CONSTRAINED MOLECULAR DYNAMICS MODEL (COMD) WITH GENERALIZED SYMMETRY ENERGY

JAIME SAHAGUN
ALDO BONASERA AND HUA ZHENG
CYCLOTRON INSTITUTE
TEXAS A&M UNIVERSITY
CONSTRAINED MOLECULAR DYNAMICS MODEL (COMD)

Computer Program (FORTRAN)

- Models interactions and dynamics of nucleon in nuclei
- Computational time is short enough to allow the study of the heaviest nuclei systems
- Study the Nuclear Equation of State
  - i. Exotic Nuclei
  - ii. Astrophysical Implications
1. Makes ground state nuclei
2. Models collisions of those nuclei
Distribution function of the $i$th nucleon:

$$f_i(r,p) = \frac{1}{(2\pi \sigma_r \sigma_p)^3} \cdot \exp \left[ -\frac{(r - \langle r_i \rangle)^2}{2\sigma_r^2} - \frac{(p - \langle p_i \rangle)^2}{2\sigma_p^2} \right]$$

Minimum Spanning tree Method:

Total Energy of the $i$th nucleon:

$$H = \sum_i \frac{\langle p_i \rangle^2}{2m} + V_i$$

Total Potential Energy:

$$V = V^{vol} + V^{(3)} + V^{sym} + V^{surf} + V^{Coul}.$$
THEORETICAL FRAMEWORK

Liquid Drop Model:

\[ E_B = a_V A - a_S A^{2/3} - a_A \frac{(A-2Z)^2}{A^{1/3}} - a_C \frac{Z(Z-1)}{A^{1/3}} + \delta(A, Z) \]

- **Volume term**
- **Surface term**
- **Asymmetry term**
- **Coulomb term**
- **Pairing term**

\[ V = V^{\text{vol}} + V^{(3)} + V^{\text{sym}} + V^{\text{surf}} + V^{\text{Coul}}. \]

- Volume term:
  \[ V^{\text{vol}} = \frac{f_0}{2 \rho_0} \sum_{i,j \neq i} \rho_{ij}, \]

- Asymmetry term:
  \[ V^{(3)} = \frac{f_3}{(\mu + 1)(\rho_0)^{\frac{1}{2}}} \sum_{i,j \neq i} \rho_{ij}^\mu, \]

- Symmetry term:
  \[ V^{\text{sym}} = \frac{a_{\text{sym}}}{2 \rho_0} \sum_{i,j \neq i} \left[ 2 \delta_{i, i} \delta_{j, j} - 1 \right] \rho_{ij}, \]

- Surface term:
  \[ V^{\text{surf}} = \frac{C_s}{2 \rho_0} \sum_{i,j \neq i} \nabla^2_{(r_j)}(\rho_{ij}), \]

- Coulomb term:
  \[ V^{\text{Coul}} = \frac{1}{2} \sum_{i,j \neq \text{protons}} \frac{e^2}{|\langle r_i \rangle - \langle r_j \rangle|} \text{erf} \left( \frac{|\langle r_i \rangle - \langle r_j \rangle|}{2 \sigma_r^2} \right). \]
Nuclear Equation Of State:

\[ \frac{E}{A}(\rho, m_x) = \left(1 + \frac{5}{9}m_x^2\right)\tilde{e}_f\tilde{\rho}^{2/3} + \left(1 + c_1m_x^2\right)\frac{A_1}{2}\tilde{\rho} + \left(1 + c_2m_x^2\right)\frac{B_1}{1 + \sigma}\tilde{\rho}^\sigma. \]

where:

\[ m_x = \frac{N - Z}{A} \]

Symmetric Energy:

\[ S(\rho) = \frac{5}{9}\tilde{e}_f\tilde{\rho}^{2/3} + c_1\frac{A_1}{2}\tilde{\rho} + c_2\frac{B_1}{1 + \sigma}\tilde{\rho}^\sigma. \]

Curvature of Symmetric Energy:

\[ L(\rho) = 3\rho_0\frac{\partial S(\rho)}{\partial \rho} = 3\left[\frac{10}{27}\tilde{e}_f\tilde{\rho}^{-1/3} + c_1\frac{A_1}{2} + c_2\frac{B_1\sigma}{1 + \sigma}\tilde{\rho}^{-1}\right], \]

Curvature of Symmetric Energy Coefficient:

\[ L(\rho_0) = L = 3\left[\frac{10}{27}\tilde{e}_f + c_1\frac{A_1}{2} + c_2\frac{B_1\sigma}{1 + \sigma}\right], \]
## CHECKING THE CODE

<table>
<thead>
<tr>
<th></th>
<th>Carbon 12</th>
<th>Oxygen 16</th>
<th>Calcium 40</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S(\rho_0) = 32.0$ MeV</td>
<td>New Code</td>
<td>Old Code</td>
<td>New code</td>
</tr>
<tr>
<td>BE/A average (MeV)</td>
<td>-11.8381</td>
<td>-11.8408</td>
<td>-10.4498</td>
</tr>
<tr>
<td>Avg Radius (fm)</td>
<td>3.497577</td>
<td>3.449</td>
<td>3.73763</td>
</tr>
</tbody>
</table>

- Similar BE/A values
- Similar Radius values
SYMMETRIC NUCLEI (N=Z)

- BE/A is not affected much by different L values

- Radius has no dependence on the curvature of symmetric energy
CALCIUM ISOTOPES ($^{34}\text{Ca}$)

- Not much change happens between $L=10-50$ (MeV)
- Only when $L$ is a large value do we see a change in binding energy and density

- Columbic force dominates
CALCIUM ISOTOPES (\(^{48}\text{Ca}\))

- Opposite behavior from \(^{34}\text{Ca}\)
- Not much change happens between 50–90 (MeV) L values

- Symmetric term dominates
NEUTRON CLUSTERS

- Neutron Cluster was affected more by the change on L as the previous results.

- Radius is negatively proportional to L.

- Creates small clusters of 2 neutrons.
HEAVIER NEUTRON CLUSTERS

- No matter the size of the cluster, it always seemed to settled at around -0.7 MeV

- Density increased with an increase of neutrons
CONCLUSION

• Code has been improved, modified with generalized symmetric energy
• Results showed interesting and promising results
• Code is ready for further research