ATIMA 1.4 Improvements

Helmut Weick, Hans Geissel,
Shivaji Purushotaman, Christoph Scheidenberger
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- ATIMA basic ingredients
- New combined mean charge formula
- Resulting improvements in dE/dx
- Numerical calculation

GSI FAIR HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

Equations in ATIMA (1)

Bethe equation (PWBA):

$$\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{m v^2} N Z_2 \left[\ln\left(\frac{2m\gamma^2 v^2}{I}\right) - \beta^2\right] \quad , \; Z_1 \alpha / \beta \ll 1$$

$\Delta L_{LS}(Z_1,v)$ exact solution for collision with one electron,
corresponds to Bloch term at low energies
big effect for high Z_1 and $\gamma > 1.5$, also includes nuclear size effect ($\gamma \gg 1$)

xB Barkas factor
(polarisation of atom)

Fermi-density effect
for relativistic velocities

$$\frac{dE}{dx} = \frac{4\pi q_1^2 e^4}{m v^2} N Z_2 \left[\ln\left(\frac{2m\gamma^2 v^2}{I}\right) - \beta^2 + \Delta L_{LS} - \delta/2\right]$$

$- c(Z_2,v)$
shell corrections
(sum rule not valid)

$+\Delta L_{screen}(Z_1,v)$

use <q> instead of Z
ΔL weight for different collisions
sum over all $dE/dx(q_i)$

Equations in ATIMA (2)

No good description based on direct theory for
eavy ions below 10 or 30 MeV/u.

Use Ziegler's scaling formula from proton dE/dx with
fitted effective charges, still an older version from 1990s.

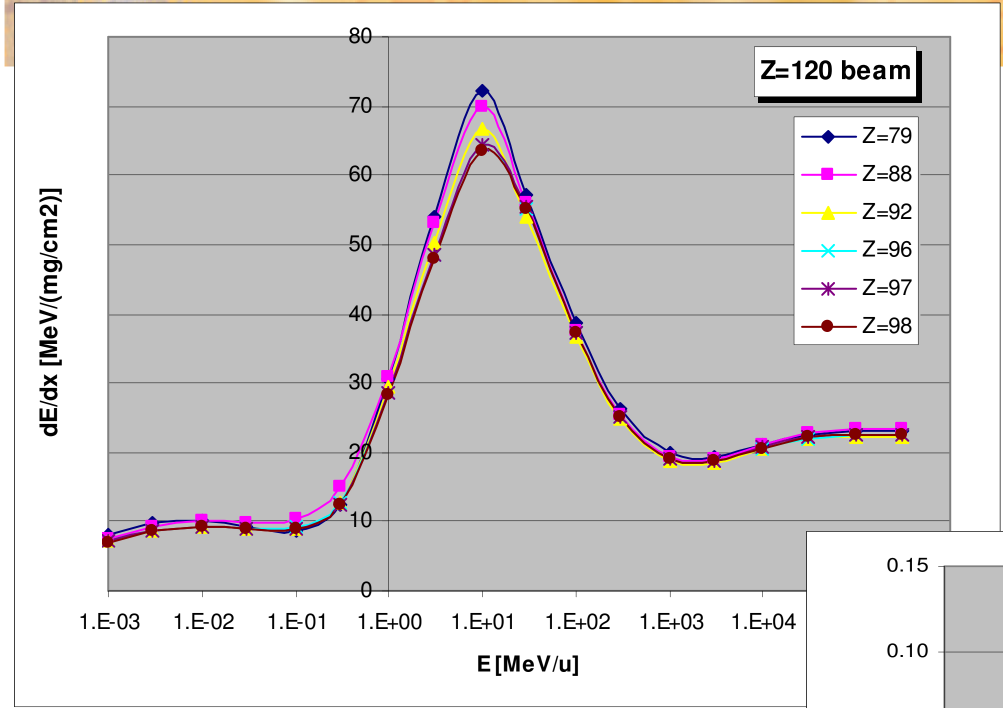
Our goal for ATIMA (at least for E > 30 MeV/u):
No fit formula, base it on theory !

Do not use effective charges as fit parameter for many
different effects, instead use only the real projectile charges.

Of course theory needs input from experiments,
but only when based on theory different physics effects
can be distinguished and understood.

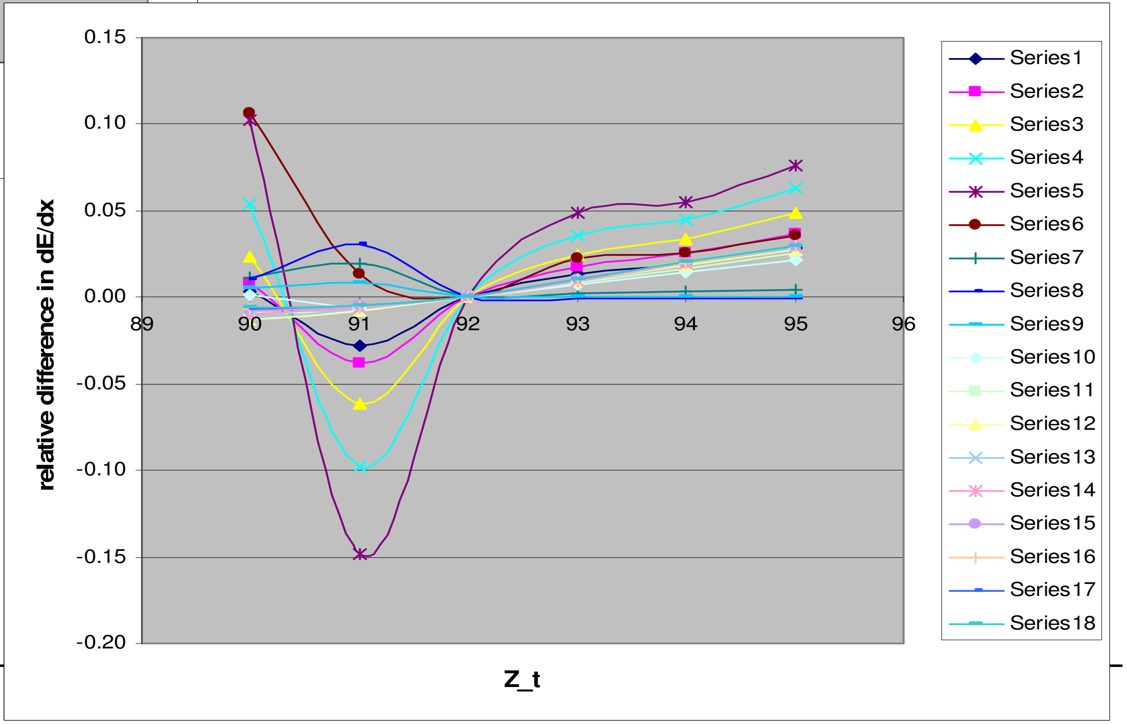
ATIMA 1.3, extension for Z_p=93-120, Z_t=93-99

done in 2012



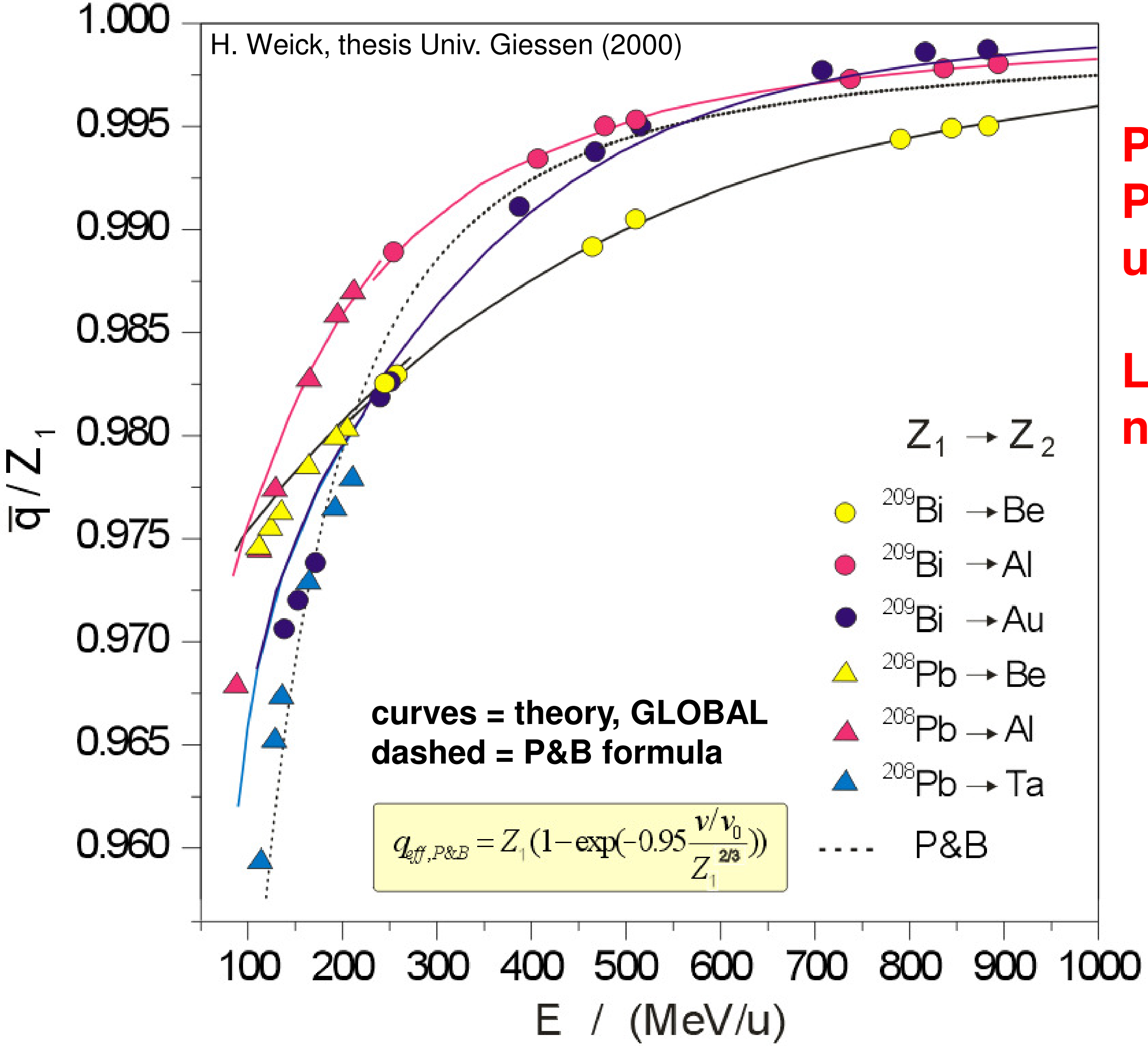
< 10 MeV/u, extrapolation in Ziegler style new calculated Fermi energies for Z_t > 92.

Theory for >30 MeV/u, but of course not tested at all.



Deviation to Stopping Power in a Uranium target.
Each curve shows one energy from 1 keV/u – 300 GeV/u for ^{246}U beam.
The large deviation for Z_t = 91 is due to a strange v_Fermi of Ziegler.

