有限振幅法による
中重領域核の光吸収断面積

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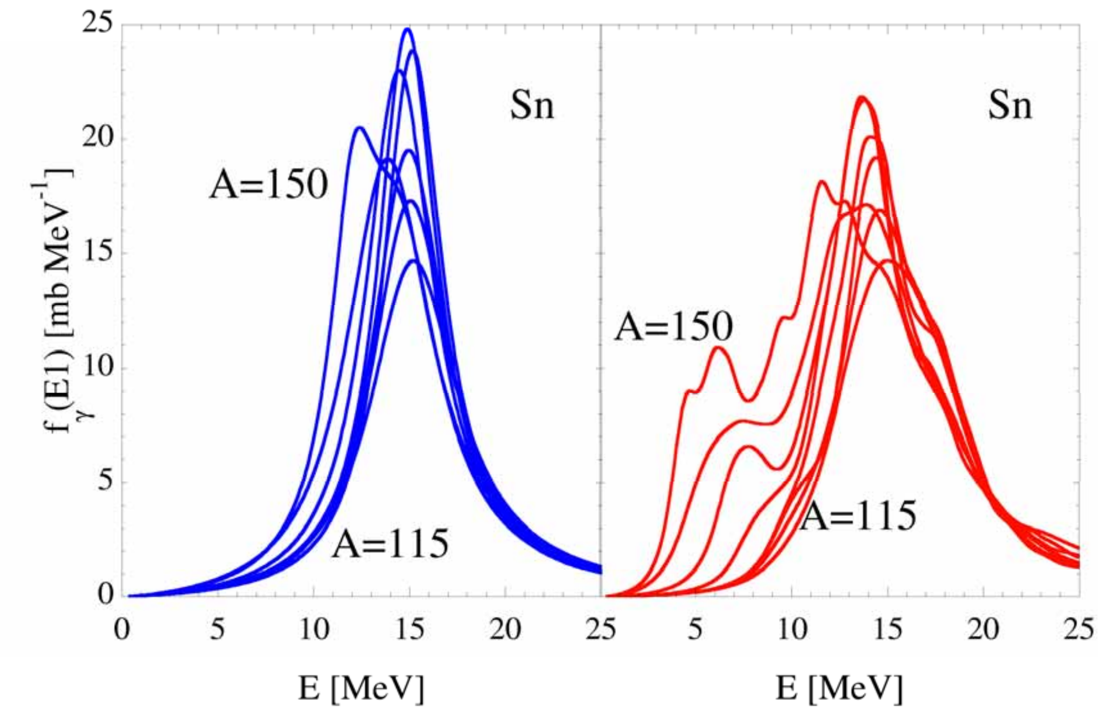
「計算科学による新たな知の発見・統合・創出」

光核反応断面積の重要性

- 最も基本的な反応断面積
- 広いエネルギー領域に渡って測定された原子核は安定核でもわずか
- 不安定核では皆無
- 応用的側面
  - クリーンな核変換
  - 元素合成ネットワーク計算

