Implementation of the ETACHA4 code to the LISE^{++} package

i. Porting from FORTRAN to C++

ii. Creation the ETACHA GUI shell for Windows OS

iii. Modify LISE^{++} to use ETACHA.dll in LISE^{++} transmission calculations

iv. Update LISE.xls to provide ETACHA calculations in MS Excel (???)

Important!!

ETACHA4 (GUI-version) is still under construction.
ODE integrator should be updated!

MICHIGAN STATE UNIVERSITY LISE++

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Extension of charge-state-distribution calculations for ion-solid collisions towards low velocities and many-electron ions

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Knowledge of the detailed evolution of the whole charge-state distribution of projectile ions colliding with targets is required in several fields of research such as material science and atomic and nuclear physics but also in accelerator physics, and in particular in regard to the several foreseen large-scale facilities. However, there is a lack of data for collisions in the nonperturbative energy domain and that involve many-electron projectiles. Starting from the ETACHA model we developed [Rozet *et al.*, Nucl. Instrum. Methods Phys. Res., Sect. B **107**, 67 (1996)], we present an extension of its validity domain towards lower velocities and larger distortions. Moreover, the system of rate equations is able to take into account ions with up to 60 orbital states of electrons. The computed data from the different new versions of the ETACHA code are compared to some test

Current LISE^{++} Development : ETACHA4

the projectile perturbation parameter K_p:

$$K_p = \frac{Z_t}{Z_p}\frac{v_e}{v_p},$$

where Z_t and Z_p are the target and projectile atomic numbers, v_e the mean orbital velocity of the active electron, and v_p the projectile velocity.

1. Beyond the perturbative regime for projectile states from n = 1 to 4

Our previous version of the ETACHA code [4] was well suited to a high-velocity and low-perturbation regime, the aim being to optimize the production of high charge states after the stripping solid foil. Therefore, the first (or plane-wave) Born approximation (PWBA) can be safely used for ionization and excitation [14,15], whereas the continuum distorted-wave (CDW) approximation [16] reproduces very well the capture cross sections. However, beside the number of states that needs to be included to handle projectile ion states up to $n = 4$, the extensions of the ETACHA code intend also to tackle collision systems in the nonperturbative regime in which those theoretical approaches are well known to fail in reproducing experimental results. In this respect, one can

1. ETACHA4 calculates evolution of charge state distributions in 10-100 MeV/u. Quality calculation for K < 1; Global works above 70 MeV/u
2. Important for the FRIB stripping foil project. NSCL database (?)
3. GLOBAL : Z-q ≤ 28, ETACHA4: Z-q ≤ 60. ETACHA5 is under development (n ≥ 5)
4. Benchmark energy range application