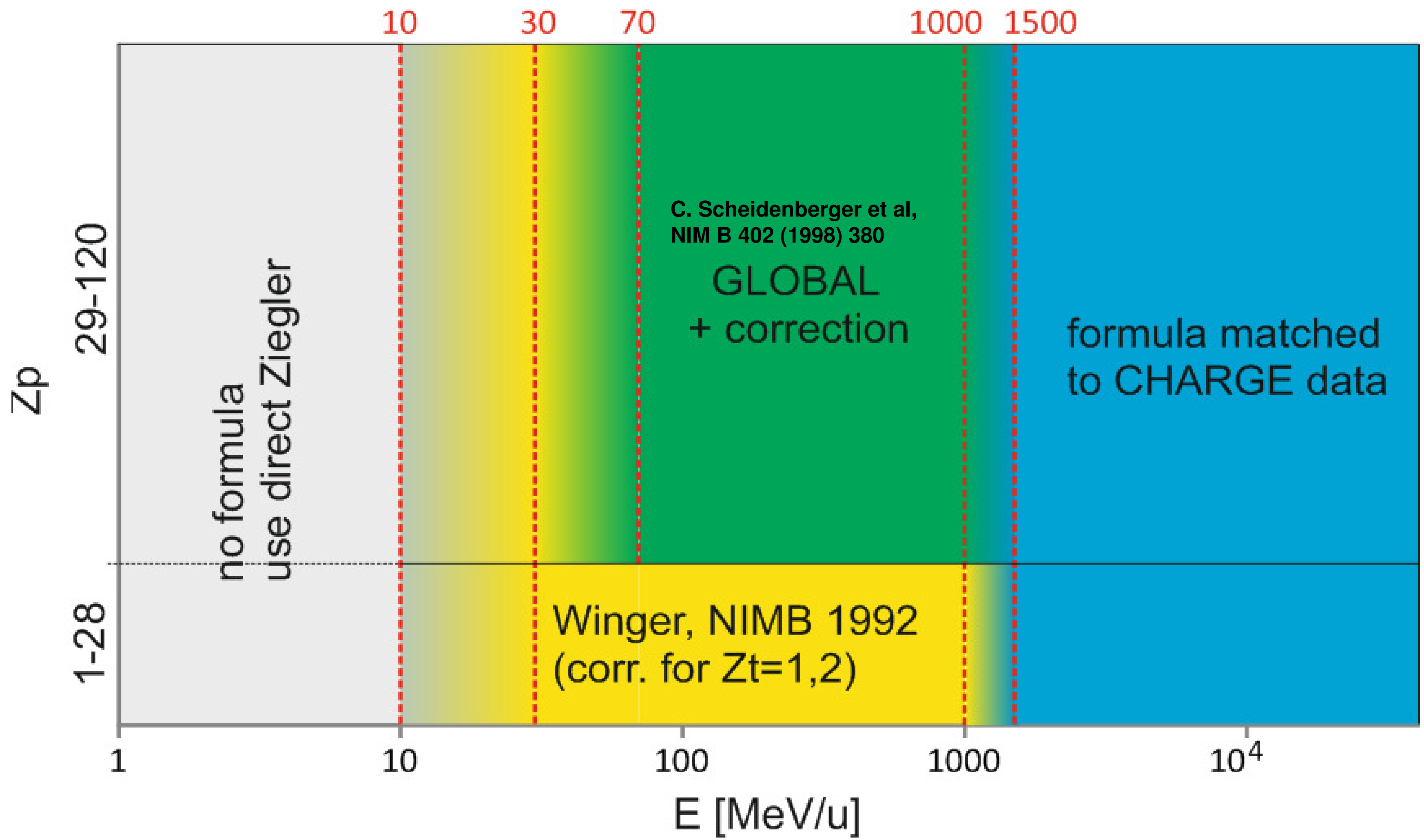
Mean Charge State of Bi, Pb Ions



Pierce & Blann formula
PR 173, 390 (1968)
used in ATIMA 1.2

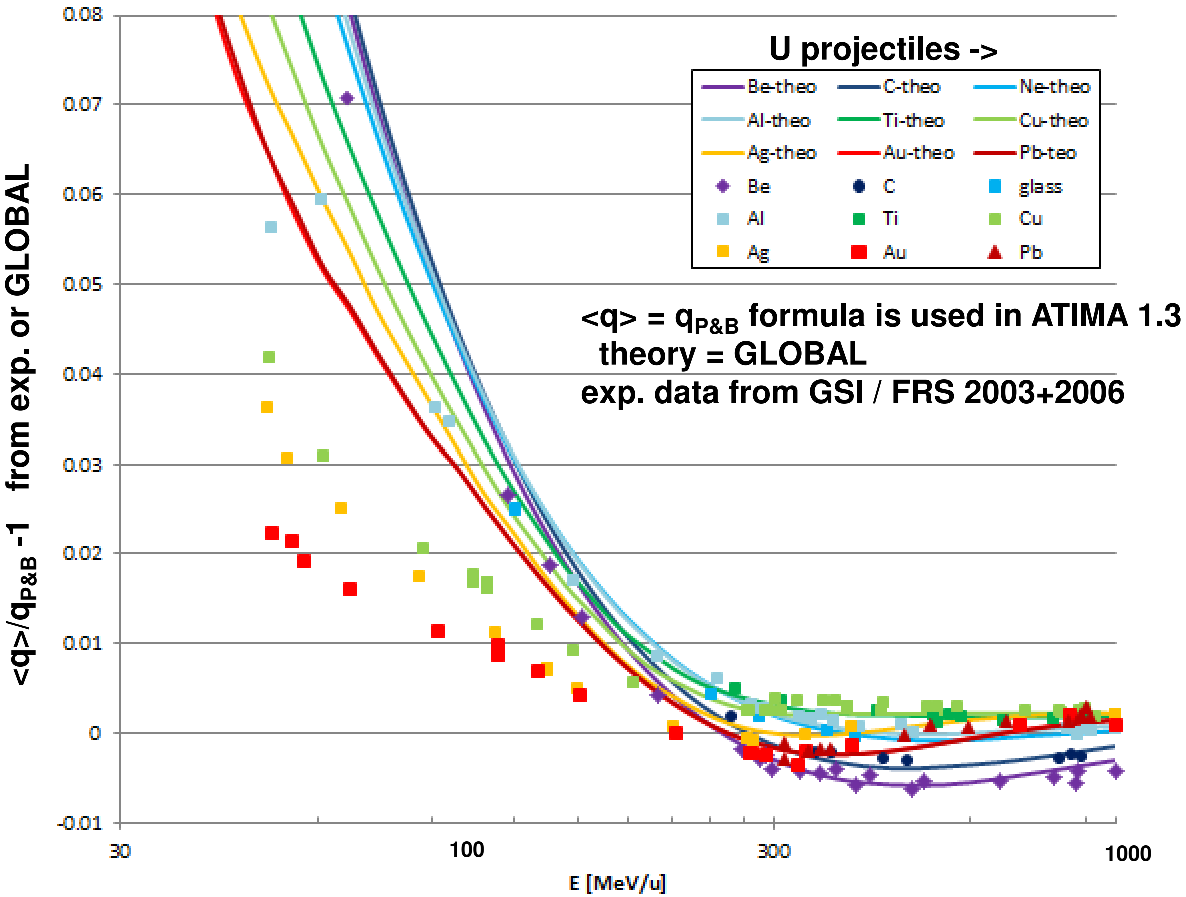
Large deviations in <q>,
no dependence on Z_2.

Combined Mean Charge State Formula for ATIMA 1.4



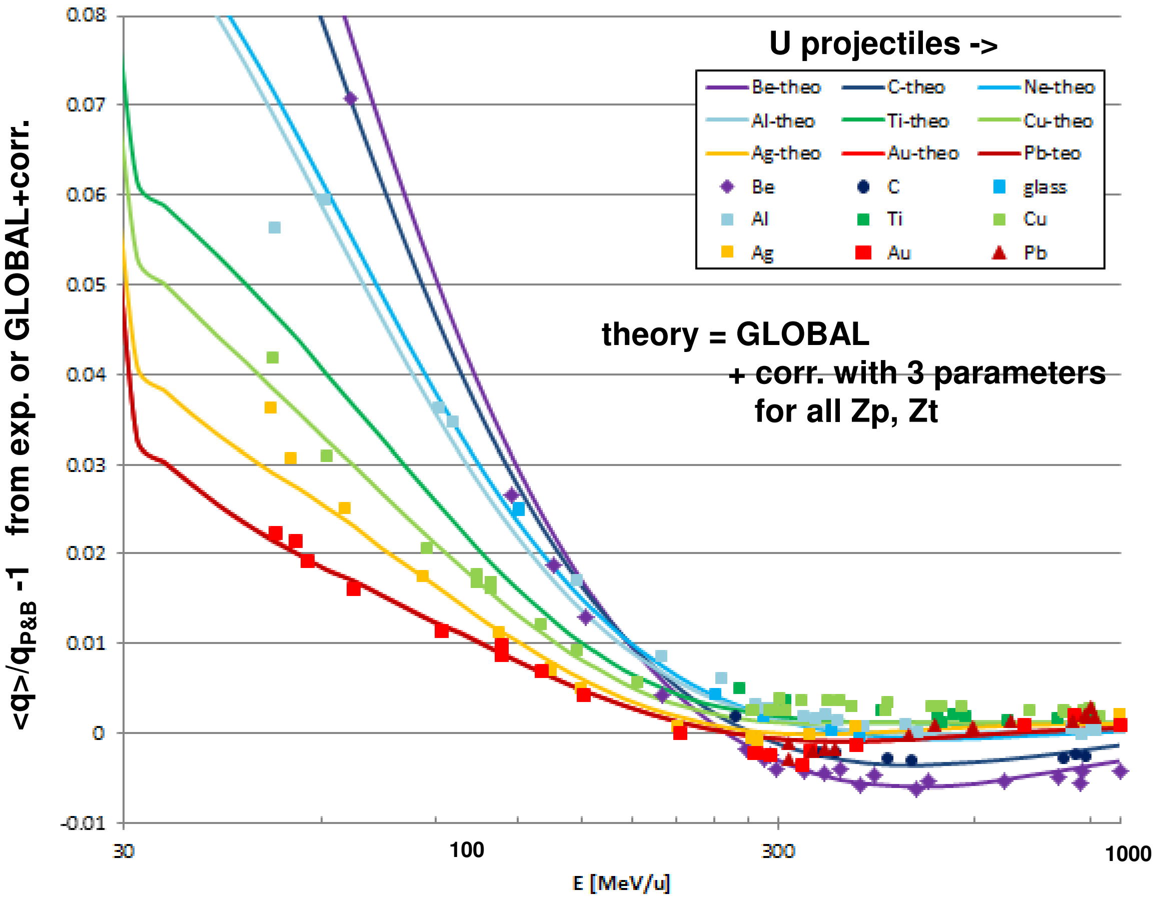
Different formulas with weighted average in overlapping energy range

