

Current Status of Vilnius Parallel Shell Model Code (VPSM)



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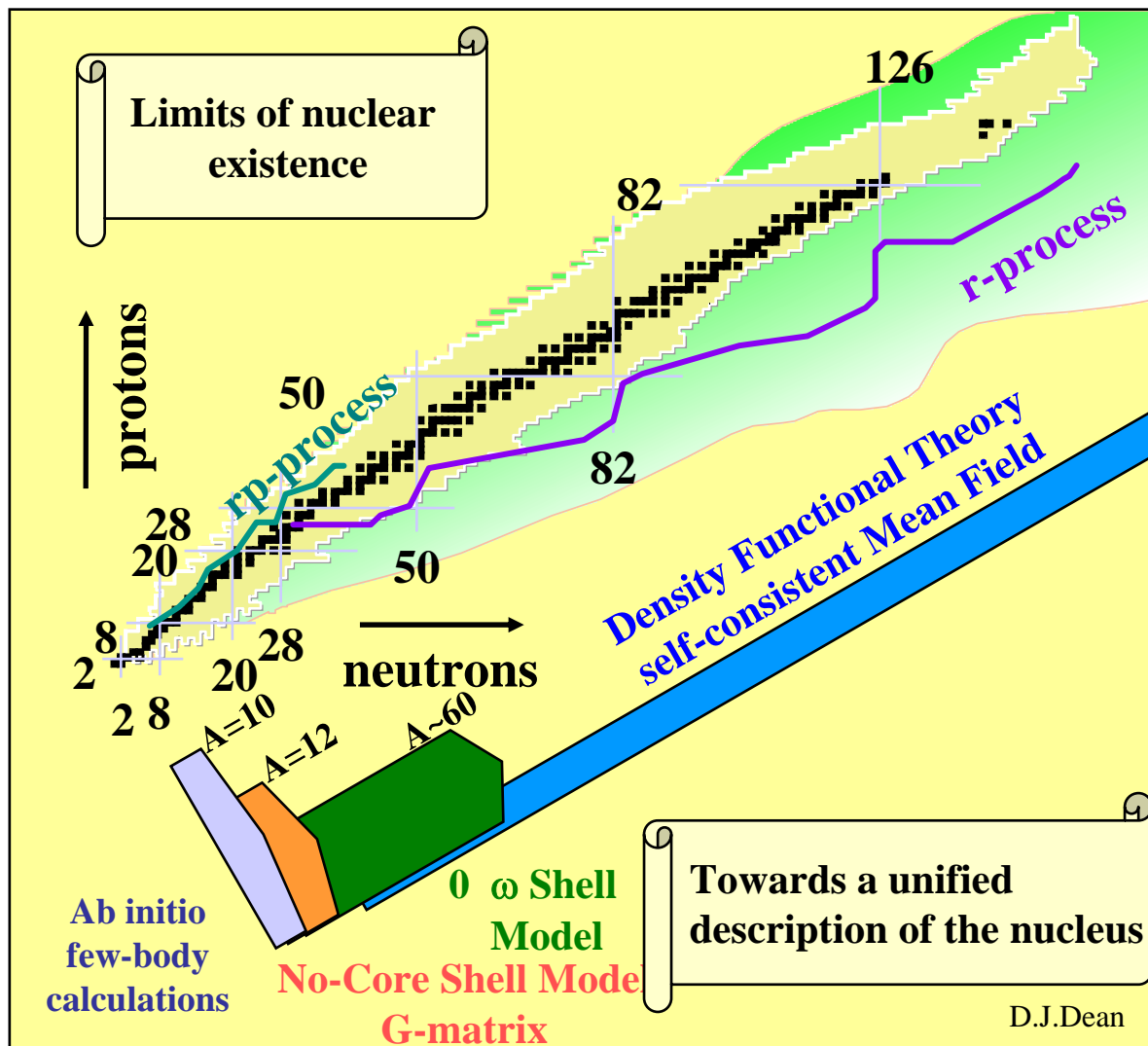
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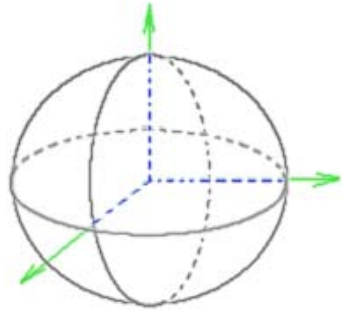
Objectives