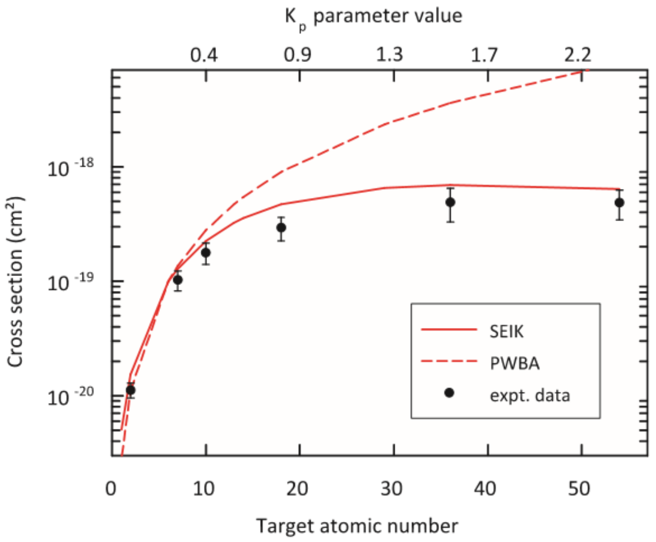
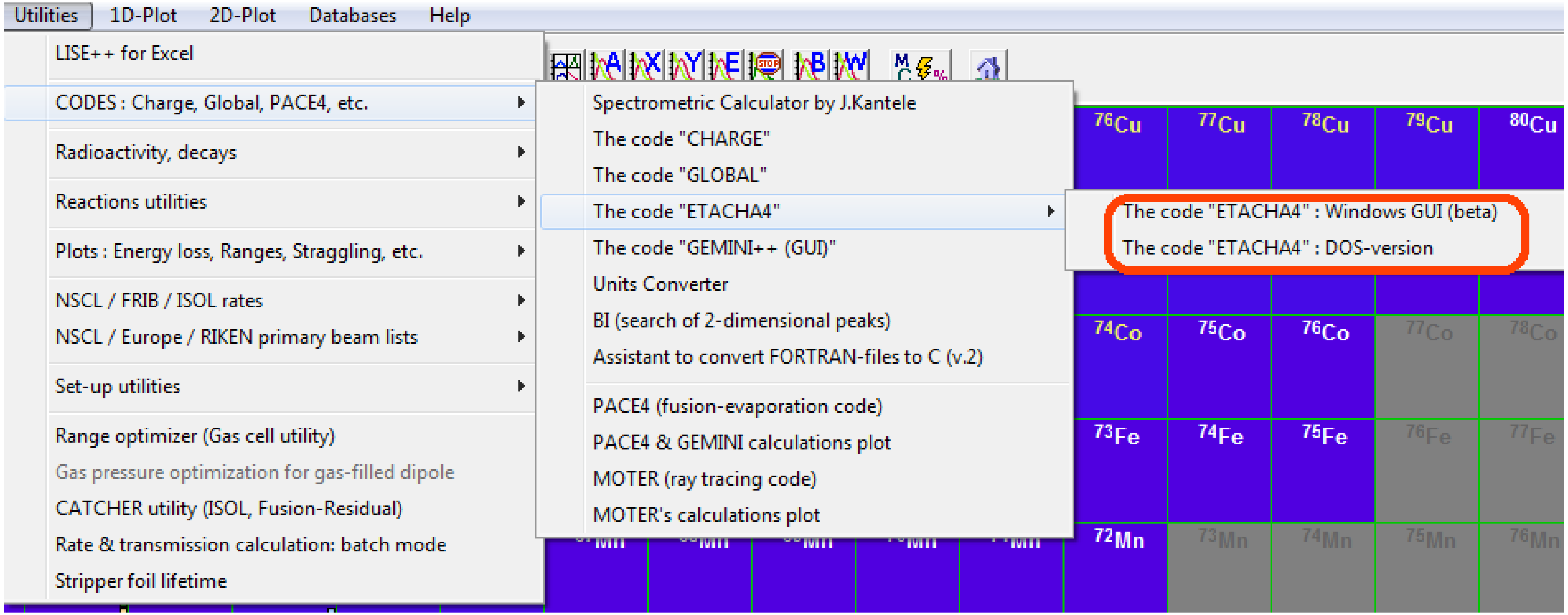


FIG. 3. (Color online) $1s-2p$ excitation cross section for Ar^{17+} ions at a fixed velocity $v_p = 23$ a.u. (13.6 MeV u^{-1}) as a function of exciting target atomic number. Dots with error bars, experiment [21];

Therefore, the ETACHA code should provide rather reliable data for some of the collision systems envisaged to cover the entire ^{100}Sn region with the Super Spectrometer Separator at SPIRAL2, as for $^{58}Ni^{19+}$ on ^{40}Ca, ^{46}Ti, ^{50}Cr, or ^{54}Fe from 3.5 to 4.5 MeV u^{-1} [8]. Nevertheless, preliminary comparisons between ETACHA and measurements performed with 11 MeV u^{-1} U^{38+} ions impinging on carbon targets (a system of importance for the design of the Rare Isotope Accelerator driver linac at Michigan State University (MSU)) [48] exhibit the requirement to even extend the ETACHA code towards the inclusion of $n \geqslant 5$. Although ETACHA4 can in principle be applied to ions with up to 60 electrons (a full $n = 4$ shell), to correctly account for the $n + 1$ level is mandatory. Future work, based on the investigations we performed, will include new tricks allowing us to fulfill this task simply enough.

[48] E. Kanter, J. Nolen, D. H. Youngblood, Y.-W. Lui, H. L. Clark, Y. Tokimoto, X. Chen, and R. L. Watson, Argonne National Laboratory (private communication).