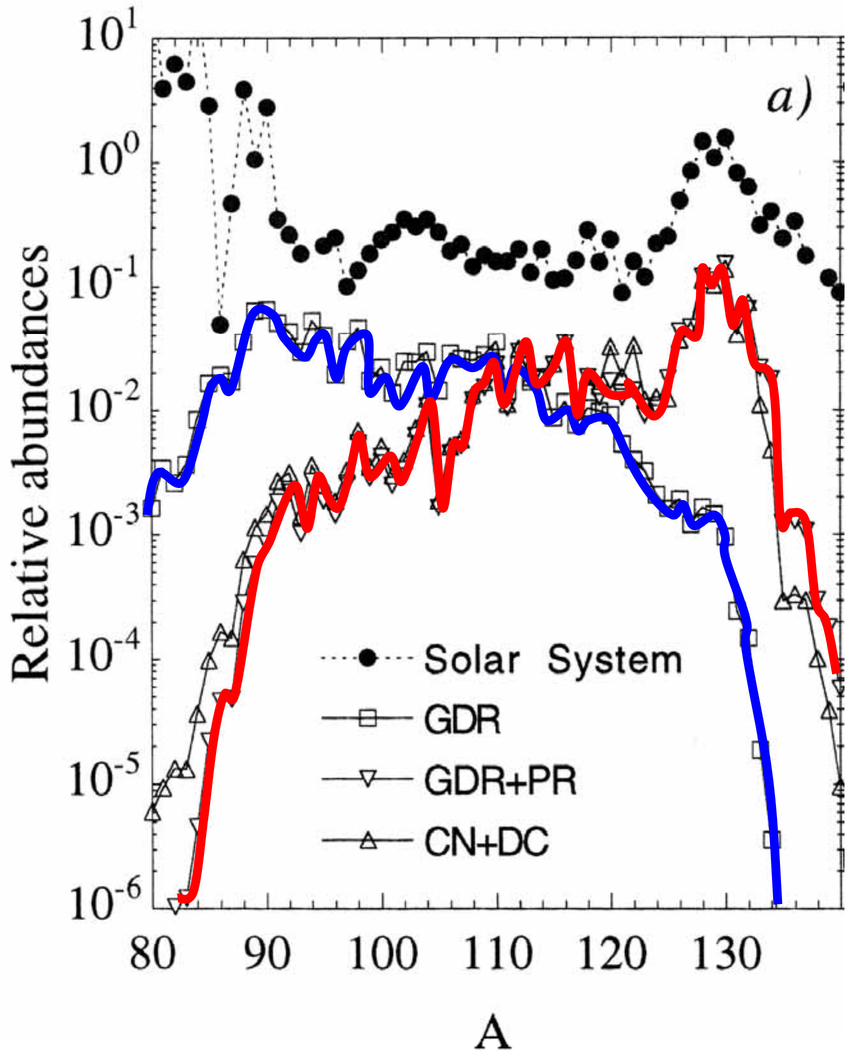
PDR: impact on the r-process

S. Goriely, Phys. Lett. **B436**, 10.



GDR
(phenom.)

GDR+pygmy
(microscopic)



Linear density response in the time-dependent density functional theory

One-body density operator under a TD external potential

$$i\frac{\partial}{\partial t}\rho(t) = \left[h_{\mathrm{KS}}[\rho(t)] + V_{\mathrm{ext}}(t), \rho(t)\right]$$

Assuming that the external potential is weak,

$$\rho(t) = \rho_0 + \delta\rho(t) \qquad h(t) = h_0 + \delta h(t) = h_0 + \left.\frac{\delta h}{\delta\rho}\right|_{\rho_0} \cdot \delta\rho(t)$$

$$i\frac{\partial}{\partial t}\delta\rho(t) = \left[h_0, \delta\rho(t)\right] + \left[\delta h(t) + V_{\mathrm{ext}}(t), \rho_0\right]$$

Let us take the external field with a fixed frequency ω,

$$V_{\mathrm{ext}}(t) = V_{\mathrm{ext}}(\omega)e^{-i\omega t} + V_{\mathrm{ext}}^{+}(\omega)e^{+i\omega t}$$

The density and residual field also oscillate with ω,

$$\delta\rho(t) = \delta\rho(\omega)e^{-i\omega t} + \delta\rho^{+}(\omega)e^{+i\omega t}$$

$$\delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t}$$

The linear response (RPA) equation

$$\omega\delta\rho(\omega) = \left[h_0, \delta\rho(\omega)\right] + \left[\delta h(\omega) + V_{\text{ext}}(\omega), \rho_0\right]$$

Note that all the quantities, except for ρ_0 and h_0, are non-hermitian.

$$\delta\rho(t) = \sum_{i=1}^{A}\left(\left|\delta\psi_i(t)\right\rangle\left\langle\phi_i\right| + \left|\phi_i\right\rangle\left\langle\delta\psi_i(t)\right|\right)$$

$$\Longrightarrow \quad \delta\rho(\omega) = \sum_{i=1}^{A}\left(\left|X_i(\omega)\right\rangle\left\langle\phi_i\right| + \left|\phi_i\right\rangle\left\langle Y_i(\omega)\right|\right)$$

This leads to the following equations for X and Y:

$$\omega\left|X_i(\omega)\right\rangle = \left(h_0 - \varepsilon_i\right)\left|X_i(\omega)\right\rangle + \hat{Q}\left\{\delta h(\omega) + V_{\text{ext}}(\omega)\right\}\left|\phi_i\right\rangle$$

$$\omega\left\langle Y_i(\omega)\right| = -\left\langle Y_i(\omega)\right|\left(h_0 - \varepsilon_i\right) - \left\langle\phi_i\right|\left\{\delta h(\omega) + V_{\text{ext}}(\omega)\right\}\hat{Q}$$

$$\hat{Q} = \sum_{i=1}^{A}\left(1 - \left|\phi_i\right\rangle\left\langle\phi_i\right|\right)$$

These are often called “RPA equations” in nuclear physics.
X and Y are called “forward” and “backward” amplitudes.