- To create a distributed-computation shell model code to study properties of nuclei in the *gds* shell ($A=80-100$):
 - Excitation spectra
 - Gamow-Teller resonances
 - Lifetimes
- Gamow-Teller resonance is important for the lepton-nucleus reaction rates and spontaneous beta-decays of nuclei
- Nuclei close to ^{100}Sn are interesting:
 - These are the last experimentally observed $N=Z$ nuclei
 - Nuclear input for fast proton capture process (rp-process) is insufficient

Computational Nuclear Structure



Spherical Shell Model



Spherically symmetric mean field

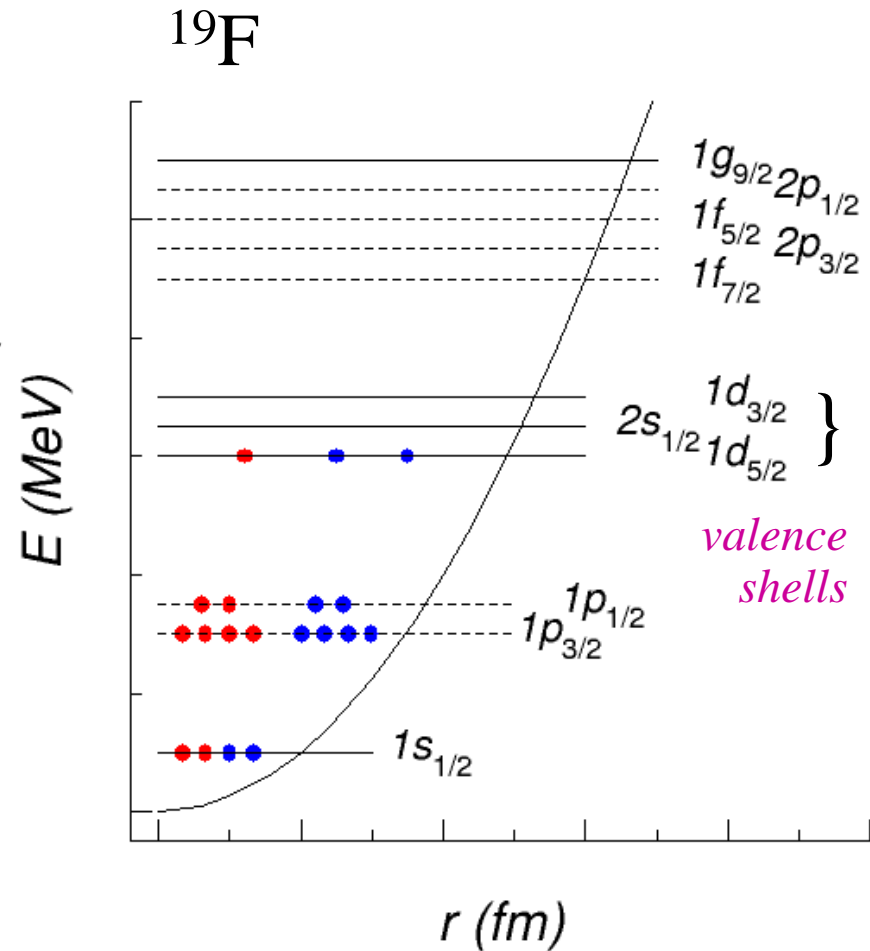
$$\hat{H} = \sum_{\alpha} \varepsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}$$

Hamiltonian has two sets of parameters:

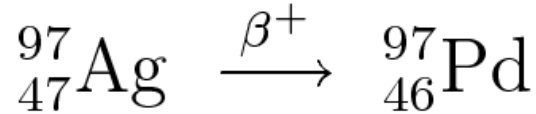
- single-particle energies
- interaction matrix elements