<q> from GLOBAL



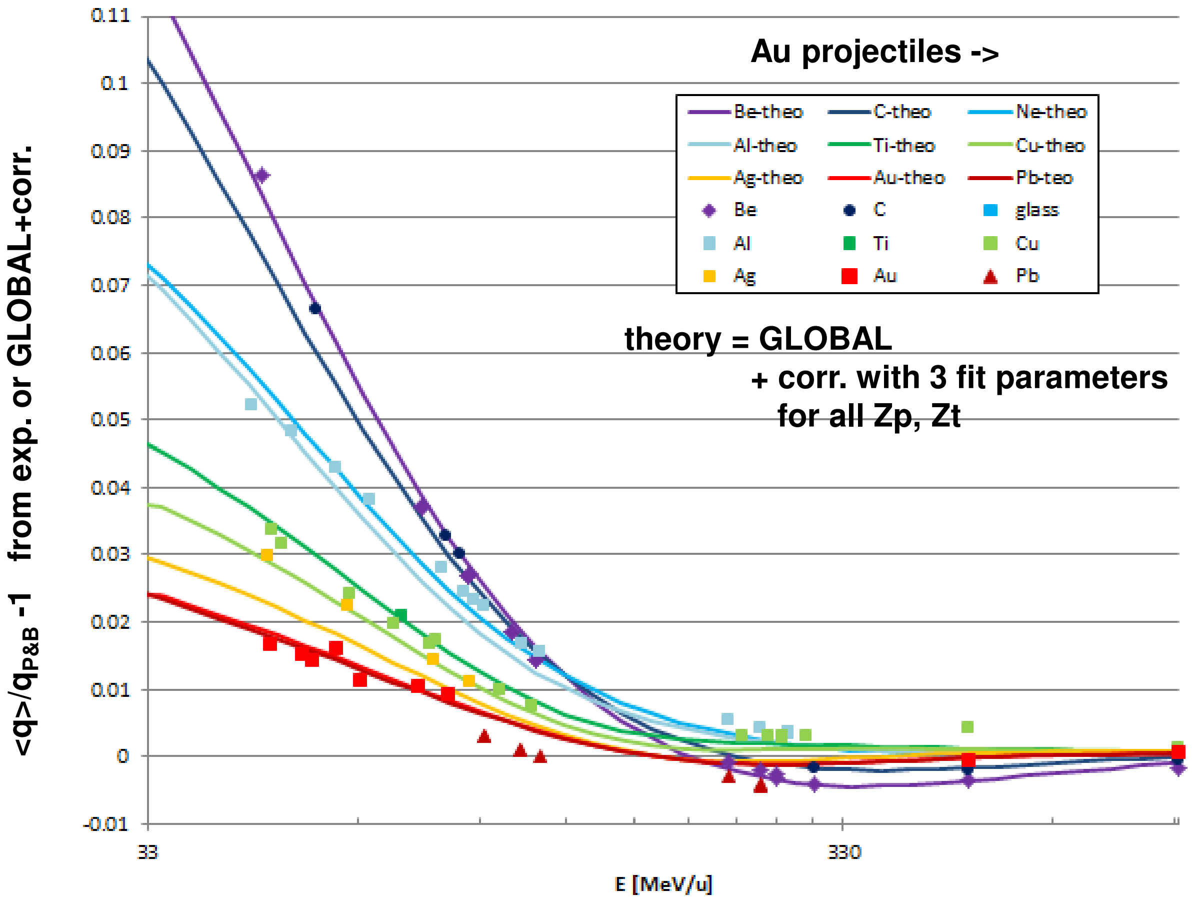
Best description of <q> at high velocities for heavy ions.

<q> from GLOBAL + correction



GLOBAL (perturbation theory) does not work well at low velocities.
=> Use simple fitted correction with increasing weight at low E.

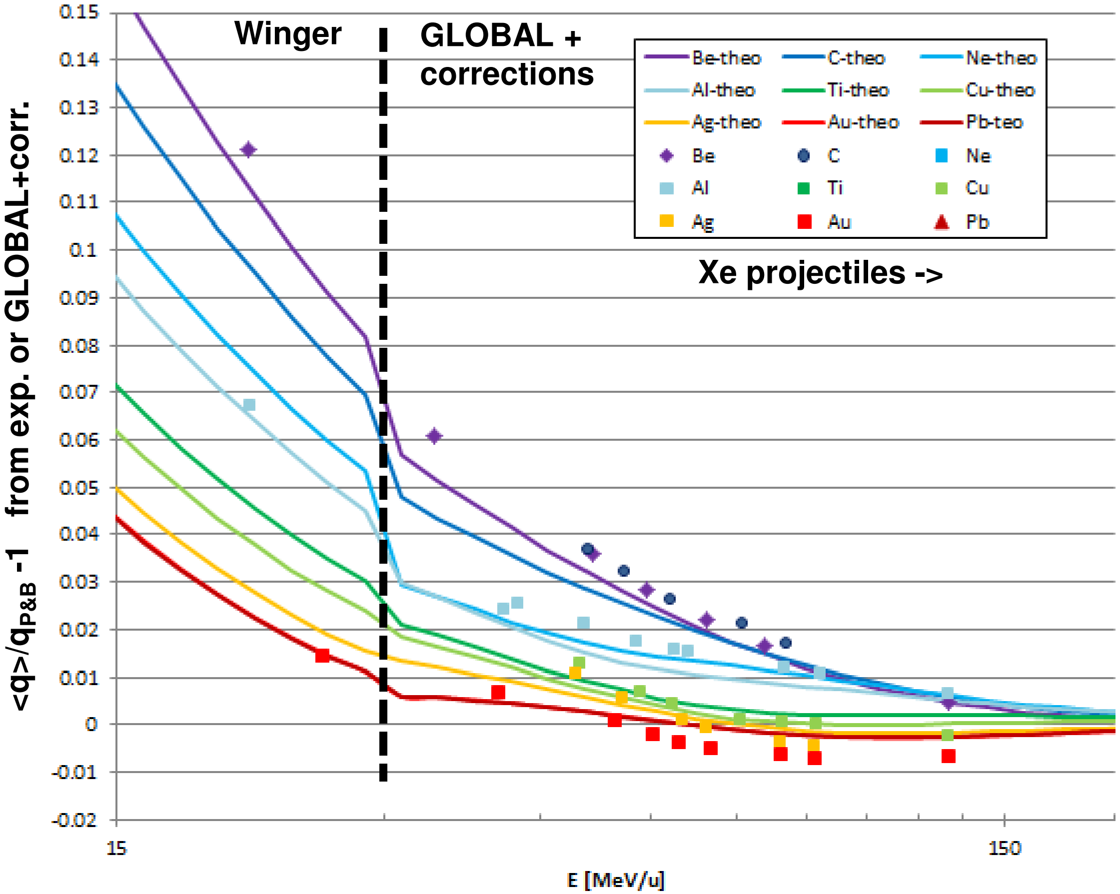
<q> from GLOBAL + correction



The same correction also works reasonably well for all Zp = 92 – 54 compared with exp. data for U, Bi, Pb, Au, Ta, Xe projectiles.

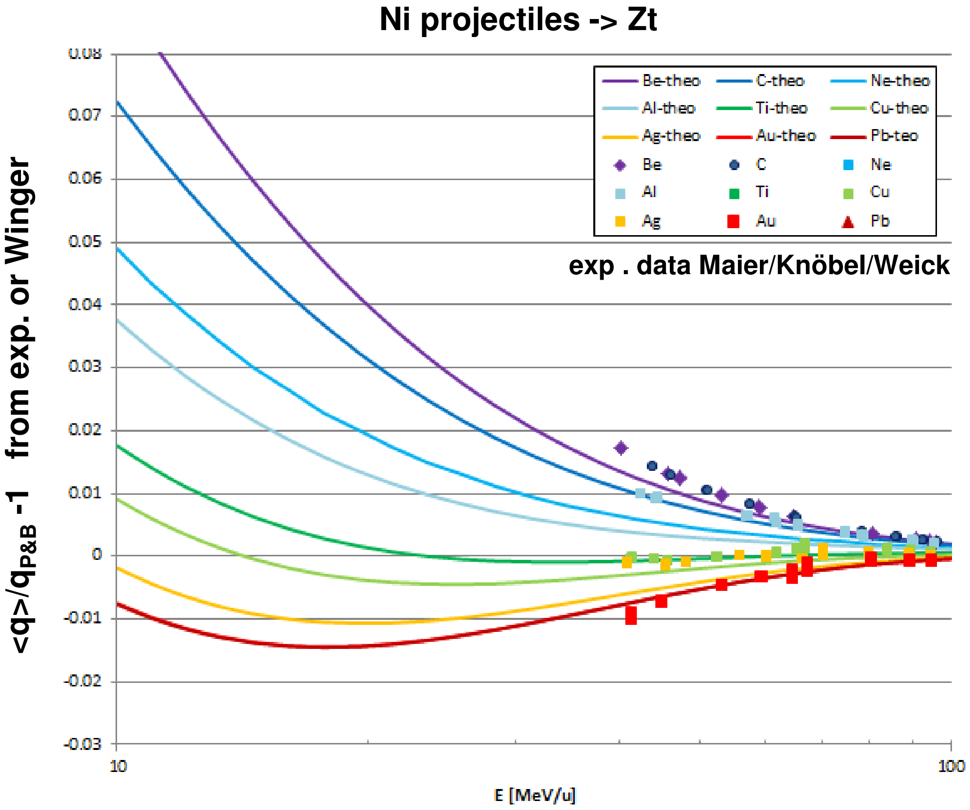
<q> from GLOBAL+corr. and Winger

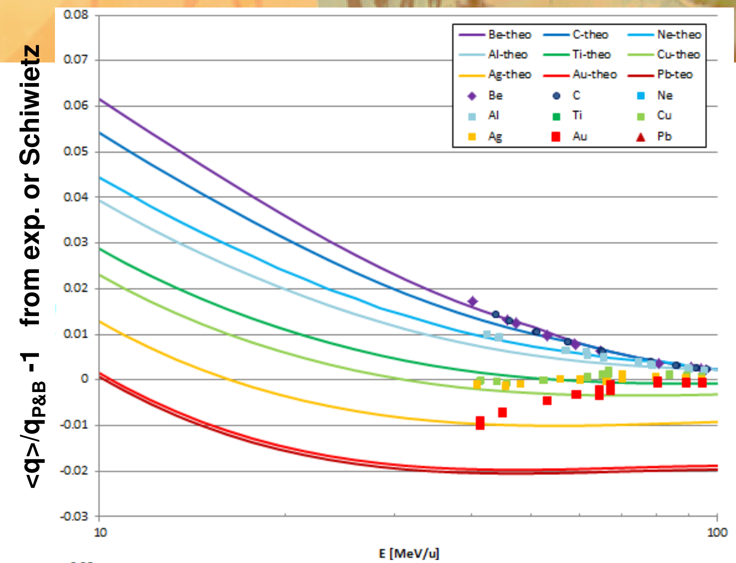
GLOBAL only for E/m > 30 MeV/u, use Winger below.

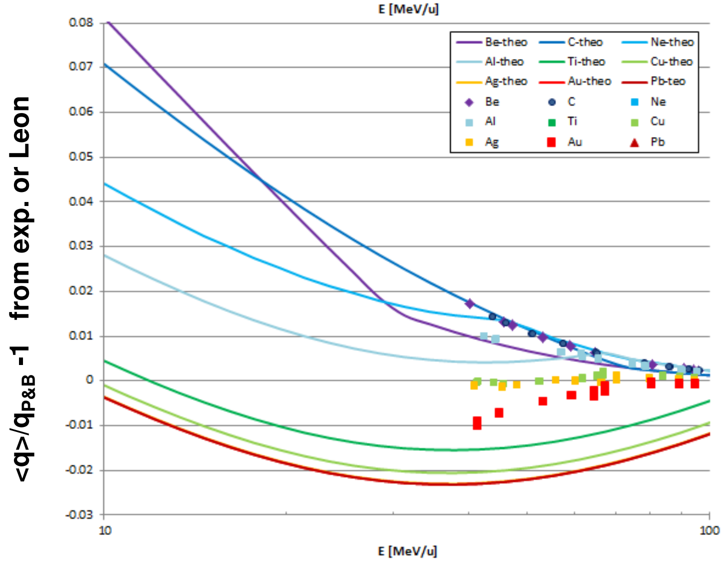


Remaining jump between GLOBAL+corr. and Winger region at 30 MeV/u.
=> Smoothen be linear weighted average over 10..70 MeV/u

<q> from Winger for Zp < 29

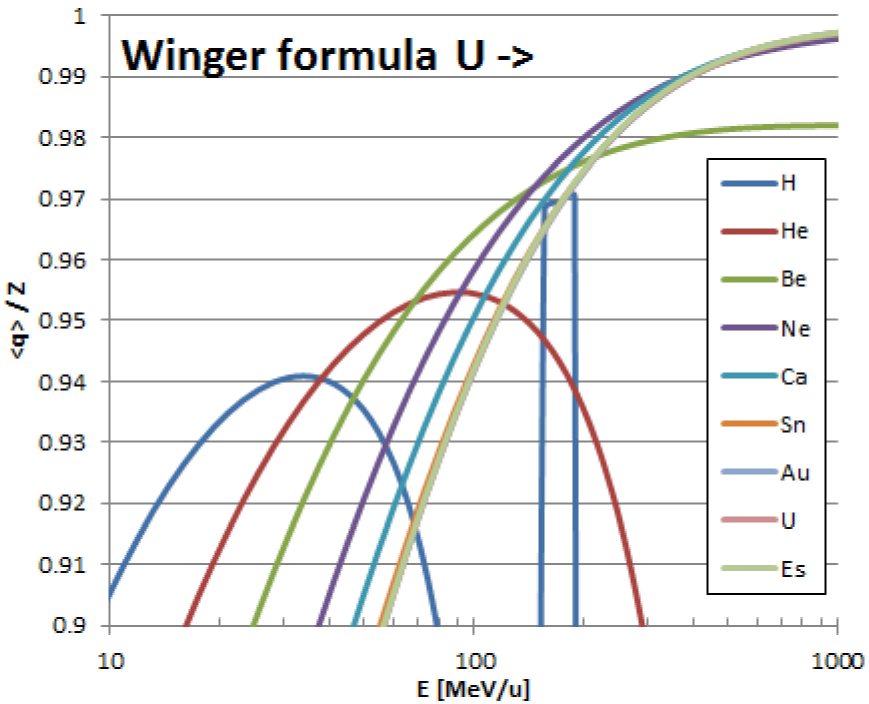






Also at low Zp the old P&B-formula shows large deviations, but GLOBAL is only for Zp>28, Winger works best.