ETACHA4 in LISE^{++}

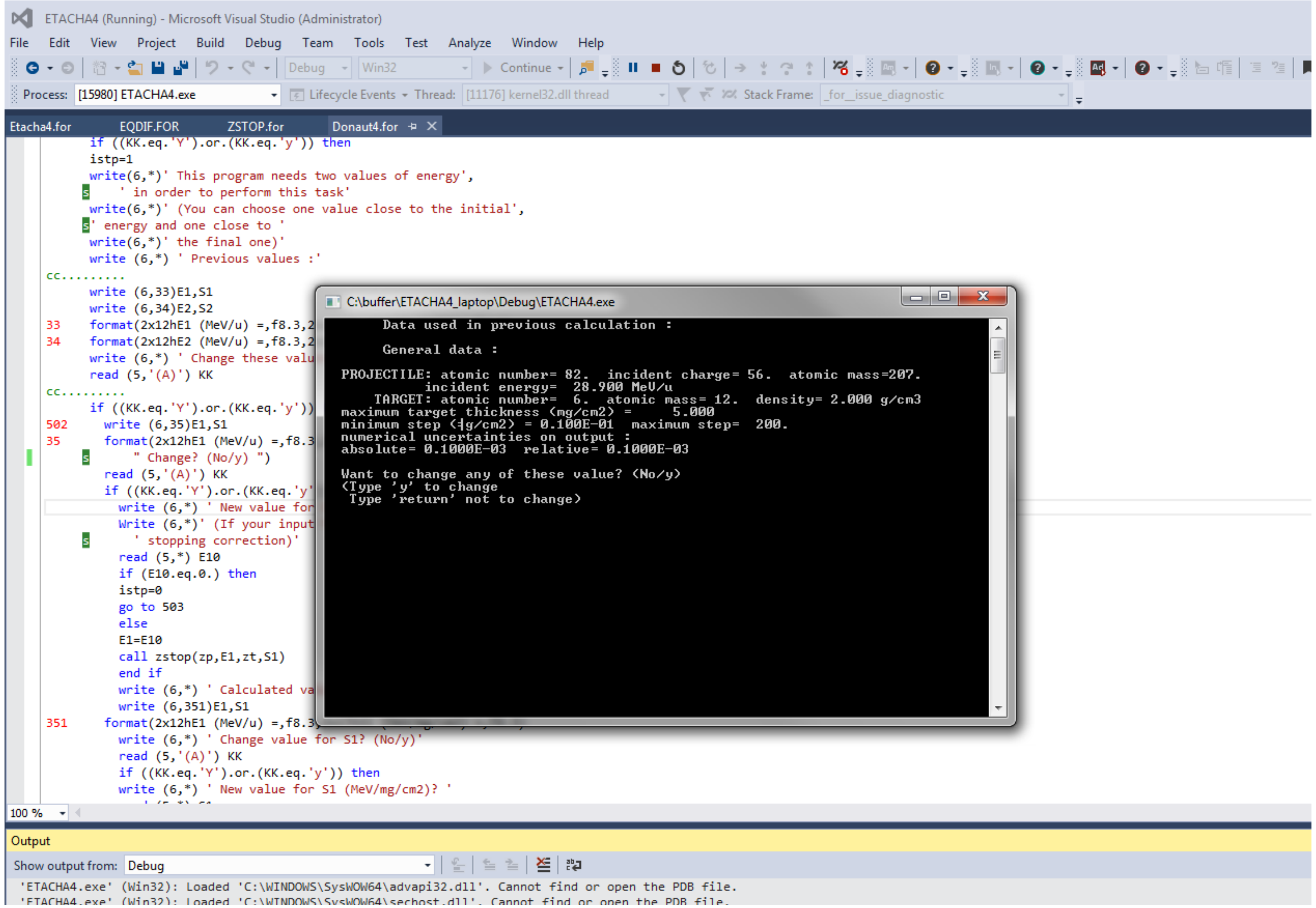


Important!!