There is a choice of the valence space

The basis dimension $D \propto \binom{N_p}{p} \binom{N_n}{n}$

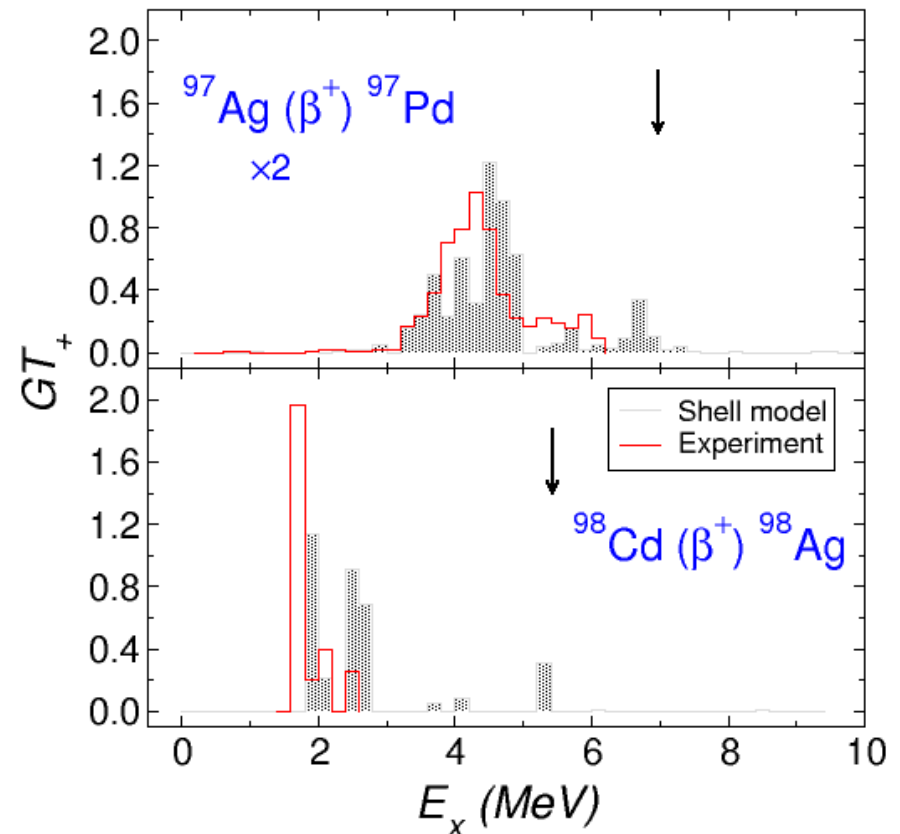
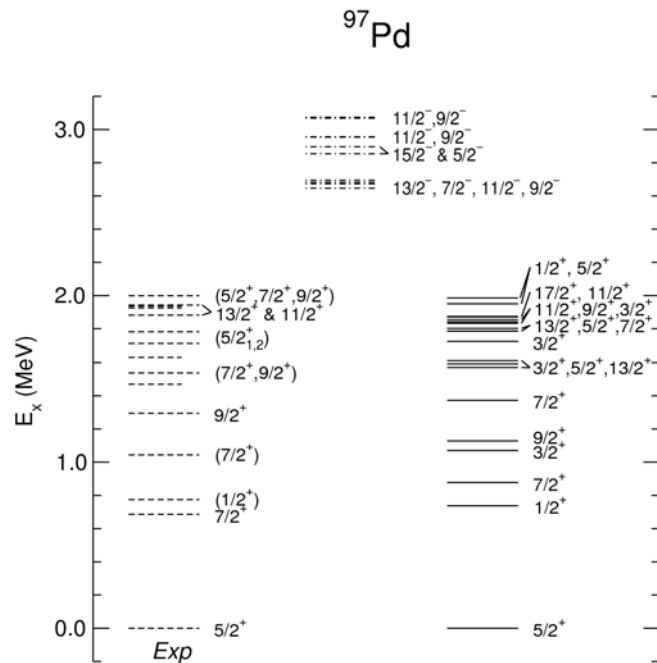


Gamow-Teller Distribution in $^{97}_{46}\text{Pd}$



$$GT_+ = \left(\frac{g_A}{g_V}\right)^2 \frac{1}{\xi_{eff}} \frac{1}{2J_i + 1} \sum_f \left| \langle \Psi_f || \sum_k \sigma(k) \tau_+(k) || \Psi_i \rangle \right|^2$$

Model space: $\pi 2p_{1/2}, 1g_{9/2};$
 $\nu 3s_{1/2}, g_{7/2}, h_{11/2}$



VPSM Status

- First version was created last year
- Programming language C/C++; 21 module
- It is suited for both uniprocessor and multiprocessor (MPI layer) computations
- On September it was used to test MPI on clusters by K.Paulikas (KTU)
- It was used for a pilot study of Gamow-Teller resonances in $A=84-87$ nuclei (not on grid!)