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

A method to avoid the explicit calculation of the residual fields (interactions)

$$\delta\rho(t) = \delta\rho(\omega)e^{-i\omega t} + \delta\rho^{+}(\omega)e^{+i\omega t}$$

$$\delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t}$$

Residual fields are proportional to $\delta\rho(\omega)$

$$\delta h(\omega) = \left.\frac{\delta h}{\delta\rho}\right|_{\rho_0} \cdot \delta\rho(\omega) \qquad \delta\rho(\omega) = \sum_{i=1}^{A}\left(\left| X_i(\omega) \right\rangle\left\langle \phi_i \right| + \left| \phi_i \right\rangle\left\langle Y_i(\omega) \right| \right)$$

This can be obtained with non-hermitian *pseudo*-density operators

$$\tilde{\rho}_\eta \equiv \rho_0 + \eta\delta\rho(\omega) = \sum_{i=1}^{A}\left(\left|\phi_i\right\rangle + \eta\left| X_i(\omega)\right\rangle \right)\left(\left\langle \phi_i \right| + \eta\left\langle Y_i(\omega)\right| \right) + O(\eta^2)$$

$$h[\tilde{\rho}_\eta] = h[\rho_0] + \eta\delta h(\omega) + O(\eta^2)$$

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

Residual fields can be estimated by the finite difference method:

$$\delta h(\omega) = \frac{1}{\eta}\left(h\left[\langle\psi'|,|\psi\rangle\right] - h_0\right)$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta|X_i(\omega)\rangle, \quad \langle\psi_i'| = \langle\phi_i| + \eta\langle Y_i(\omega)|$$

Starting from initial amplitudes $X^{(0)}$ and $Y^{(0)}$, one can use an iterative method to solve the following linear-response equations.

$$\omega|X_i(\omega)\rangle = (h_0 - \varepsilon_i)|X_i(\omega)\rangle + \hat{Q}\{\delta h(\omega) + V_{\text{ext}}(\omega)\}|\phi_i\rangle$$

$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \varepsilon_i) - \langle\phi_i|\{\delta h(\omega) + V_{\text{ext}}(\omega)\}\hat{Q}$$

Programming of the RPA code becomes very much trivial, because we only need calculation of the single-particle potential, with different bras and kets.

Numerical Algorithm

T.N., Inakura, Yabana, PRC76 (2007) 024318.

We want to solve the following linear-response equations:

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = -\begin{pmatrix} (V_{\text{ext}})_{mi} \\ (V_{\text{ext}})_{im} \end{pmatrix}$$

This is the linear algebraic equation of the form:

$$\mathbf{A}\vec{x} = \vec{b}$$

Starting from an initial vector $\vec{x}^{(0)}$, one can use an iterative method to solve the equations.
In the iterative algorithm, we do not need an explicit matrix of **A**, but only need to calculate $\mathbf{A}\vec{x}^{(n)}$

For non-hermitian matrix **A**, Bi-Conjugate Gradient Method, Generalized Conjugate Residual Method, etc.