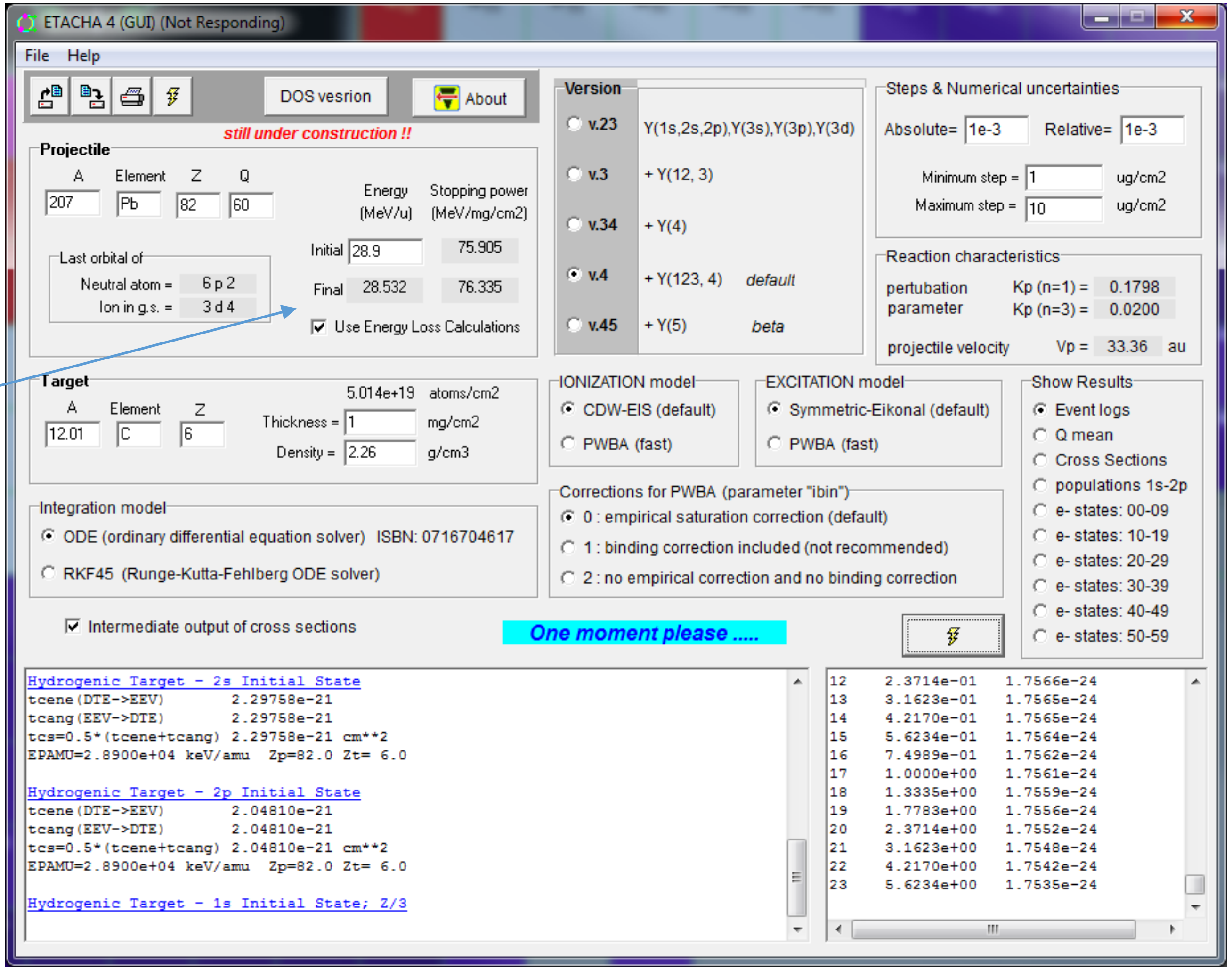
ETACHA4 (GUI-version) is still under construction.
ODE integrator should be updated!

ETACHA4 - DOS version (original) / FORTRAN/

1. The current ETACHA version is “DOS-window” (“terminal” window) application
2. To compile the current version you need MS Visual Studio (project) and Intel Parallel Studio XE2016 (FORTRAN)
3. Long-long manual data entry
4. The user should manually entry final energy at the exit of material



ETACHA4 - GUI version (original) / C++/



Calculated within the code

Important!!

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ETACHA4 - GUI version (original) / C++/

Cross sections can be edited in the current dialog appeared after calculation were started

ETACHA cross sections

Information

N	(sub)shell	Capture (MEC+REC)	IONization (includes n>4)
1	1s	5.7635e-1	1.5660e-3
2	2s	9.8725e-2	2.2976e-1
3	2p	1.6881e-1	2.0481e-1
4	3s	6.9094e-2	1.1414e+0
5	3p	1.6954e-1	1.1414e+0
6	3d	2.3890e-1	1.1414e+0
7	n=4	9.2897e-1	3.1926e+0

From / To	2s	2p	3s	3p	3d	n=4
1s	3.4723e-3	5.9665e-3	5.6845e-4	8.6390e-4	7.3594e-5	5.1577e-4
2s		6.8601e+0	1.3095e-1	1.2979e-1	4.7504e-1	1.3828e-1
2p			1.4638e-2	1.5797e-1	5.8280e-1	1.3981e-1
3s				2.5257e+1		4.4038e+0
3p					1.1368e+1	4.8968e+0
3d						6.5724e+0