Computation diagram: Spectrum

To get excitation spectra

- Read input
 - Prepare temporary tables
 - Prepare matrices needed for computation
 - Iterate Matrix-Vector multiplication, until desired convergence is achieved
 - Obtain eigenvectors and eigenvalues and print output
-
- Some of the temporary tables can be reused for another nucleus
 - The matrices can be reused for operations in the same nuclear system

Computation diagram: GT distributions

To get Gamow-Teller distribution

- Get excitation spectrum (or at least the ground state) of the parent nucleus (Z,N)
- Act with GT operator and obtain the doorway state into the daughter nucleus $(Z-1,N+1)$
- Get excitation spectrum (or at least the ground state) of the daughter nucleus $(Z-1,N+1)$
- Use matrices of the daughter nucleus to obtain the GT strength distribution
- Use information about the daughter nucleus ground state energy to adjust distribution's excitation spectrum

Difficulties and Problems

- The matrix dimension grows exponentially as more nucleons or more orbits are active
- The program is very memory-intensive (both RAM and disk)

For example: ^{87}Mo nuclear system modelled as

2 active protons in $g_{9/2}d_{5/2}s_{1/2}$ (18 orbits) and

5 active neutrons in $g_{9/2}d_{5/2}s_{1/2}g_{7/2}d_{3/2}$ (30 orbits)

$D=1.5 \cdot 10^6$; The matrix was divided into 20 rows

Temporary files 9.9 Gb (the largest one – 429Mb)

Out of these 7.1 Gb are taken by files needed for the computation

Check-point file after 100 iterations – 1.2 Gb (this is the amount of RAM needed + 0.3 Gb for the largest table).

This gave energies of 4 lowest states

VPSM Outlook

- Identify the steps requiring most disk space and the largest amount of RAM. Try to amend the demands (maybe by doing more computations)
- Implement storage of the vectors on disk, instead of keeping them in memory (at the moment only the matrix can be split into pieces).
Maybe implement splitting of the vectors themselves
- Implement a multistep calculation where data would be sent and received from the storage elements

Grid Experience

- The grid is not “MPI-friendly”
- The test problem: Gamow-Teller decay of the ^{44}V ground state.
 - Dimensions are small: $D(^{44}\text{V})$ and $D(^{44}\text{Ti})$ are less than 4000.

Computations in the Grid I

5 lentelė: Proposed clusters to solve the test problem $^{44}\text{V}(\text{GT}_+)^{44}\text{Ti}$ and computational success

`glite-job-list-match --vo balticgrid gt_44VTi.jdl`

No.	Cluster	Node number, N_p	Was it ok?	Remarks
1	atomas.itpa.lt	6 [†]	+	64-bit cluster, "non-standard" compilation
2	birzs.latnet.lv	16	+	One day tasks were aborted
3	grid2.mif.vu.lt	22	–	It was unable to complete. The system was always waiting for one computer to respond
4	grid5.mif.vu.lt	22	–	Tasks were aborted
5	kriit.eenet.ee	10	–	Computation ran to unfinity (no results)
6	pupa.elen.ktu.lt	10	+	Computation ran fast
7	zeus02.cyf-kr.edu.pl	272	–	Was unable to compute: non-standard system?

[†] The cluster Atomas has 8 CPU, but only 6 were available during the days of studies (end of November, 2006).

Computations in the Grid II

6 lentelė: Calculation of Gamow-Teller distributions in ^{44}Ti on cluster Atomas. The matrix was divided into 6 pieces by rows. The time is averaged over two runs. t_{N_p} is the computation time using N_p processors.

Number of processors, N_p	Execution time (mins)	Speed-up t_1/t_{N_p}	Effectiveness $t_1/(N_p t_{N_p})$
<i>Over grid</i>			
1	12.74	1.00	1.00
2	8.16	1.56	0.78
4	6.85	1.86	0.46
6	3.44	3.70	0.62
<i>Interactively on a 2-CPU node</i>			
1	1.32	1.00	1.00
2	0.70	1.89	0.94

Note: Cluster Atomas is heterogeneous: 4CPU + 2x2CPU

Computations in the Grid III

7 lentelė: Calculation of Gamow-Teller distributions in ^{44}Ti on BalticGrid clusters. Computation time when $N_p = 1, 6$ and 8 . The matrix divided into 6 pieces by rows. The time is averaged over 3 runs discarding one, if it is notably greater.

Cluster	Computation time (mins)			Speed-up	Effectiveness
	t_1	t_6	t_8 †	t_1/t_6	$t_1/(6t_6)$
Atomas (VU ITPA, over grid)	12.52	3.51	–	3.6	0.60
Birzs (Latvia)	–*	1.00 ^a	0.95	–	–
Pupa (Kaunas)	1.36	0.52	0.59 ^b	2.6	0.44
Zeus02 (Poland)	1.04	–	–	–	–

† The matrix is split into 8 rows.

