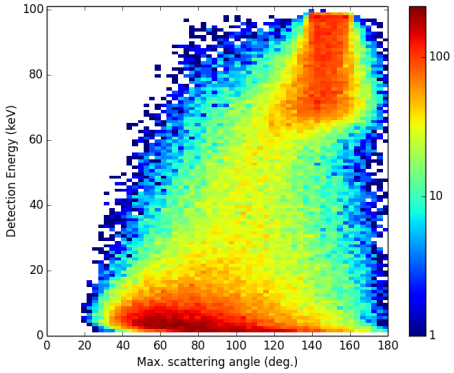
Multiple scattering simulation: effects at medium energy

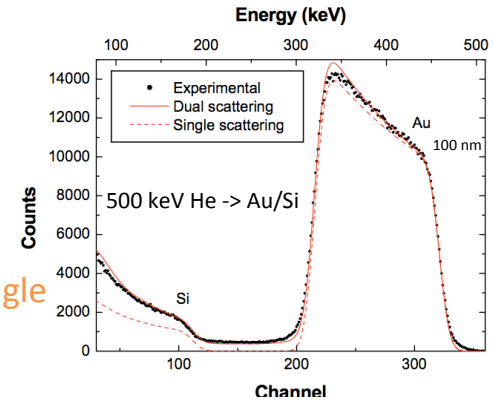


François Schiettekatte
Université de Montréal

HRDP 8, August 2016

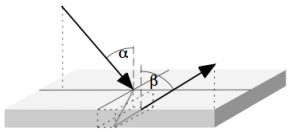
Multiple scattering (MS)

Broadening
Background
Low energy tails
Asymmetry at grazing angle



Important whenever
cross-section x distance = large

large at low energy or high Z



Source: SimNRA manual

Analytical theory ("<20°")
Double scattering (SimNRA, NDF)
Monte Carlo (TRBS, MCERD, Corteo)

Why Monte Carlo?

Full trajectory simulation for each ion

Takes many/most effects into account, e.g.:

Multiple/plural scattering

Full geometry

But… full trajectory simulation for each ion!

Running SRIM: 10 nC = months, years

Yet, TRIM already fast: RPA, CPA, BCA, MAGIC

MCERD:

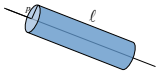
main collision approximation x 10^3-10^5

virtual detector x 10-100

$$n = Nt\left(\frac{1}{\lambda}\sum_{\lambda}\frac{d\sigma}{d\Omega}\right)q\Delta\Omega$$

Corteo: replaces trigonometric and transcendental function calls…

- Poisson's probability:
  $P(\ell)d\ell = e^{-\ell/\ell_0}d\ell \Rightarrow \ell = -\ell_0 \ln r_1$
  $\pi p_0^2 \ell N = 1 \quad \Rightarrow p = \sqrt{\frac{r_2}{\pi \ell N}}$

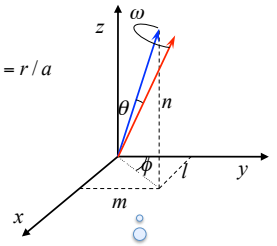


- Scattering angle: $s = p/a, \quad \varepsilon = E_{CM}\cdot a/Z_1Z_2e^2$
  - $\Theta_{CM}(\varepsilon,s) = \pi - 2\int_{\rho_0}^{\infty}\frac{s\,d\rho}{\rho^2\sqrt{1-\frac{\Phi(\rho)}{\rho\varepsilon}-\left(\frac{s}{\rho}\right)^2}}, \quad \Phi(\rho) = \sum_{i=1}^{4}a_i e^{-b_i r}, \quad \rho = r/a$
  - MAGIC:
    - $\sin^2\frac{\Theta_{CM}}{2}(s,\varepsilon)$
    - Needs to compute screening
  - Lab ref. frame: $\theta = \arctan\left(\sin\Theta_{CM}\Big/\left(\cos\Theta_{CM}+\frac{M_1}{M_2}\right)\right)$
  - Azimuthal angle: $\omega = 2\pi r_3$
  - Rotation l, m, n: directional cosines

$$l' = l\cos\theta + \frac{\sin\theta}{\sqrt{1-n^2}}(ln\cos\omega + m\sin\omega)$$

$$m' = m\cos\theta + \frac{\sin\theta}{\sqrt{1-n^2}}(mn\cos\omega - l\sin\omega)$$