Skyrme FAM in 3D real space

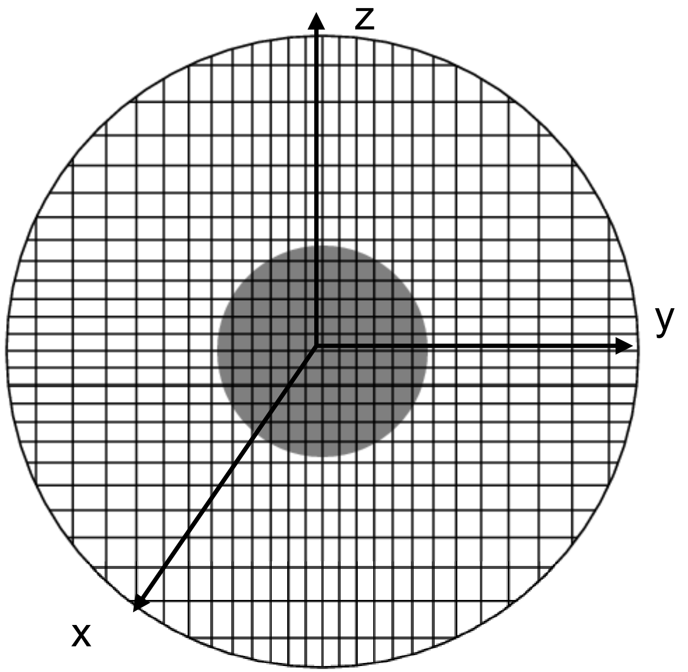
Linear response equations

$$\omega X_i(\omega;\vec{r}) = (h_0 - \varepsilon_i) X_i(\omega;\vec{r}) + \hat{Q}\{\delta h(\omega) + V_{\rm ext}(\omega)\}\phi_i(\vec{r})$$

$$-\omega^* Y_i(\omega;\vec{r}) = (h_0 - \varepsilon_i) Y_i(\omega;\vec{r}) + \hat{Q}\{\delta h^+(\omega) + V_{\rm ext}^+(\omega)\}\phi_i(\vec{r})$$

3D space is discretized in lattice

F & B amplitudes: $X_i(\mathbf{r},\omega) = \{X_i(\mathbf{r}_k,\omega_n)\}_{k=1,\ldots Mr}^{n=1,\ldots ME}, \quad i = 1,\ldots,N$



N: Number of particles

Mr: Number of mesh points

ME: Number of energy points

Spatial mesh size is about 0.8 fm.

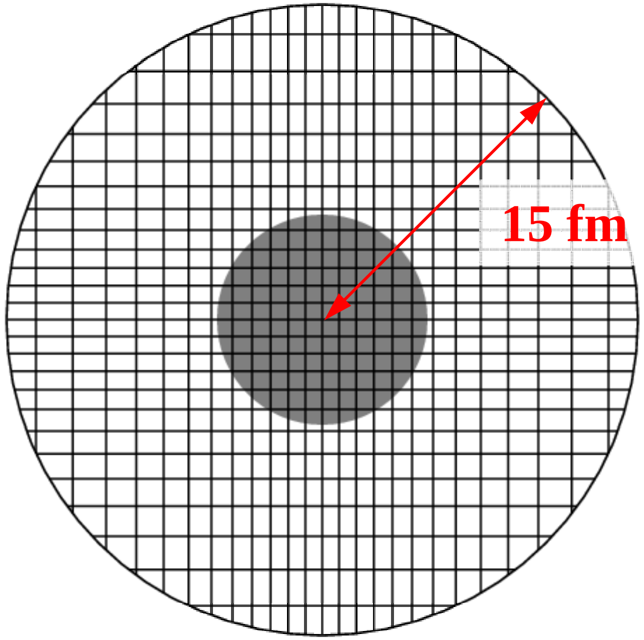
Energy mesh size is about 0.3 MeV

Inakura, Nakatsukasa, Yabana, in preparation.

Numerical Details

- SkM* interaction
- 3D mesh in **adaptive coordinate**
- R_{box} = 15 fm, about 10,000 grid points
- Complex energy with Γ = 1.0 MeV
- ΔE = 0.3 MeV