^a Discarded time 9.0 mins

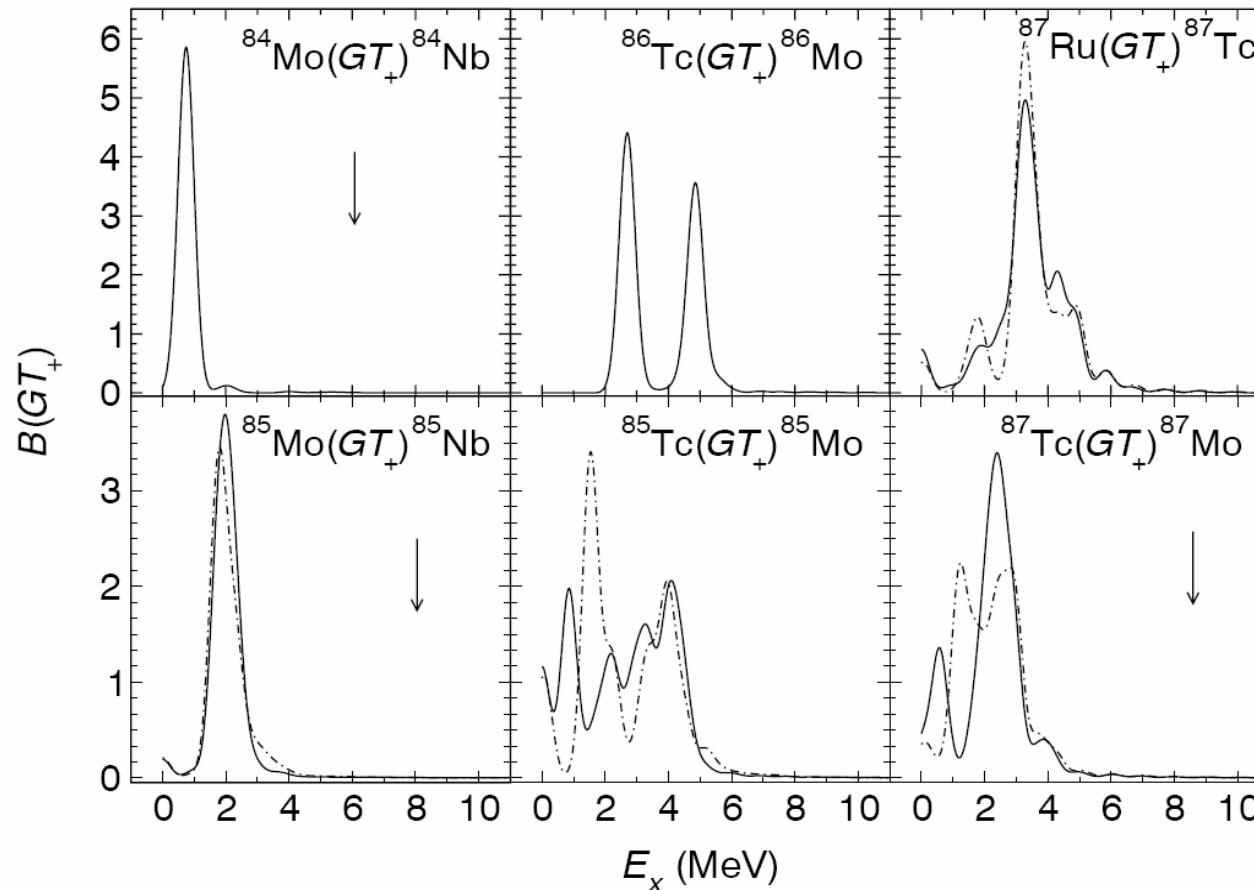
^b Discarded time 1.3 mins

* The cluster refused to run MPI code with only one process

Note: last week I got an email from Zeus02 administrator that the file system for BalticGrid VO was changed to NTFS. The feasibility of calculation is not tested yet.

Distributions of the Gamow-Teller Strength

Calculated using a PC with large RAM



2 pav.: Gamow-Teller distributions in nuclei with $A = 84-87$. Arrows indicate the value of Q_{Ec} , if it is smaller than 10 MeV. The discrete distributions were Gaussian-smoothed using $\sigma = 0.5$ MeV. In some nuclei the decay of both the ground state (solid line) and the calculated first excited state (dashed line) are shown.