Fix Winger problem for low Zt



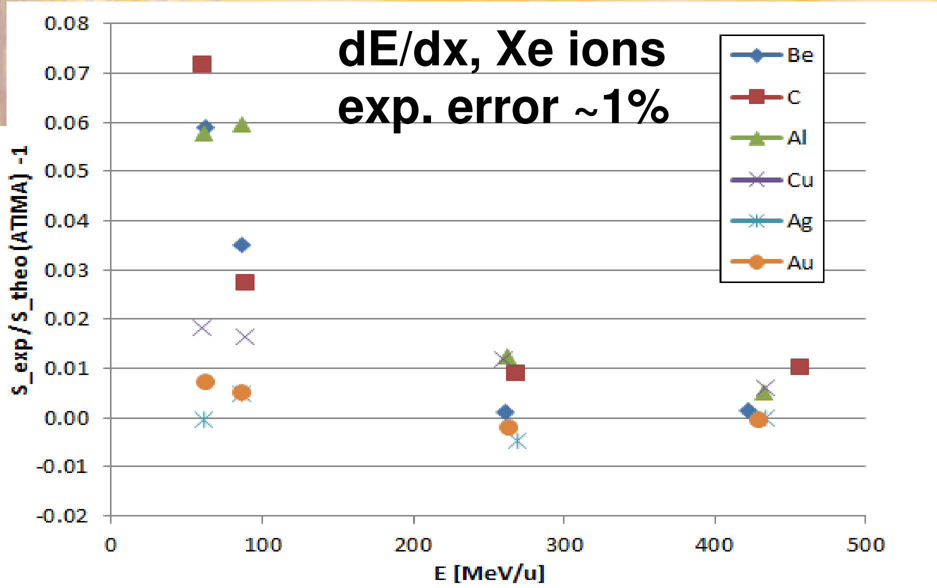
Parametrization not good for H+He,
Polynomial out of good range,
⇒ use a simple correction

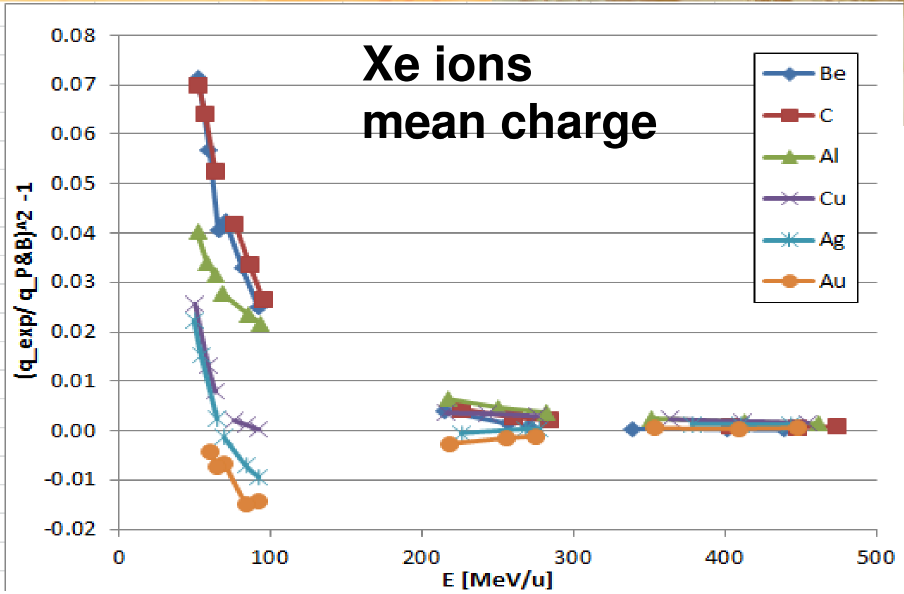
```
quick fix for 10 < E <100 MeV/u
if (I_Zt.eq.2) then
     Zt=2.8
elseif (I_Zt.eq.1) then
     Zt=2.6
endif
```

No such problem for Zp < 29.

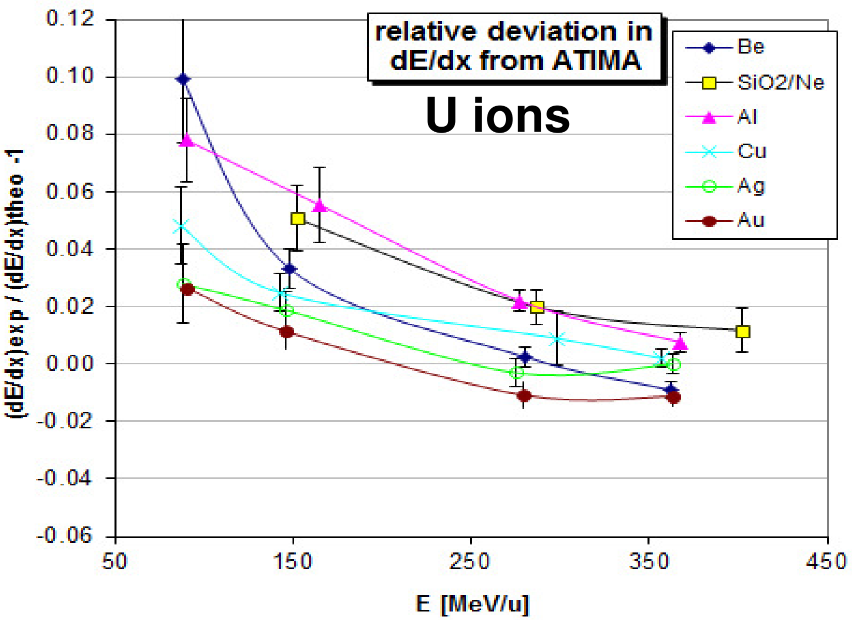
Formula is useful for Zt > 92, also for Zp up to 120.

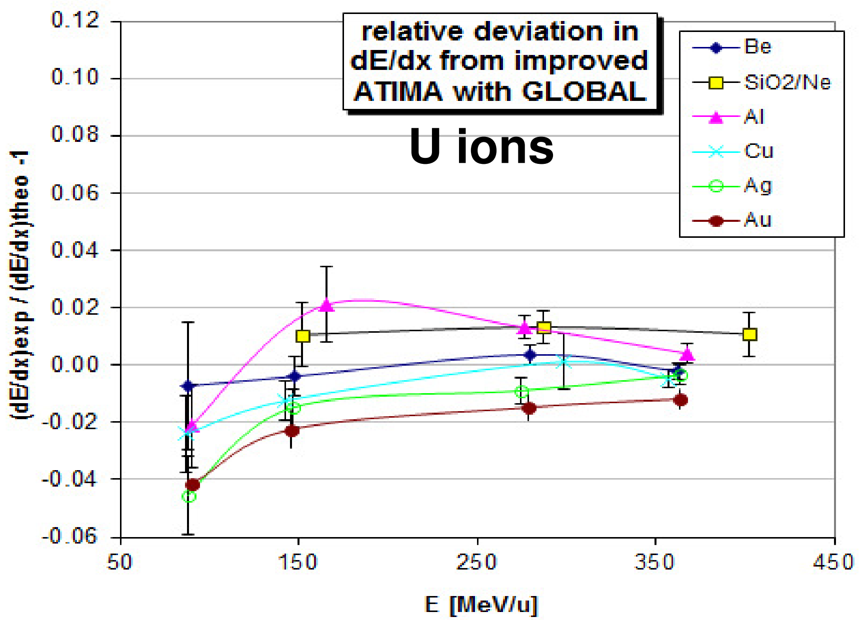
Measured deviation from ATIMA 1.3



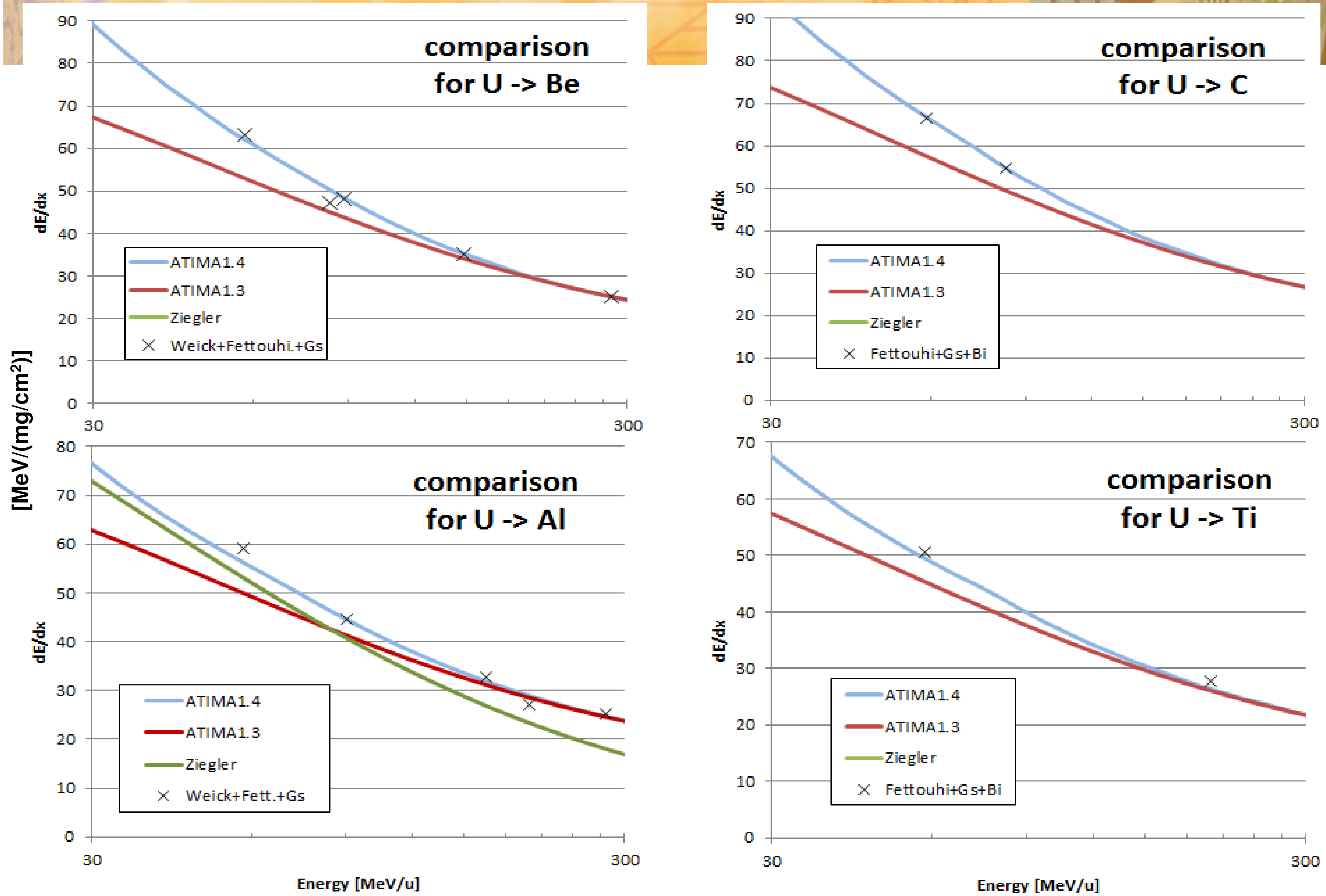


mostly unpublished data from FRS (Maier, Portillo, Weick, et al.)

