

- 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!

PHYSICAL REVIEW A **92**, 042703 (2015)

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

E. Lamour,^{1,2} P. D. Fainstein,³ M. Galassi,⁴ C. Prigent,^{1,2} C. A. Ramirez,⁴ R. D. Rivarola,⁴ J.-P. Rozet,^{1,2}
M. Trassinelli,^{1,2} and D. Vernhet^{1,2,*}

¹*CNRS, UMR 7588, Institut des NanoSciences de Paris (INSP), 4 Place Jussieu, 75005 Paris, France*

²*Sorbonne Universités, UPMC Université Paris 06, INSP, UMR 7588, F-75005 Paris, France*

³*Centro Atómico Bariloche, Comisión Nacional de Energía Atómica and Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), 8400 San Carlos de Bariloche, Río Negro, Argentina*

⁴*Laboratorio de Colisiones Atómicas, Instituto de Física Rosario (CONICET-UNR) and Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Avenida Pellegrini 250, 2000 Rosario, Argentina*

(Received 4 June 2015; published 12 October 2015)

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

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 : $Z-q \leq 28$, ETACHA4: $Z-q \leq 60$. ETACHA5 is under development ($n \geq 5$)
4. Benchmark energy range application

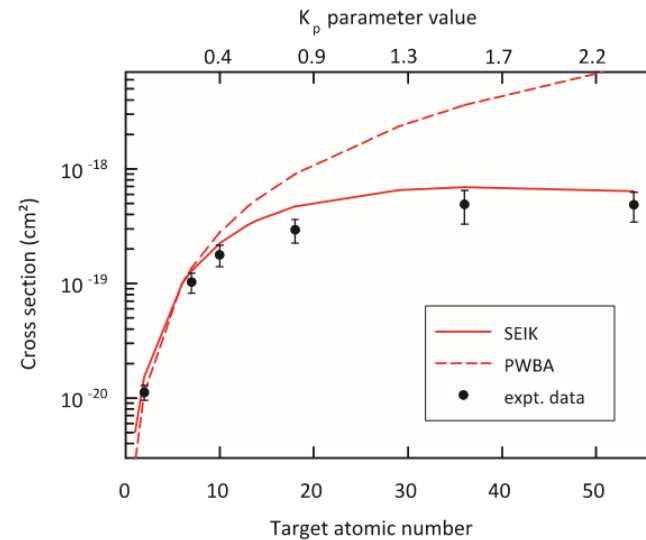
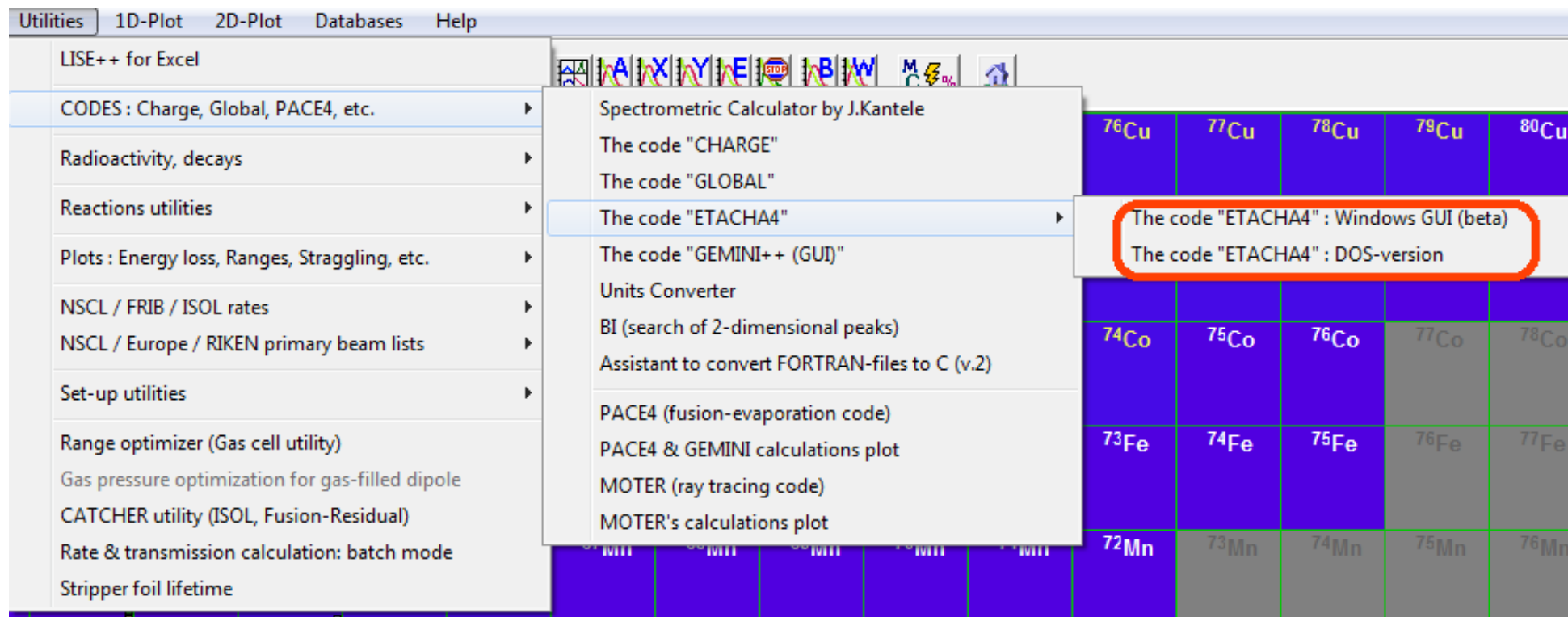