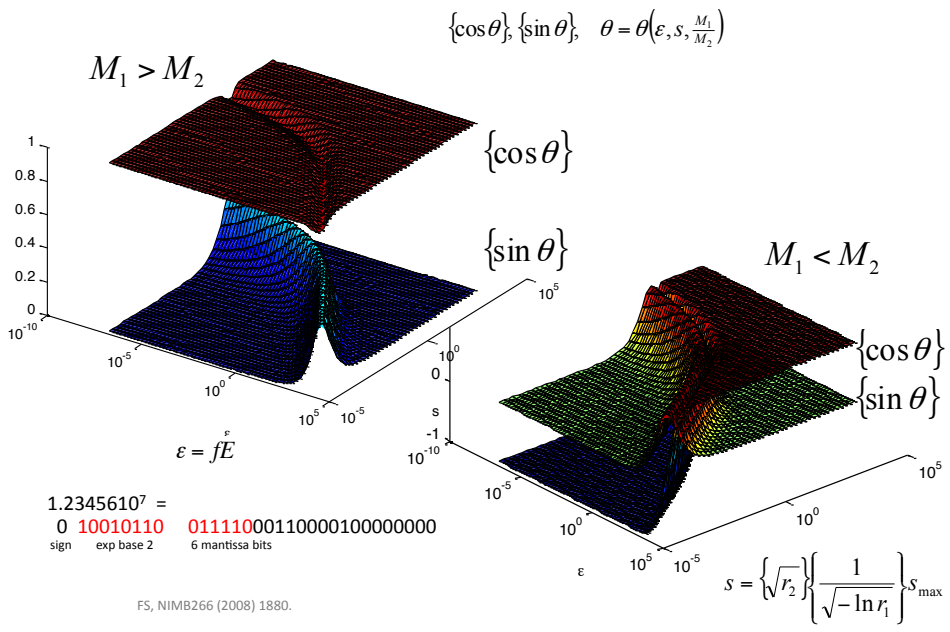
$$n' = n\cos\theta - \sqrt{1-n^2}\sin\theta\cos\omega$$



BILLIONS OF TIMES

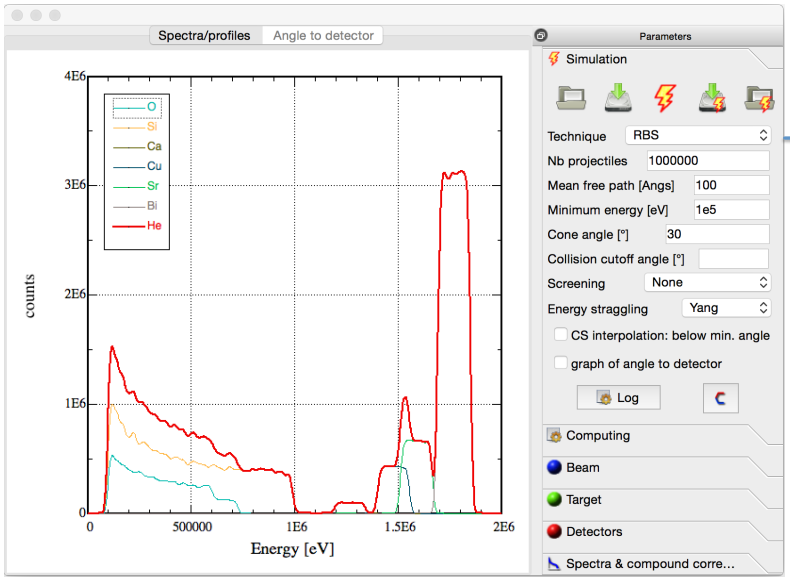
- Energy loss: $E' = E - E\frac{4M_1M_2}{(M_1+M_2)^2}\sin^2\Theta_{CM}/2 - \left(\frac{dE}{dx}\right)_e \ell - (\Delta E)_{straggling}\sqrt{\ell}$

… by lookup in tables indexed using binary representation of floats



FS, NIMB266 (2008) 1880.