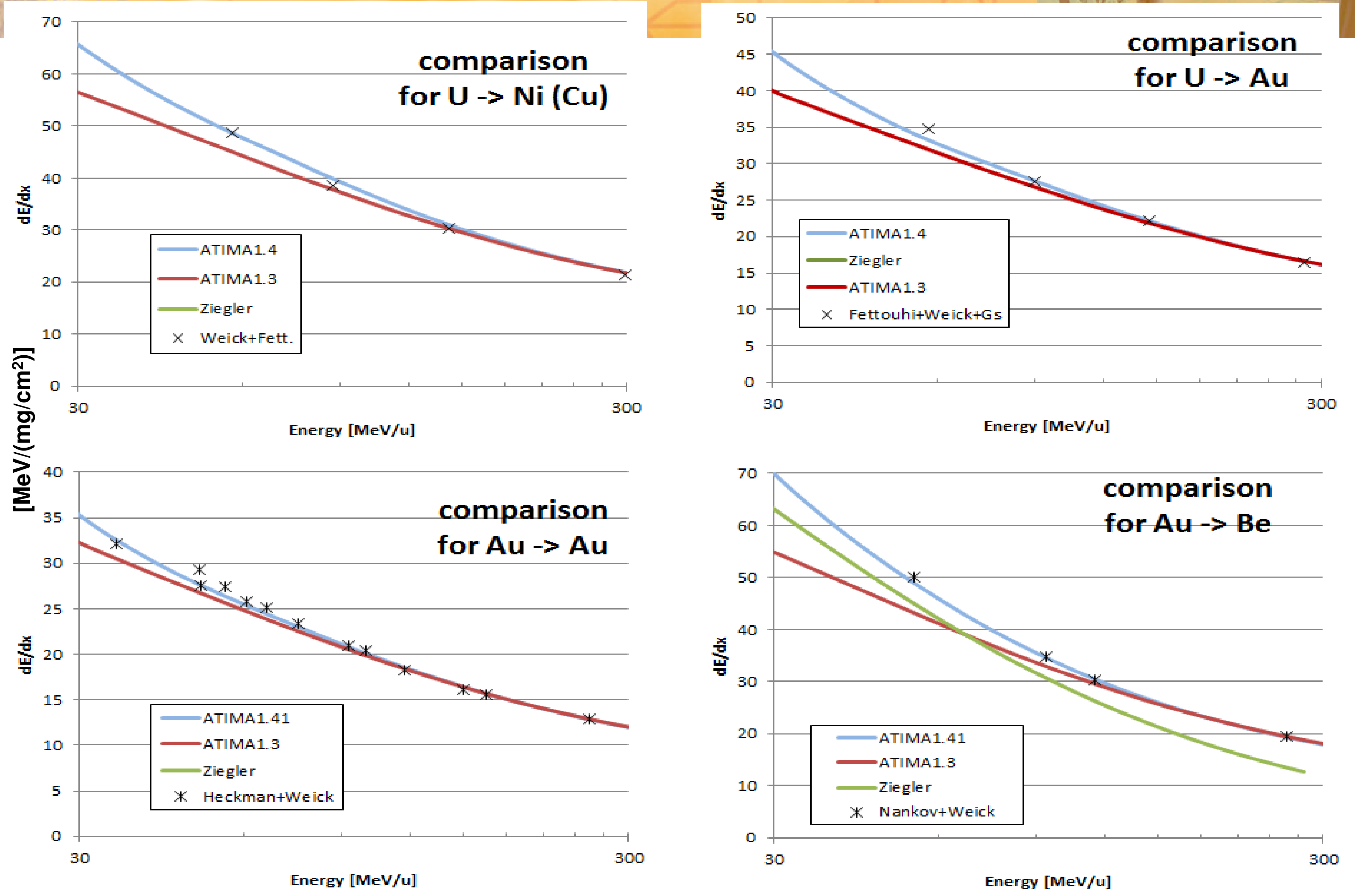




ATIMA 1.4 vs 1.3, zoom above 30 MeV/u

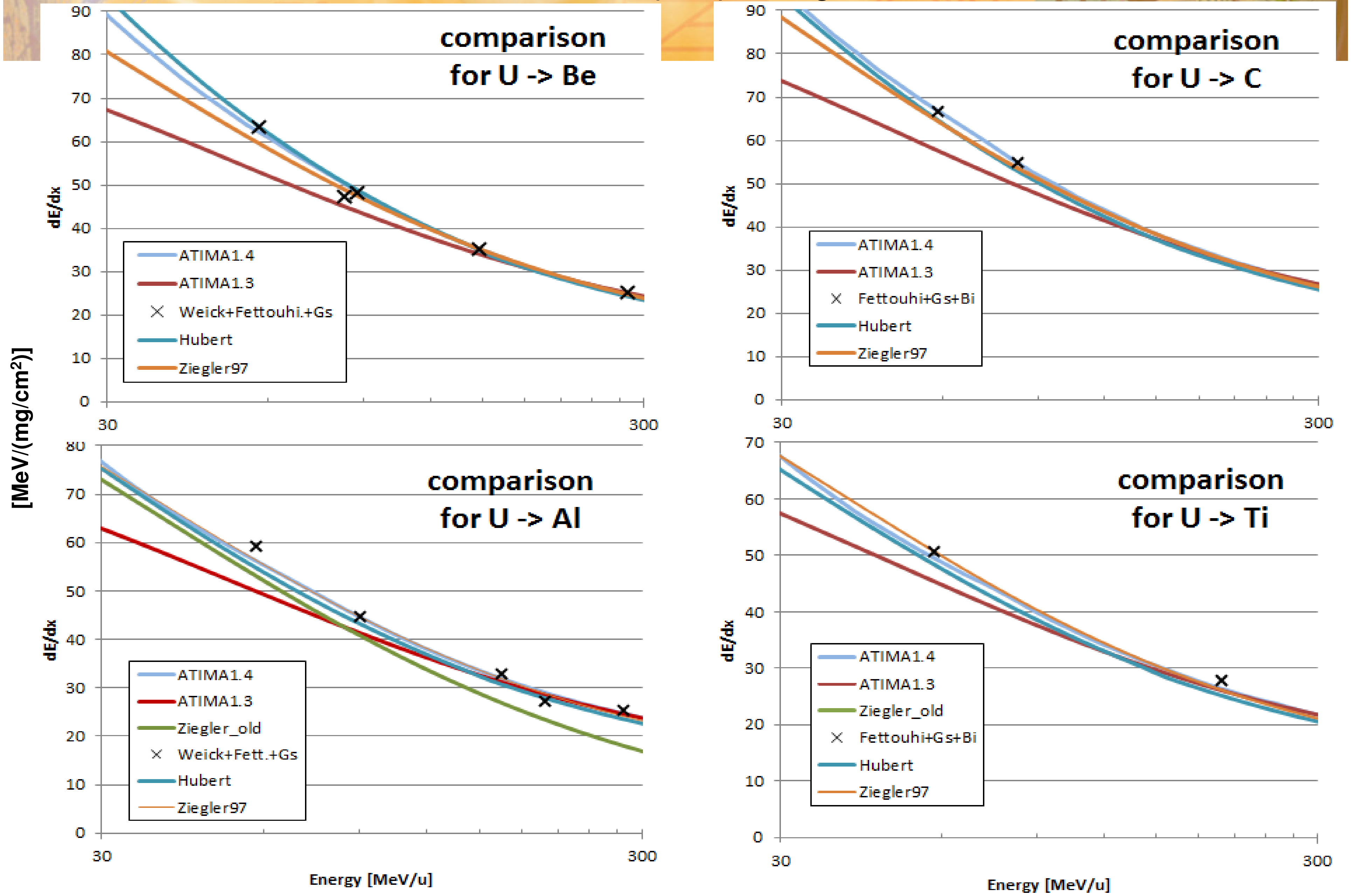


ATIMA 1.4 vs 1.3, zoom above 30 MeV/u

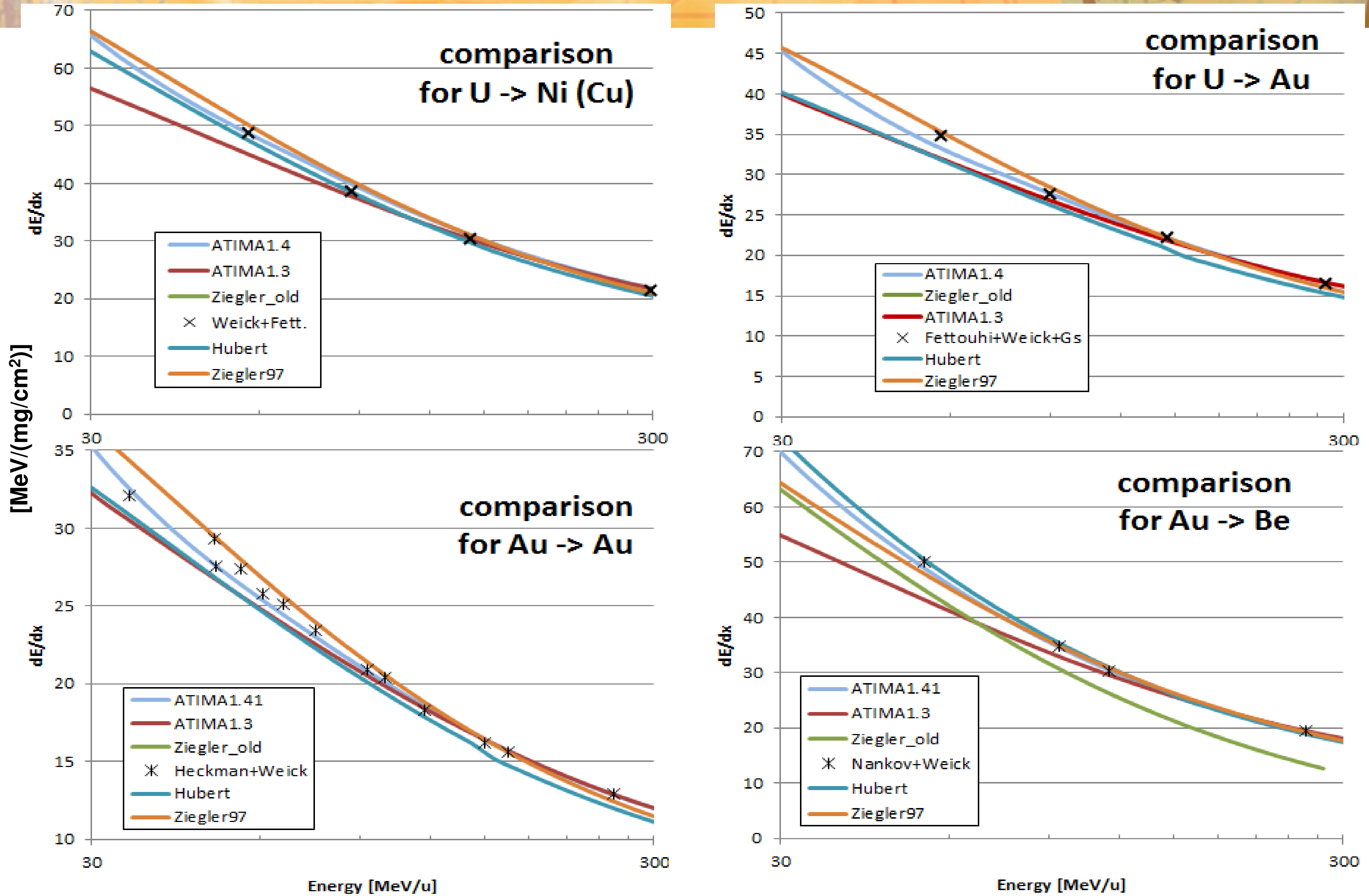


ATIMA 1.4 vs Hubert, Ziegler97

AtNDT 49 (1990) 1 Pergamon Press 1985



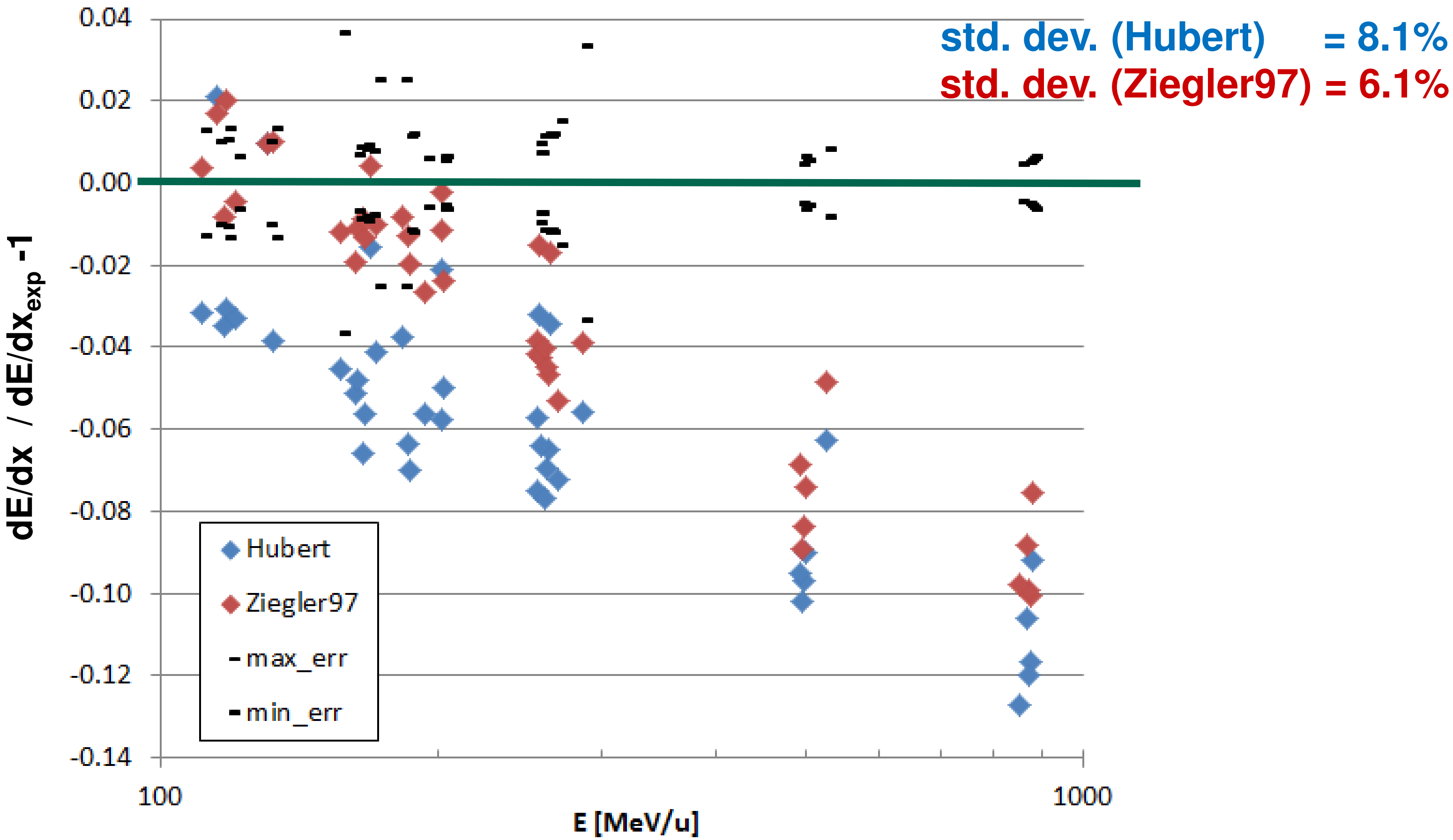
ATIMA 1.4 vs Hubert, Ziegler97



Hubert, Ziegler97 look good ?

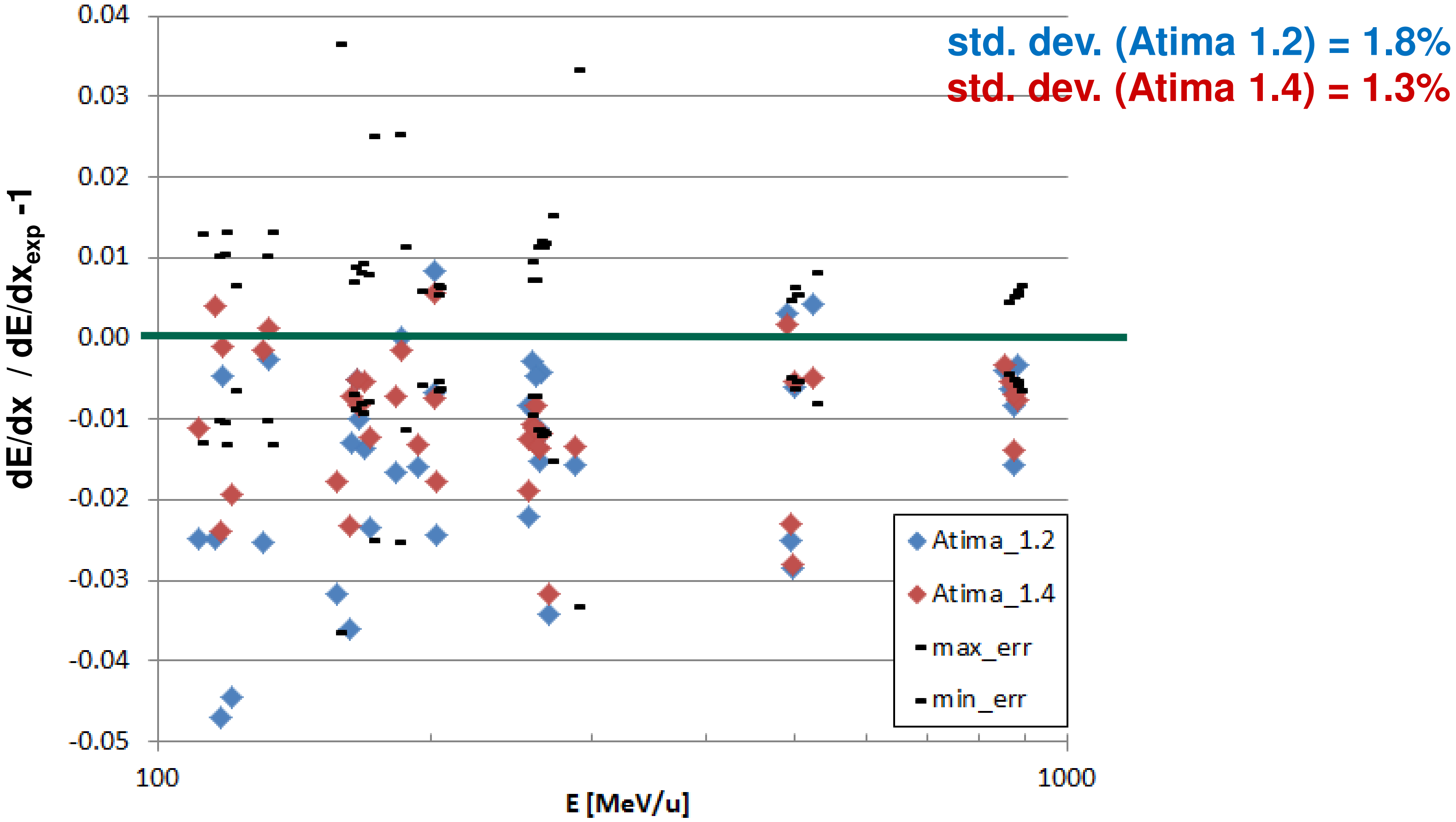