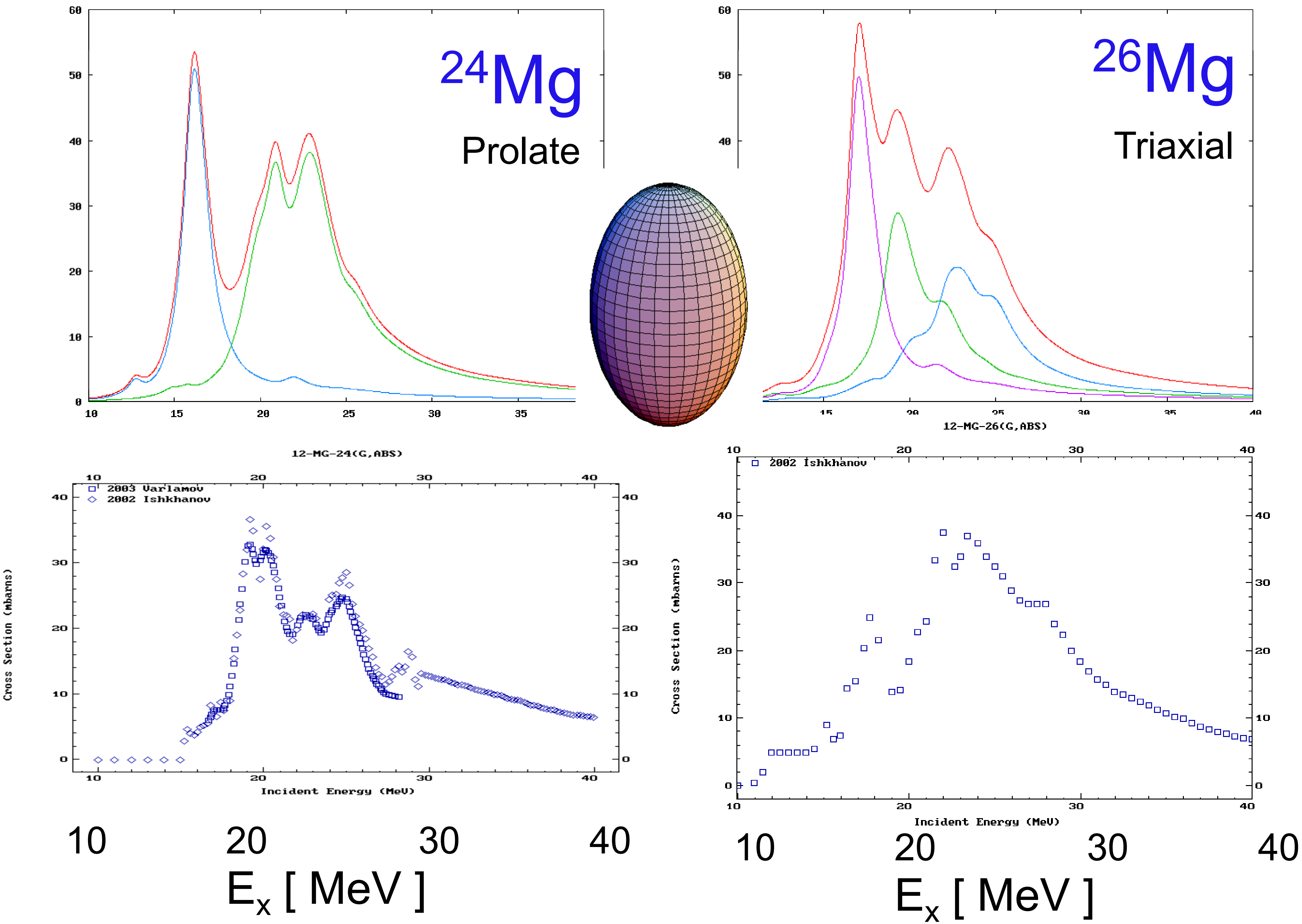
  up to E = 38.1 MeV (128 points)
- **Energy-paralleled** calculation



