{}_{33}\mathbb{L}_{32}$.

Using Singular Value Decomposition (**SVD**) we have: $\mathbb{L}^{-1}{}_{22}\mathbb{L}_{23} = \mathbb{U}_{23}\mathbb{S}_{23}\mathbb{V}^{*}{}_{23}$ (for some relatively small rank R)

Our original decomposition becomes:

$$\begin{vmatrix} \mathbb{I}_{n1} & \mathbb{L}^{-1}{}_{11}\mathbb{L}_{12} & 0 \\ \mathbb{L}^{-1}{}_{22}\mathbb{L}_{21} & \mathbb{I}_{n2} & \mathbb{L}^{-1}{}_{22}\mathbb{L}_{23} \\ 0 & \mathbb{L}^{-1}{}_{33}\mathbb{L}_{32} & \mathbb{I}_{n3} \end{vmatrix} =$$

$$\left| \begin{bmatrix} \mathbb{I}_{n1} & 0 & 0 \\ 0 & \mathbb{I}_{n2} & 0 \\ 0 & 0 & \mathbb{V}^{*}{}_{23} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{n1} & \mathbb{L}^{-1}{}_{11}\mathbb{L}_{12} & 0 \\ \mathbb{L}^{-1}{}_{22}\mathbb{L}_{21} & \mathbb{I}_{n2} & \mathbb{L}^{-1}{}_{22}\mathbb{L}_{23} \\ 0 & \mathbb{L}^{-1}{}_{33}\mathbb{L}_{32} & \mathbb{I}_{n3} \end{bmatrix} \begin{bmatrix} \mathbb{I}_{n1} & 0 & 0 \\ 0 & \mathbb{I}_{n2} & 0 \\ 0 & 0 & \mathbb{V}_{23} \end{bmatrix} \right| =$$

$$\begin{vmatrix} \mathbb{I}_{n1} & \mathbb{L}^{-1}{}_{11}\mathbb{L}_{12} & 0 \\ \mathbb{L}^{-1}{}_{22}\mathbb{L}_{21} & \mathbb{I}_{n2} & \mathbb{U}_{23}\mathbb{S}_{23} \\ 0 & \mathbb{V}^{*}{}_{23}\mathbb{L}^{-1}{}_{33}\mathbb{L}_{32} & \mathbb{I}_{n3} \end{vmatrix}$$

# Low Rank of matrices (cont...)

Since the matrix $\mathbb{U}_{23}\mathbb{S}_{23}$ has rank **R**, it implies that the last **(n3 - R)** columns will have a single 1 from lower right $\mathbb{I}$ as shown in example below:

Let **n1 = 2, n2 = 2** and **n3 = 3**. So our original decompsition of the matrix will be:

$$\begin{vmatrix} 1 & 0 & b_{11} & b_{12} & 0 & 0 & 0 \\ 0 & 1 & b_{21} & b_{22} & 0 & 0 & 0 \\ c_{11} & c_{12} & 1 & 0 & d^*_{11} & d^*_{12} & 0 \\ c_{21} & c_{22} & 0 & 1 & d^*_{21} & d^*_{22} & 0 \\ 0 & 0 & e_{11} & e_{12} & 1 & 0 & 0 \\ 0 & 0 & e_{21} & e_{22} & 0 & 1 & 0 \\ 0 & 0 & e_{31} & e_{32} & 0 & 0 & 1 \end{vmatrix}$$

So, the final **(n3 - R)** rows do not contribute to the determinant. Therefore we can drop the last **(n3 - R)** rows and columns from the matrix while calculating the determinat which will **SPEED UP** the whole process.

For instance, for the above 7x7 orginal matrix, the code takes about 20 seconds to run. However after including the SVD modification, the code runs in 5-8 seconnds!!!. So, for a 7x7 matrix if the run time gain is around 10 seconds, **GAIN could be HIGH** for large nxn matrices.

# Status and Future Work

**Status:**

- Formula that establishes the interaction between Three groups and taking advantage of Low rank of matrices for accelerating the running time has been implemented in Python and tested.
- The finer details of figuring out Zero-Minors in $\mathbb{M}_{23}$ have been worked out and proved.

**Future Work:**

- Finding Zero-Minors in $\mathbb{M}_{12}$ and modifying the formula (2).
- Implementing acceleration related modification for $\mathbb{M}_{12}$ .
- Modifying the overall formula (2) to include Zero-Minor deletion.
- Generalizing the formula (2) for more than three groups.