You can EDIT these cross sections

N	(sub)shell	MEC (capture)	REC (capture)	IONization
1	1s	7.4753e-5	5.7628e-1	1.5660e-3
2	2s	1.0215e-2	8.8511e-2	2.2976e-1
3	2p	3.0644e-2	1.3817e-1	2.0481e-1
4	3s	4.2868e-2	2.6225e-2	1.1414e+0
5	3p	1.2860e-1	4.0938e-2	1.1414e+0
6	3d	2.1434e-1	2.4563e-2	1.1414e+0
7	n=4	9.0063e-1	2.8335e-2	3.1926e+0

From / To	2s	2p	3s	3p	3d	n=4
1s	3.4723e-3	5.9665e-3	5.6845e-4	8.6390e-4	7.3594e-5	5.1577e-4
2s		6.8601e+0	1.3095e-1	1.2979e-1	4.7504e-1	1.3828e-1
2p			1.4638e-2	1.5797e-1	5.8280e-1	1.3981e-1
3s				2.5257e+1		4.4038e+0
3p					1.1368e+1	4.8968e+0
3d						6.5724e+0

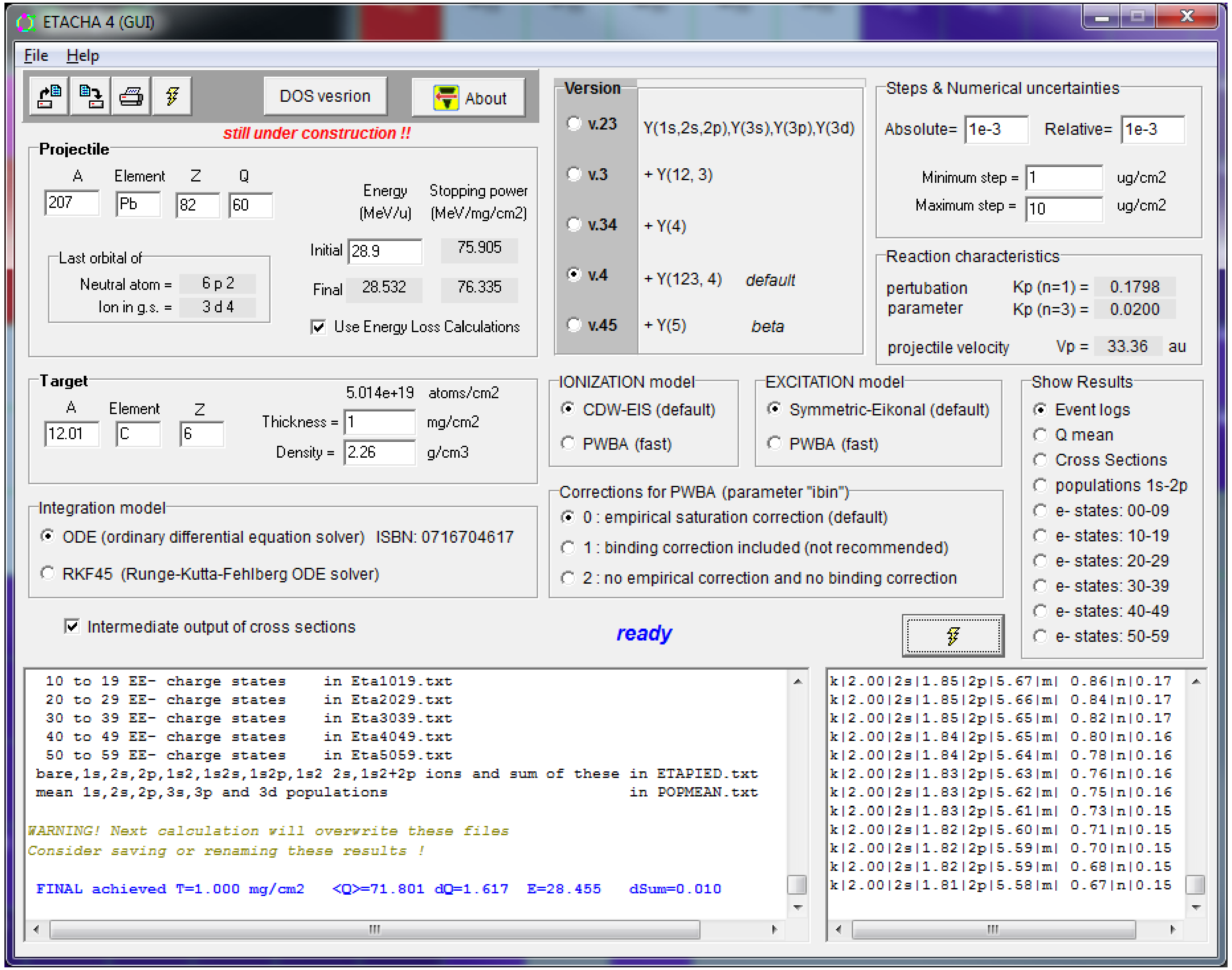
Version 4

Ionization:: CDW-EIS
Excitation:: SE
207Pb (28.9MeV/u) + C

Accept   Quit

All cross sections in 1e-20 cm2

Results:


ETACHA 4 (GUI)
File
Help
DOS vesrion
About
still under construction !!
Projectile
A
Element
Z
Q
207
Pb
82
60
Energy (MeV/u)
Stopping power (MeV/mg/cm2)
Initial
28.9
75.905
Final
28.532
76.335
Last orbital of
Neutral atom = 6 p 2
Ion in g.s. = 3 d 4
Use Energy Loss Calculations
Target
A
Element
Z
12.01
C
6
5.014e+19 atoms/cm2
Thickness = 1 mg/cm2
Density = 2.26 g/cm3
Integration model
ODE (ordinary differential equation solver) ISBN: 0716704617
RKF45 (Runge-Kutta-Fehlberg ODE solver)
Intermediate output of cross sections
Version
v.23 Y(1s,2s,2p),Y(3s),Y(3p),Y(3d)
v.3 + Y(12, 3)
v.34 + Y(4)
v.4 + Y(123, 4) default
v.45 + Y(5) beta
Steps & Numerical uncertainties
Absolute= 1e-3
Relative= 1e-3
Minimum step = 1 ug/cm2
Maximum step = 10 ug/cm2
Reaction characteristics