Yes, just above 30 MeV/u, but not when looking more closely for E > 100 MeV/u

Experiment data from thesis H. Weick, JLU Giessen 2000
Bi, Pb, Au projectiles on Be, Al, Cu, Ag, Ta, Au, Pb targets
41 points with average error 1%.



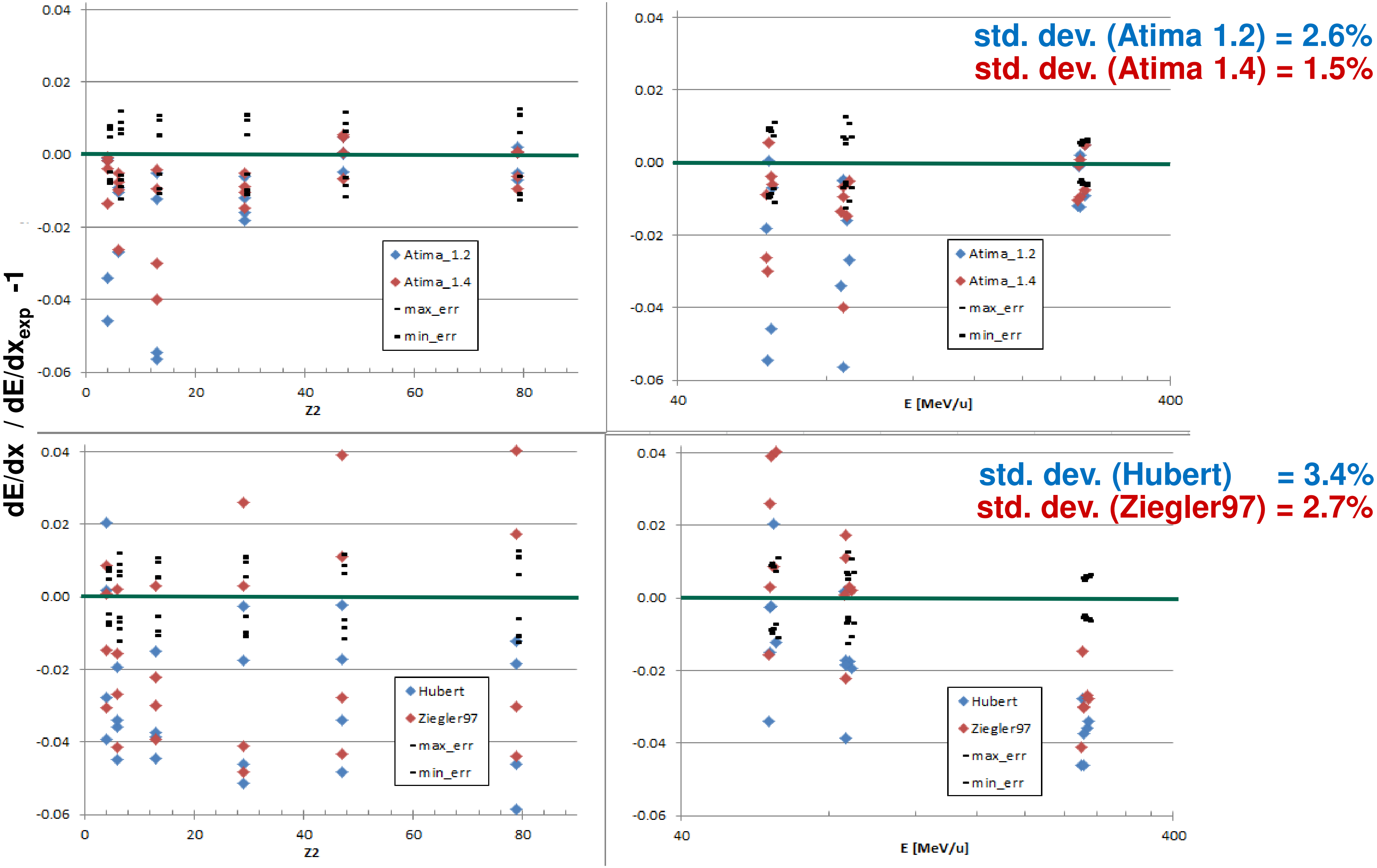
ATIMA for E > 100 MeV/u

Experiment data from thesis H. Weick, JLU Giessen 2000
Bi, Pb, Au projectiles on Be, Al, Cu, Ag, Ta, Au, Pb targets
41 points with average error 1.1%.