FIG. 3. (Color online) $1s-2p$ excitation cross section for Ar^{17+} ions at a fixed velocity $v_p = 23$ a.u. (13.6 MeV u^{-1}) as a function of exciting target atomic number. Dots with error bars, experiment [21];

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 $^{58}\text{Ni}^{19+}$ 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 $11 \text{ MeV u}^{-1} \text{ U}^{38+}$ 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 $n \geq 5$. 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.

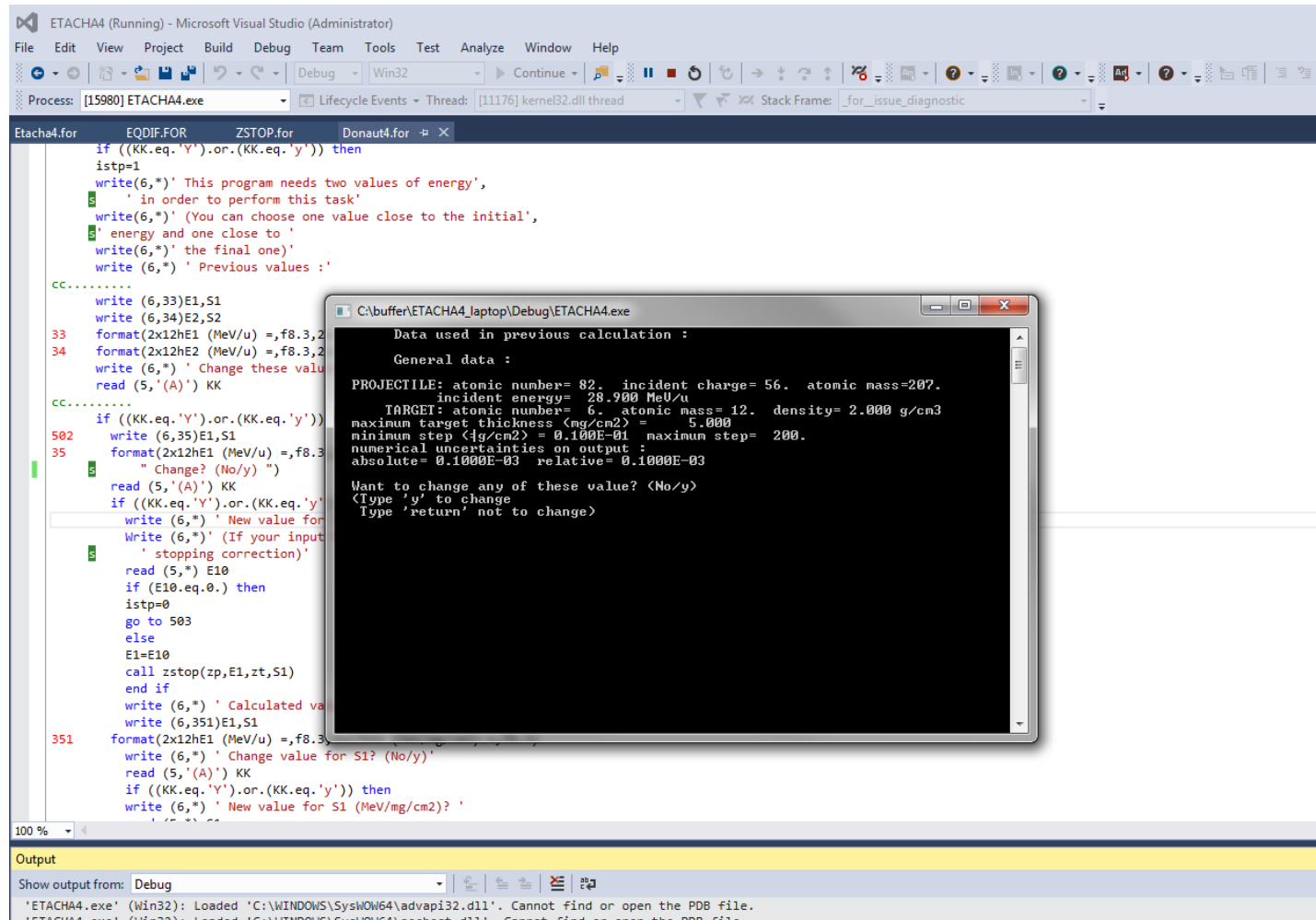
[48] E. Kanter, J. Nolen, D. H. Youngblood, Y.-W. Lui, H. L. Clark, Y. Tokimoto, X. Chen, and R. L. Watson, Argonne National Laboratory (private communication).