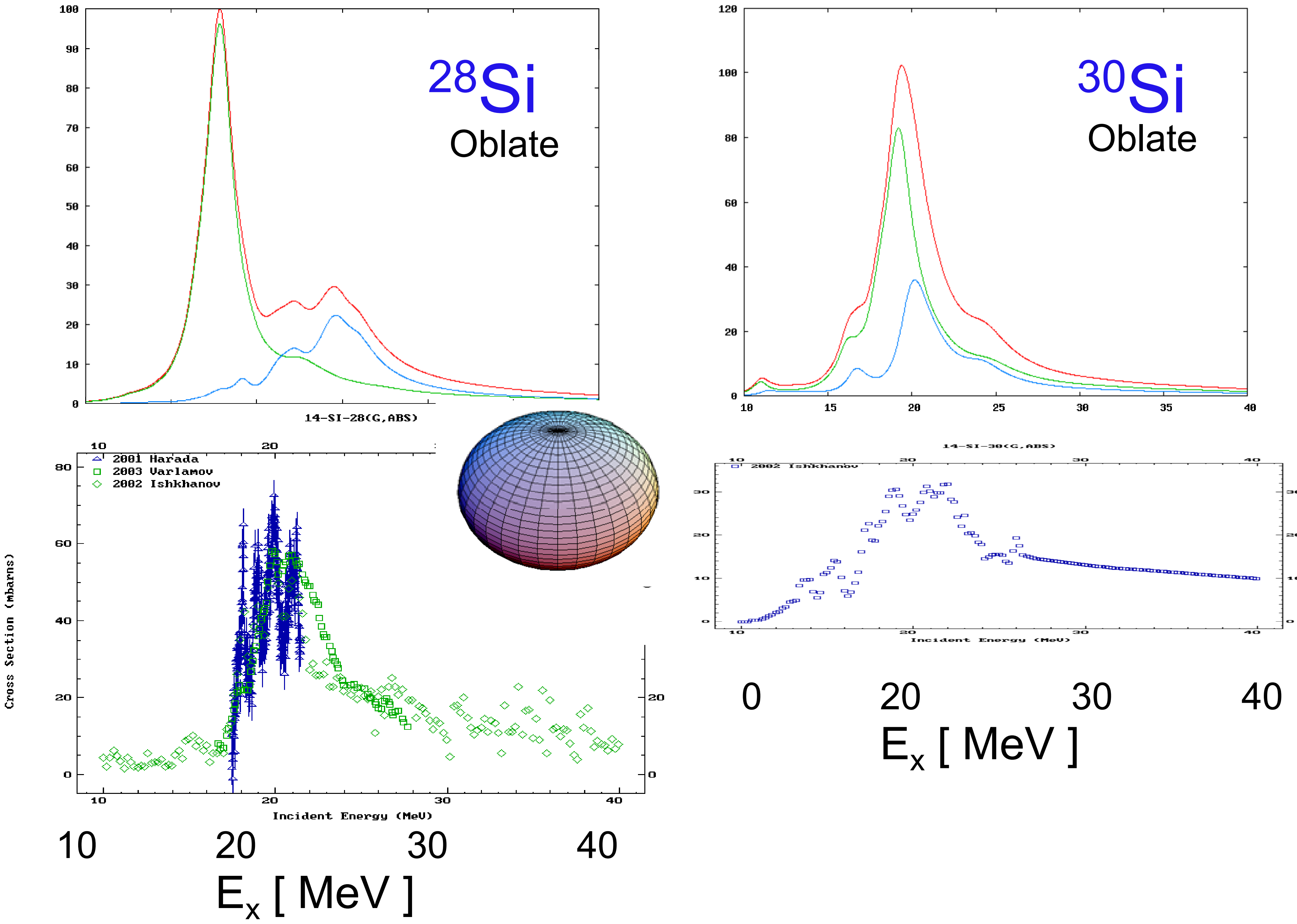
adaptive coordinate
PRC71, 024301