Xe Projectiles

Data from FRS Run95 (Weick, M. Maier)
reanalyzed in 2017, 21 points with average error 0.9%.

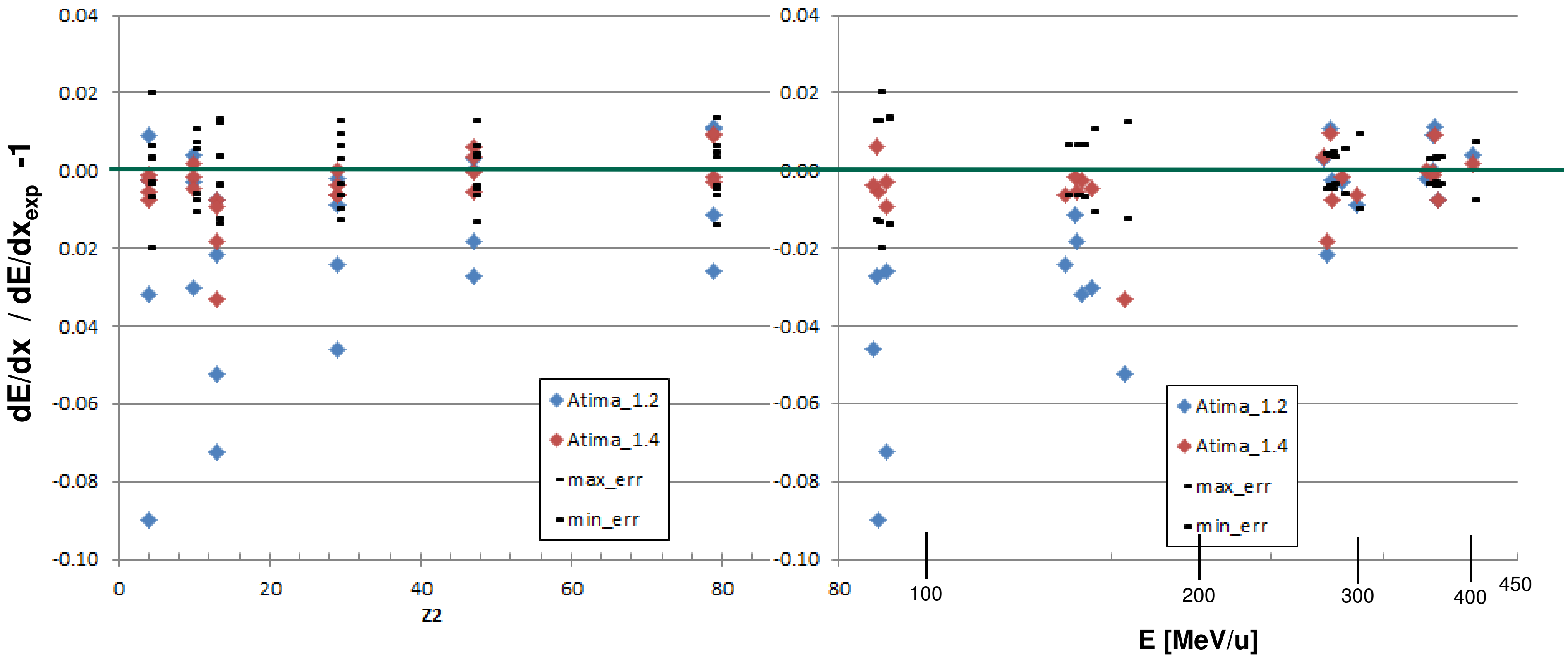


Uranium Projectiles

Data from FRS Run87, evaluated in 2006, H. Weick (unpublished)
23 points, U-> Be, SiO_2, Al, Cu, Ag, Au with average error 0.8%

std. dev. (Atima 1.2) = 1.52%
std. dev. (Atima 1.4) = 0.78%

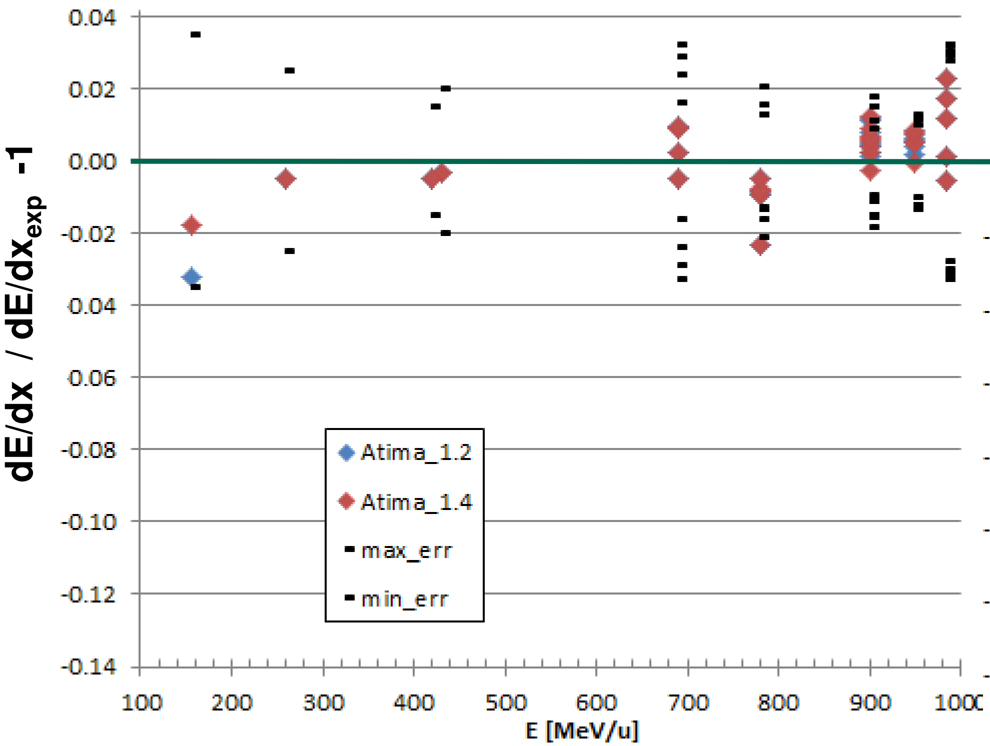
std. dev. (Hubert) = 5.0%
std. dev. (Ziegler97) = 1.8%
both not plotted



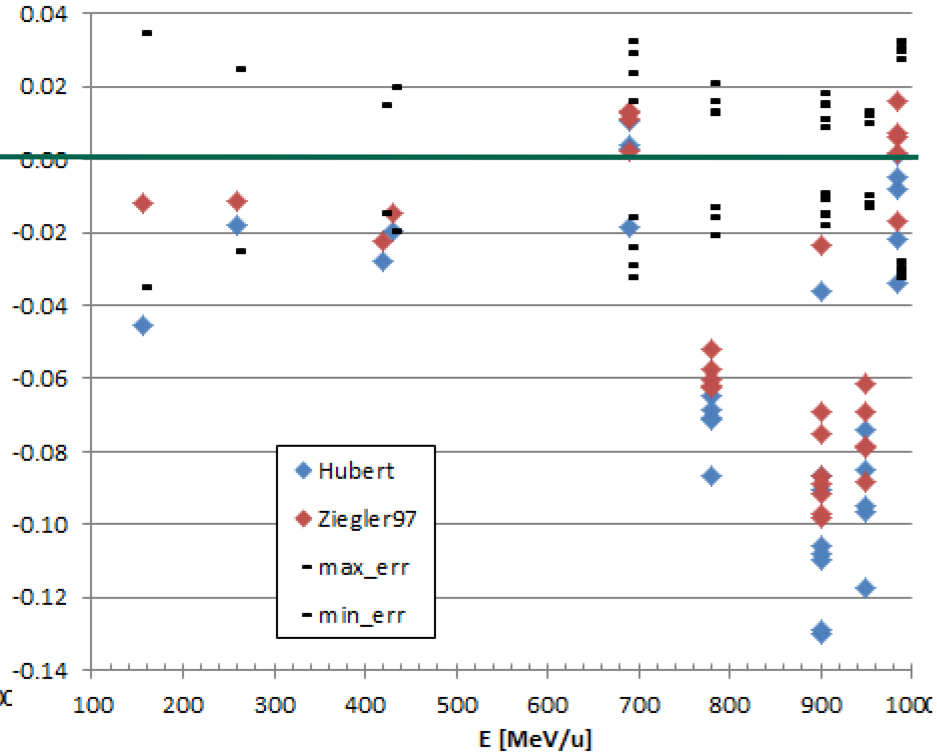
Higher E Projectiles

Data from thesis C. Scheidenberger, JLU Giessen 1994
31 points (Zp=8-92, Zt=4-82) with average error 1.8%

std. dev. (Atima 1.2) = 0.88%
std. dev. (Atima 1.4) = 0.84%



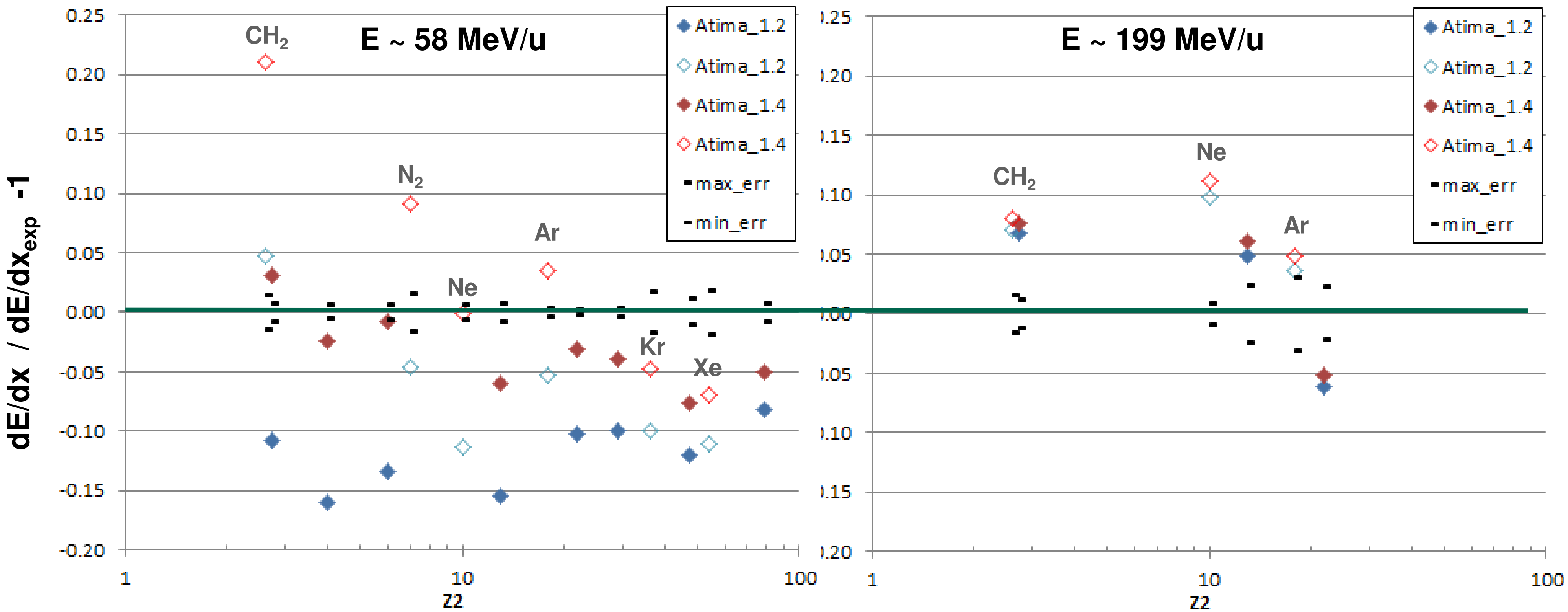
std. dev. (Hubert) = 8.6%
std. dev. (Ziegler97) = 6.7%