Beta-decay of ^{86}Mo

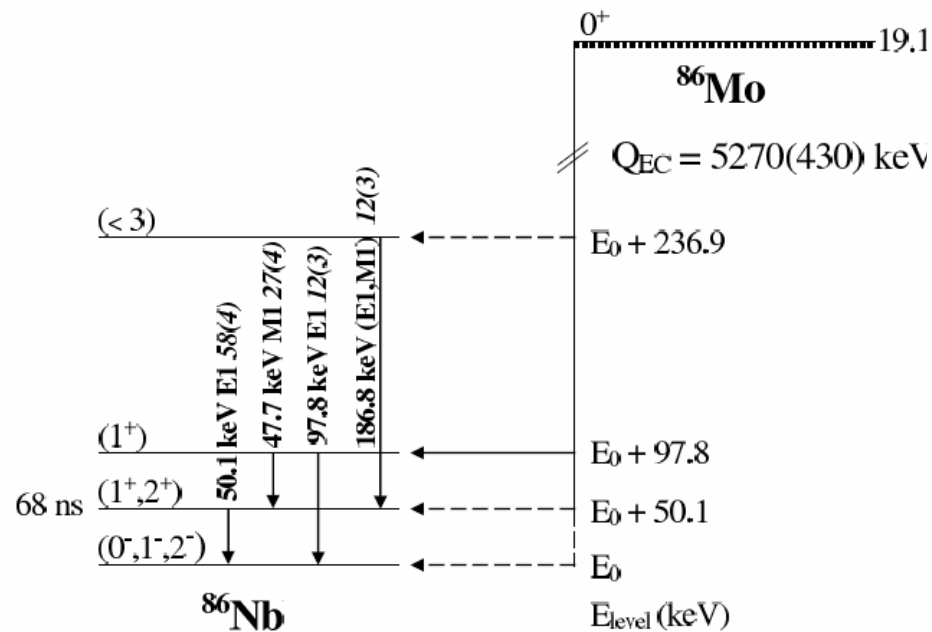
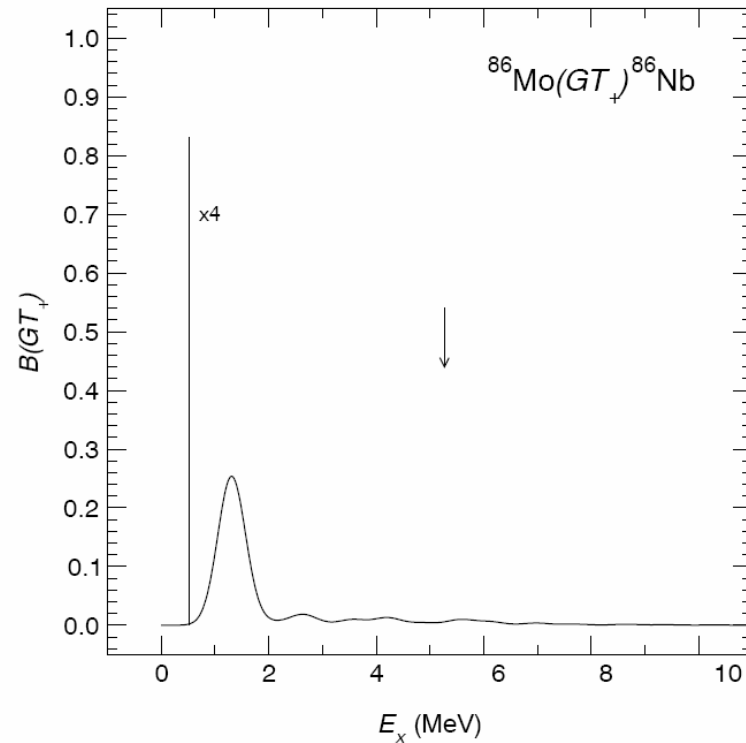


Fig. 18. A proposed decay scheme of ^{86}Mo . The γ -intensities are normalised by the 50.1 keV transition. The Q -value is taken from ref. [21].



Conclusions

- The first version of a distributed-memory shell model code VPSM was created. It works both on a PC and on a computer cluster with MPI installed.
- Computations are resource-intensive, which limits possibilities to run on the grid clusters. Main problem, so far, is the demand of RAM. This should be targeted first.
- Using this code, the Gamow-Teller strength distributions in the *gds* nuclei with the mass numbers $A \leq 87$ were calculated.