User interface (decoupled from the simulation engine)



- RBS
- RBS-TOF
- EBS
- ERD
- ERD-TOF
- Coincidence
- Implantation?
- …and more

Corteo is distributed free of charge under the GPL
New version of the program and manual to be release next week

The simulation engine produces a “list mode” output

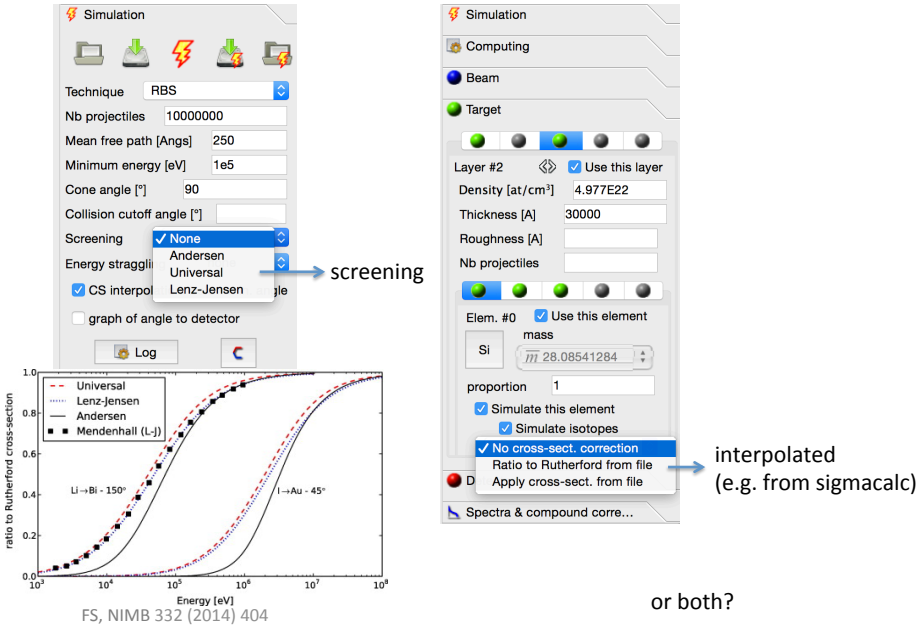
HRDP8 — bash — 122×34

```
#E crosssect Nt_Omega/Num_det_part E_before_coll cos_coll_angle cos_angle_det0 colldepth Z2 collision_layer CS_stamp
9.729337e+04  8.245721e-05 7.099999e-07  9.992724e+04 -9.552660e-01  9.981990e-01 6.166160e-04  79 0 0
9.733486e+04  8.065614e-05 7.099999e-07  9.987301e+04 -9.781078e-01  9.815761e-01 1.761760e-03  79 0 0
9.676336e+04  8.378043e-05 7.099999e-07  9.932591e+04 -9.505420e-01  9.992237e-01 3.051048e-03  79 0 0
3.846742e+04  8.047430e-05 7.099999e-07  9.995191e+04 -9.789067e-01  9.029862e-01 2.962960e-03  79 0 0
7.548544e+04  8.674742e-05 7.099999e-07  9.902866e+04 -9.220068e-01  8.713186e-01 3.499496e-03  79 0 0
9.696864e+04  8.342670e-05 7.099999e-07  9.949509e+04 -9.516202e-01  9.956357e-01 3.947944e-03  79 0 0
9.899748e+04  8.031445e-05 7.099999e-07  1.007060e+05 -9.671348e-01  9.997319e-01 5.469464e-03  79 0 0
9.785949e+04  8.156944e-05 7.099999e-07  9.996920e+04 -9.651796e-01  9.999252e-01 6.678673e-03  79 0 0
9.760051e+04  8.111264e-05 7.099999e-07  9.972666e+04 -9.751807e-01  9.986120e-01 6.038032e-03  79 0 0
9.818277e+04  8.129710e-05 7.099999e-07  1.000129e+05 -9.676926e-01  9.997465e-01 9.353345e-03  79 0 0
9.826693e+04  7.971957e-05 7.099999e-07  1.000486e+05 -9.865297e-01  9.994971e-01 9.753744e-03  79 0 0
9.806474e+04  8.233791e-05 7.099999e-07  9.987404e+04 -9.576566e-01  9.996516e-01 1.093092e-02  79 0 0
9.745153e+04  8.628382e-05 7.099999e-07  9.922914e+04 -9.235911e-01  9.984483e-01 1.285284e-02  79 0 0
9.822863e+04  8.154536e-05 7.099999e-07  1.002766e+05 -9.598871e-01  9.980919e-01 1.306105e-02  79 0 0
7.276030e+04  8.004707e-05 7.099999e-07  1.000061e+05 -9.832168e-01  9.081724e-01 1.531930e-02  79 0 0
9.820904e+04  8.014528e-05 7.099999e-07  1.004544e+05 -9.737949e-01  9.998249e-01 1.659258e-02  79 0 0
9.873623e+04  8.017551e-05 7.099999e-07  1.008565e+05 -9.661258e-01  9.999943e-01 2.114112e-02  79 0 0
5.505002e+04  7.992076e-05 7.099999e-07  1.000889e+05 -9.832718e-01  9.065257e-01 2.237435e-02  79 0 0
9.840020e+04  8.039379e-05 7.099999e-07  1.002720e+05 -9.740455e-01  9.985154e-01 2.236635e-02  79 0 0
9.109164e+04  8.157906e-05 7.099999e-07  9.968234e+04 -9.703019e-01  8.740464e-01 2.570568e-02  79 0 0
6.682575e+04  7.952032e-05 7.099999e-07  9.976044e+04 -9.943555e-01  9.358528e-01 2.549747e-02  79 0 0
9.561658e+04  7.921019e-05 7.099999e-07  1.000223e+05 -9.934314e-01  9.537800e-01 3.013411e-02  79 0 0
```