=> only small difference because ions are almost bare,
only one point for Bi->Al at 159 MeV/u really improved

Low E, gases + solids

Data from thesis A. Fettouhi, JLU Giessen 2006
U -> Be, N_2, Ne, CH_2, Al, Ar, Ti, Cu, Kr, Ag, Xe, Au (full = solid, empty = gas)
21 points with average error 1.1%

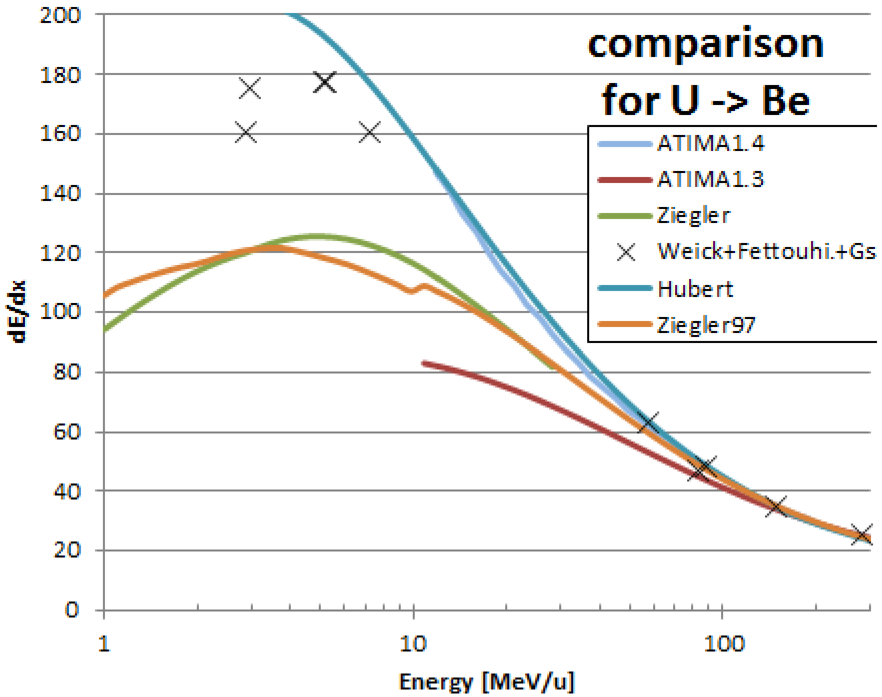


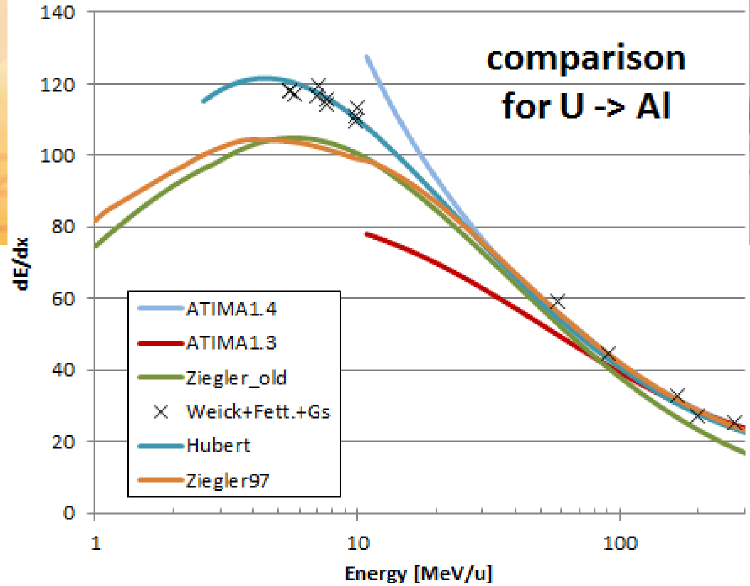
std. dev. (Atima 1.2) = 10%
std. dev. (Atima 1.4) = 3.6%

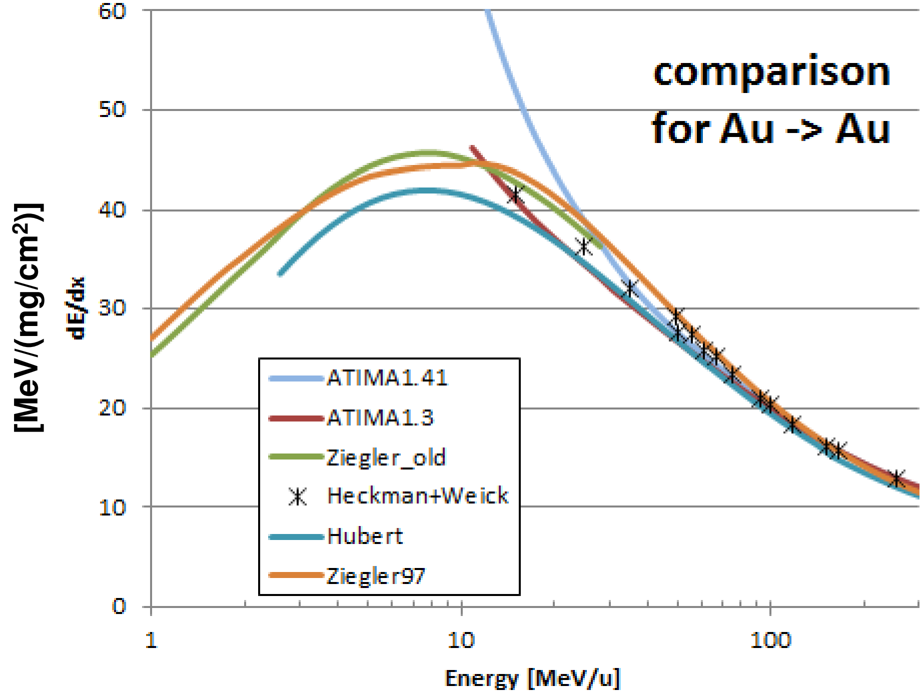
std. dev. (Hubert) = 4.6%
std. dev. (Ziegler97) = 3.3%
both not plotted

No gas-solid effect included in these programs

Behavior <30 MeV/u







Needs weighted average with Ziegler (SRIM) for 10-30 MeV/u, otherwise divergence at 10 MeV/u.

Numerical Calculation (only for ATIMA splines)

Range (R) and range straggling integrals stored as splines.

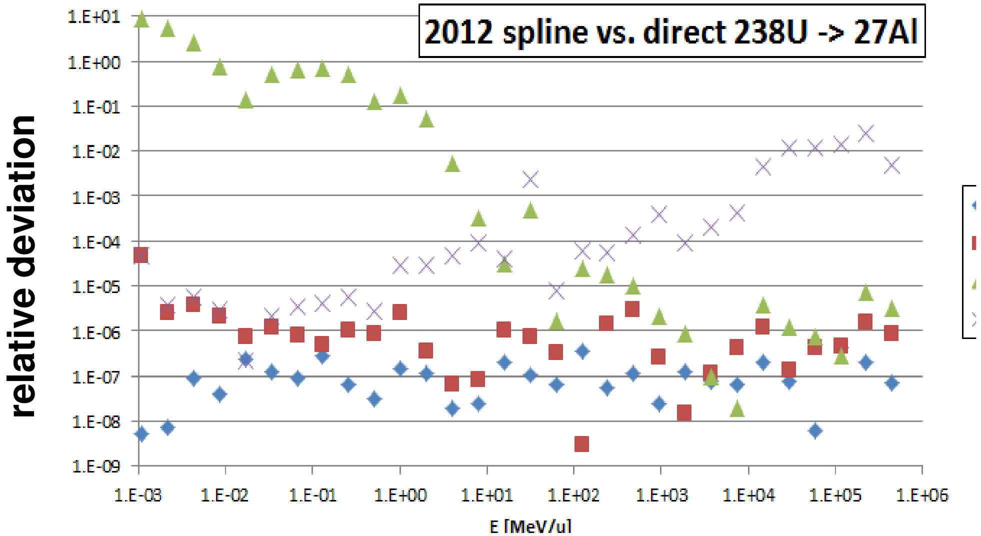
$$t = R(E_{in}) - R(E_{out})$$

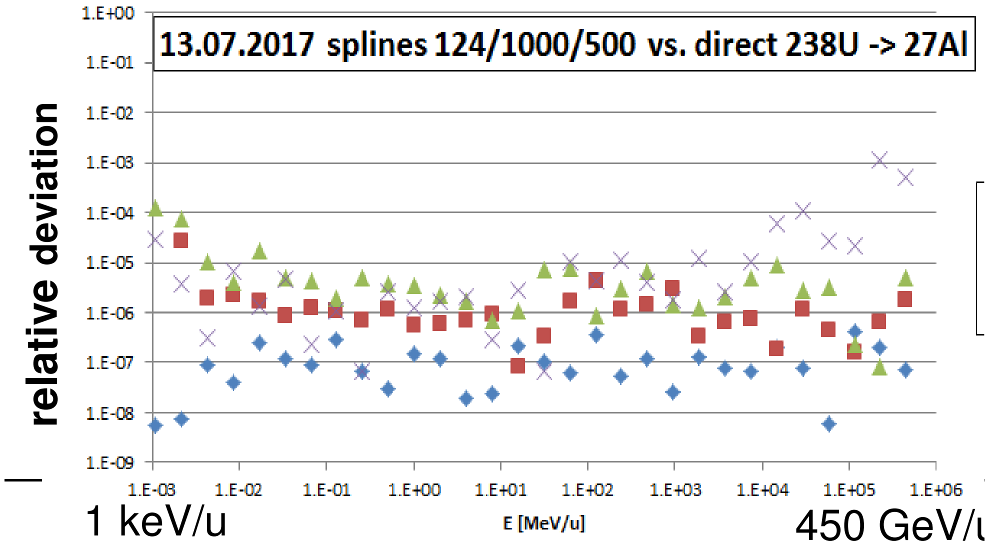
root solve to find E_{out}.
Similar for $\sigma_R^2 \to \sigma_E$, σ_α

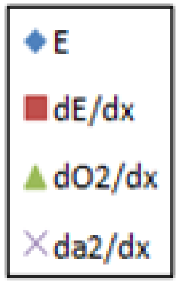
Integration done by solving
1st order ODE with COLSYS routines.

Integration is critical:
$d\Omega^2/dx$ varies by many orders
of magnitude.
-> use better start points on log scale.

All combinations -> 1.3 GB
(version 1.31 July 2017)







Summary / Conclusion

- ATIMA1.2 was best program for dE/dx (E>100 MeV/u)
- New ATIMA1.4 should be best down to 30 MeV/u.
  Hubert and Ziegler are similar in this range, but not above.
  Also improvements at energies > 100 MeV/u with Atima 1.4
- No changes on energy or angular straggling in Atima 1.4
  also no ultra relativistic enhancement yet.
- Intended release early 2018, avoid many versions.
- Even lower energies, gas-solid effects, require more input
  for now use the old Ziegler, update to new SRIM possible.