Important!!

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

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.FOR
      if ((KK.eq.'Y').or.(KK.eq.'y')) then
        istp=1
        write(6,*) ' This program needs two values of energy',
          ' in order to perform this task'
        write(6,*) ' (You can choose one value close to the initial',
          ' energy and one close to '
        write(6,*) ' the final one)'
        write(6,*) ' Previous values : '
      cc.....
        write (6,33)E1,S1
        write (6,34)E2,S2
      33 format(2x12hE1 (MeV/u) =,f8.3,2
      34 format(2x12hE2 (MeV/u) =,f8.3,2
        write (6,*) ' Change these values?'
        read (5,'(A)') KK
      cc.....
      502 if ((KK.eq.'Y').or.(KK.eq.'y'))
        write (6,35)E1,S1
      35 format(2x12hE1 (MeV/u) =,f8.3,2
        write (6,*) ' Change? (No/y) '
        read (5,'(A)') KK
        if ((KK.eq.'Y').or.(KK.eq.'y'))
          write (6,*) ' New value for '
          write (6,*) ' (If your input '
          ' stopping correction)'
          read (5,*) E10
          if (E10.eq.0.) then
            istp=0
            go to 503
          else
            E1=E10
            call zstop(zp,E1,zt,S1)
          end if
          write (6,*) ' Calculated value '
          write (6,35)E1,S1
      351 format(2x12hE1 (MeV/u) =,f8.3,2
        write (6,*) ' Change value for S1? (No/y)'
        read (5,'(A)') KK
        if ((KK.eq.'Y').or.(KK.eq.'y')) then
          write (6,*) ' New value for S1 (MeV/mg/cm2)? '

```

```

Data used in previous calculation :
General data :
PROJECTILE: atomic number= 82. incident charge= 56. atomic mass=207.
            incident energy= 28.900 MeV/u
TARGET: atomic number= 6. atomic mass= 12. density= 2.000 g/cm3
maximum target thickness (mg/cm2) = 5.000
minimum step (g/cm2) = 0.100E-01 maximum step= 200.
numerical uncertainties on output :
absolute= 0.1000E-03 relative= 0.1000E-03
Want to change any of these value? <No/y>
<Type 'y' to change
Type 'return' not to change>

```

```

Output
Show output from: Debug
'ETACHA4.exe' (Win32): Loaded 'C:\WINDOWS\SysWOW64\advapi32.dll'. Cannot find or open the PDB file.
'ETACHA4.exe' (Win32): Loaded 'C:\WINDOWS\SysWOW64\sechost.dll'. Cannot find or open the PDB file.

```

Calculated
within the code

ETACHA 4 (GUI) (Not Responding)

File Help

still under construction !!

Projectile

A	Element	Z	Q	Energy (MeV/u)	Stopping power (MeV/mg/cm2)
207	Pb	82	60		

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	Thickness (mg/cm2)	Density (g/cm3)
12.01	C	6	1	2.26

5.014e+19 atoms/cm2

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

perturbation Kp (n=1) = 0.1798
parameter 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)

Corrections for PWBA (parameter "ibin")

☒ 0 : empirical saturation correction (default)
☐ 1 : binding correction included (not recommended)
☐ 2 : no empirical correction and no binding correction

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

One moment please

Hydrogenic Target - 2s Initial State

```
tcene (DTE->EEV) 2.29758e-21
tcang (EEV->DTE) 2.29758e-21
tcs=0.5*(tcene+tcang) 2.29758e-21 cm**2
EPAMU=2.8900e+04 keV/amu Zp=82.0 Zt= 6.0
```

Hydrogenic Target - 2p Initial State

```
tcene (DTE->EEV) 2.04810e-21
tcang (EEV->DTE) 2.04810e-21
tcs=0.5*(tcene+tcang) 2.04810e-21 cm**2
EPAMU=2.8900e+04 keV/amu Zp=82.0 Zt= 6.0
```

Hydrogenic Target - 1s Initial State; Z/3

12	2.3714e-01	1.7566e-24
13	3.1623e-01	1.7565e-24
14	4.2170e-01	1.7565e-24
15	5.6234e-01	1.7564e-24
16	7.4989e-01	1.7562e-24
17	1.0000e+00	1.7561e-24
18	1.3335e+00	1.7559e-24
19	1.7783e+00	1.7556e-24
20	2.3714e+00	1.7552e-24
21	3.1623e+00	1.7548e-24
22	4.2170e+00	1.7542e-24
23	5.6234e+00	1.7535e-24

Important!!

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

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