Detailed output mode also provides

- minimal approach distance
- collision locus and $\hat{v}$ before and after collision
- exit point from the target and $\hat{v}$
- intersection point on the detector and $\hat{v}$ in detector frame

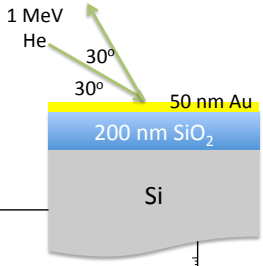
Cross-section

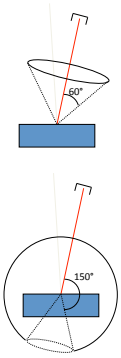


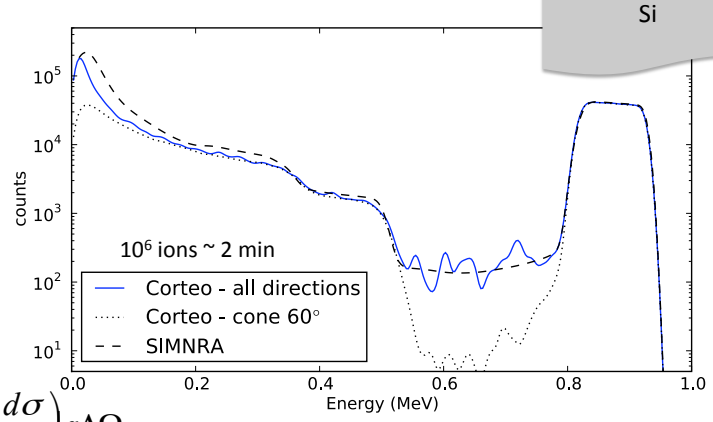
FS, NIMB 332 (2014) 404

or both?