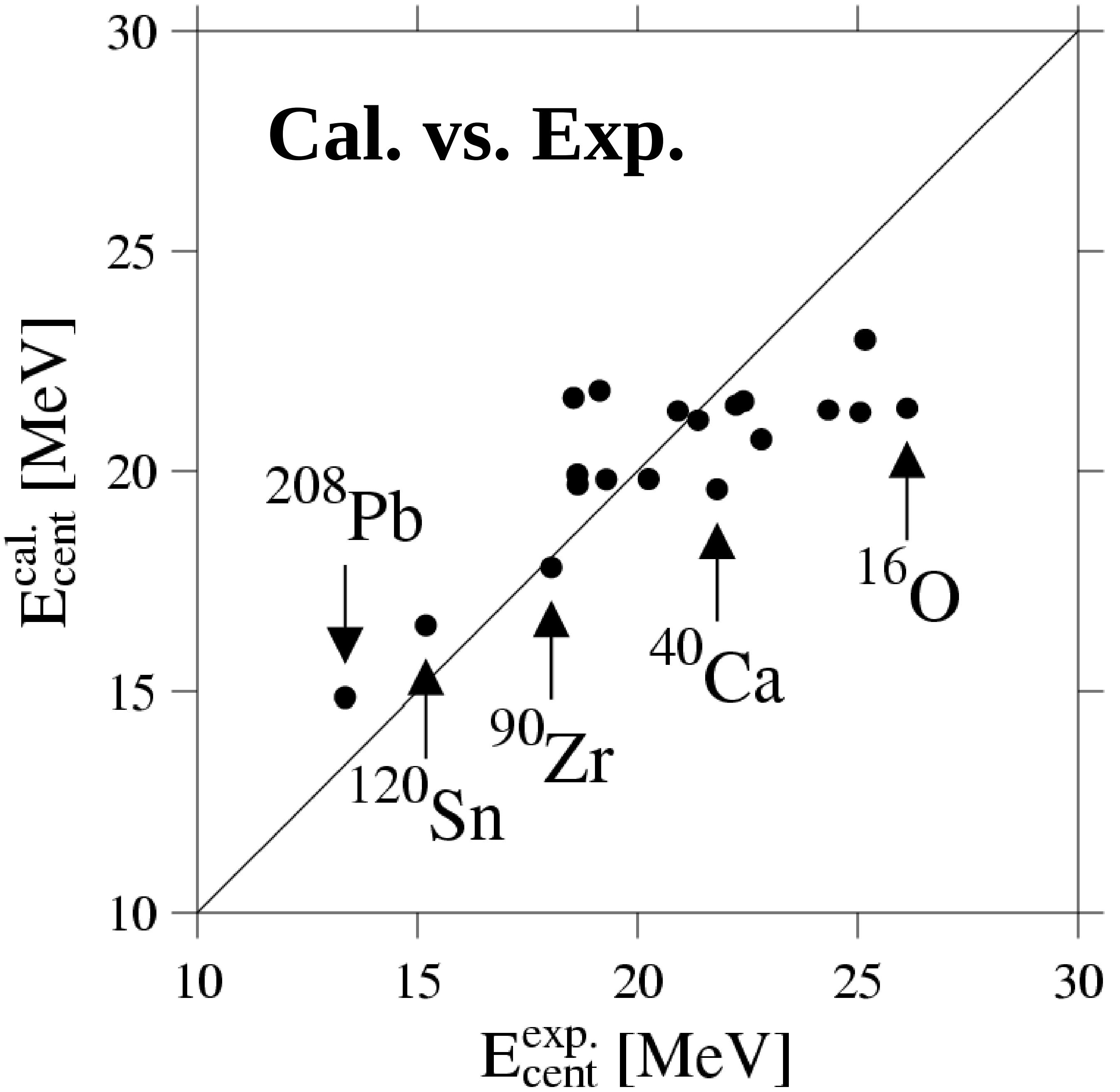
PACS-CS
Parallel Array Computer System
for Computational Sciences