pertubation parameter
Kp (n=1) = 0.1798
Kp (n=3) = 0.0200
projectile velocity Vp = 33.36 au
IONIZATION model
CDW-EIS (default)
PWBA (fast)
EXCITATION model
Symmetric-Eikonal (default)
PWBA (fast)
Show Results
Event logs
Q mean
Cross Sections
populations 1s-2p
e- states: 00-09
e- states: 10-19
e- states: 20-29
e- states: 30-39
e- states: 40-49
e- states: 50-59
Corrections for PWBA (parameter "ibin")
0 : empirical saturation correction (default)
1 : binding correction included (not recommended)
2 : no empirical correction and no binding correction
ready
10 to 19 EE- charge states in Eta1019.txt
20 to 29 EE- charge states in Eta2029.txt
30 to 39 EE- charge states in Eta3039.txt
40 to 49 EE- charge states in Eta4049.txt
50 to 59 EE- charge states in Eta5059.txt
bare,1s,2s,2p,1s2,1s2s,1s2p,1s2 2s,1s2+2p ions and sum of these in ETAPIED.txt
mean 1s,2s,2p,3s,3p and 3d populations in POPMEAN.txt
WARNING! Next calculation will overwrite these files
Consider saving or renaming these results !
FINAL achieved T=1.000 mg/cm2 <Q>=71.801 dQ=1.617 E=28.455 dSum=0.010
k|2.00|2s|1.85|2p|5.67|m| 0.86|n|0.17
k|2.00|2s|1.85|2p|5.66|m| 0.84|n|0.17
k|2.00|2s|1.85|2p|5.65|m| 0.82|n|0.17
k|2.00|2s|1.84|2p|5.65|m| 0.80|n|0.16
k|2.00|2s|1.84|2p|5.64|m| 0.78|n|0.16
k|2.00|2s|1.83|2p|5.63|m| 0.76|n|0.16
k|2.00|2s|1.83|2p|5.62|m| 0.75|n|0.16
k|2.00|2s|1.83|2p|5.61|m| 0.73|n|0.15
k|2.00|2s|1.82|2p|5.60|m| 0.71|n|0.15
k|2.00|2s|1.82|2p|5.59|m| 0.70|n|0.15
k|2.00|2s|1.82|2p|5.59|m| 0.68|n|0.15
k|2.00|2s|1.81|2p|5.58|m| 0.67|n|0.15