PACS-CS @ Univ. of Tsukuba   T2K@ Univ. of Tsukuba



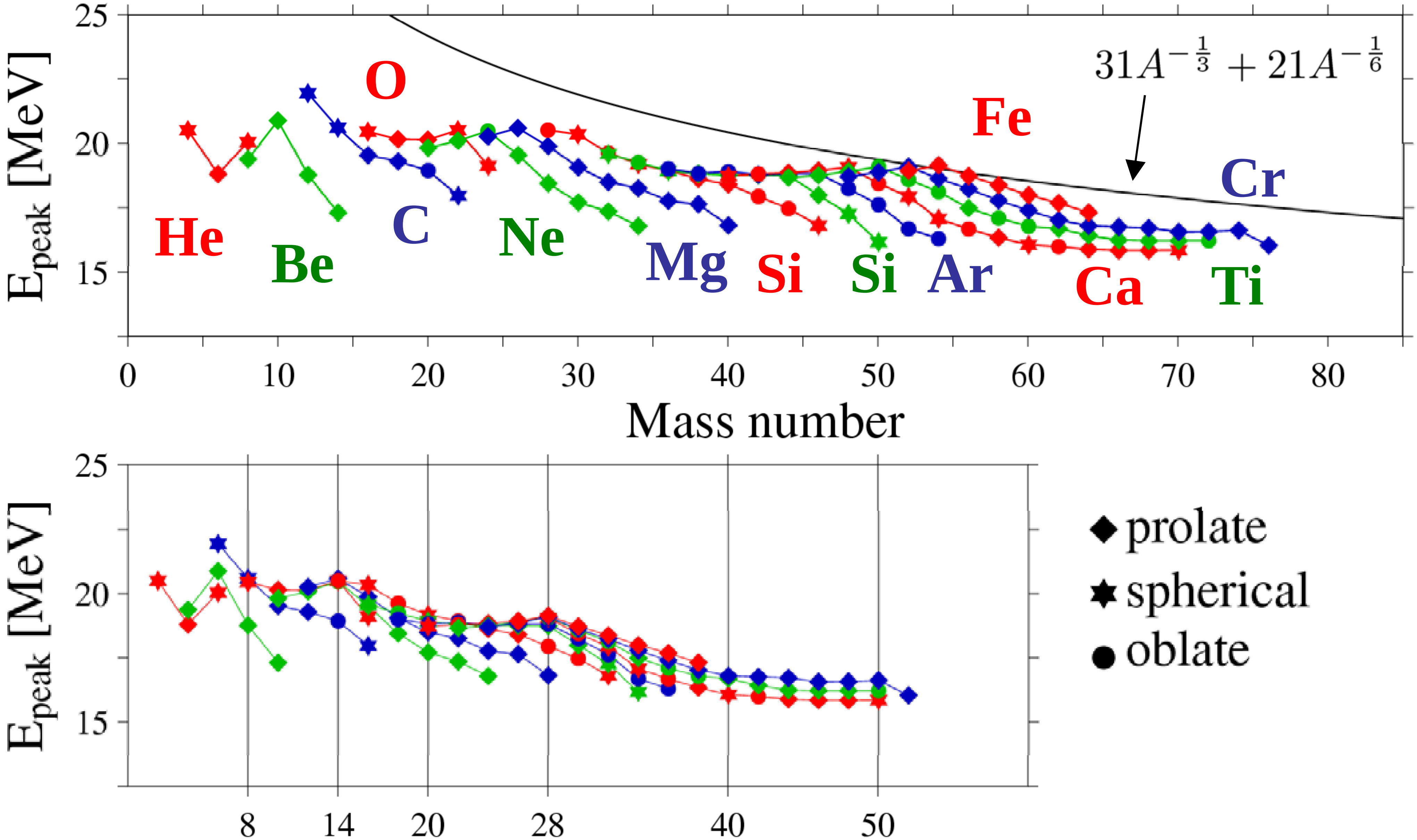
24Mg
Prolate
26Mg
Triaxial
12-MG-24(G,ABS)
12-MG-26(G,ABS)
2003 Varlamov
2002 Ishkhanov
2002 Ishkhanov
Cross Section (mbarns)
Cross Section (mbarns)
Incident Energy (MeV)
Incident Energy (MeV)
10 20 30 40
E_x [MeV]
10 20 30 40
E_x [MeV]


28Si
Oblate
14-SI-28(G,ABS)
2001 Harada
2003 Varlamov
2002 Ishkhanov
Cross Section (mbarns)
Incident Energy (MeV)
10 20 30 40
Ex [MeV]
30Si
Oblate
14-SI-30(G,ABS)
2002 Ishkhanov
Incident Energy (MeV)
0 20 30 40
Ex [MeV]



Cal. vs. Exp.
^{208}Pb
^{120}Sn
^{90}Zr
^{40}Ca
^{16}O
30
25
20
15
10
10
15
20
25
30
$E_{cent}^{cal.}$ [MeV]
$E_{cent}^{exp.}$ [MeV]

Centroid energy of IVGDR



Summary

- 有限振幅法に基づく光核反応のＴＤＤＦＴ計算
  - 通常の行列形式では大変なプログラミング作業が必要
  - 有限振幅法では、プログラミング作業が非常に小さい
  - 光子エネルギーを固定することで、単純な並列化が可能
  - Z=30領域核までの偶々核の光吸収断面積
  - 軽い核ではピークエネルギーを２～３ＭｅＶ過小評価
  - 重い核ではほぼ実験データを再現
  - ピークエネルギーに殻効果
- さらに大きな質量数領域に向けて
  - 超流動原子核を扱える準粒子形式に拡張