Effect of cone angle in which ions are thrown during main collision



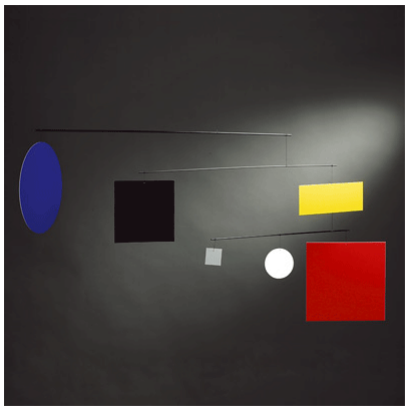




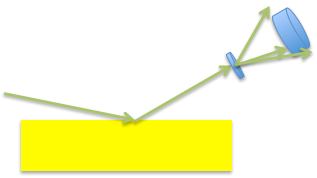
$$n = Nt\left(\frac{1}{\lambda}\sum_{\lambda}\frac{d\sigma}{d\Omega}\right)q\Delta\Omega$$

FS, NIMB266 (2008) 1880

Arbitrarily oriented rectangular and elliptically shaped detectors (including annular detectors, TOF)

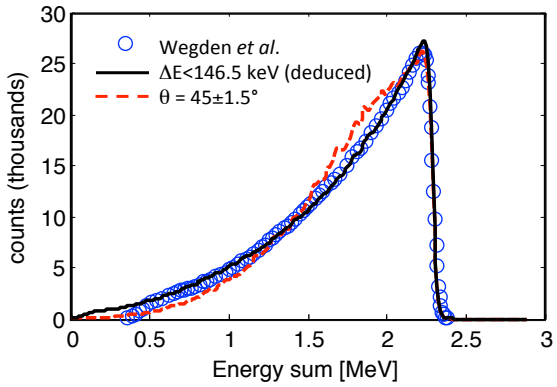


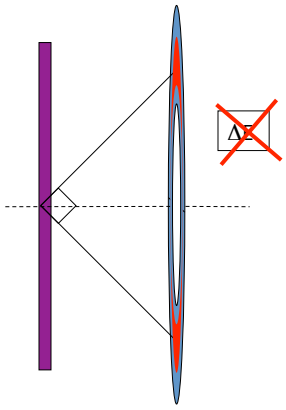
Flensted mobile, Guggenheim museum



Considers real space geometry

Coincidence





⇒ Can't be assumed that a ΔE discr. is equivalent to an angular restriction

FS, Simulation of Multiple Scattering: Effects on Coincidence, AIP Conf. Proc. 1099 (2009) 314

11

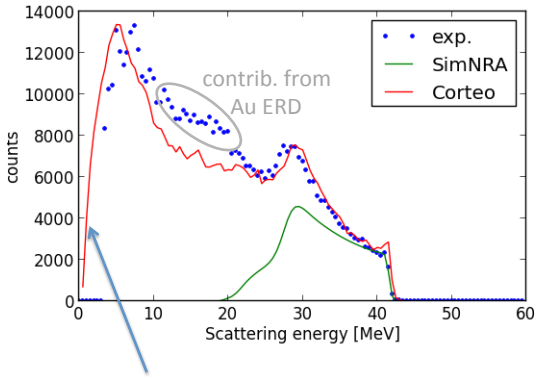
Full RBS simulations (i.e. no "main scattering" approx.)

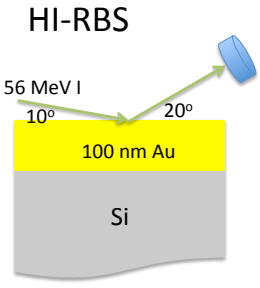
just like running SRIM for 40 years!

RBS spectrum in 1-25 core-days with Corteo

10^9-10^{11} ions in 10-2000 core-hours

higher cross-section (low energy, heavy ions) = less ions

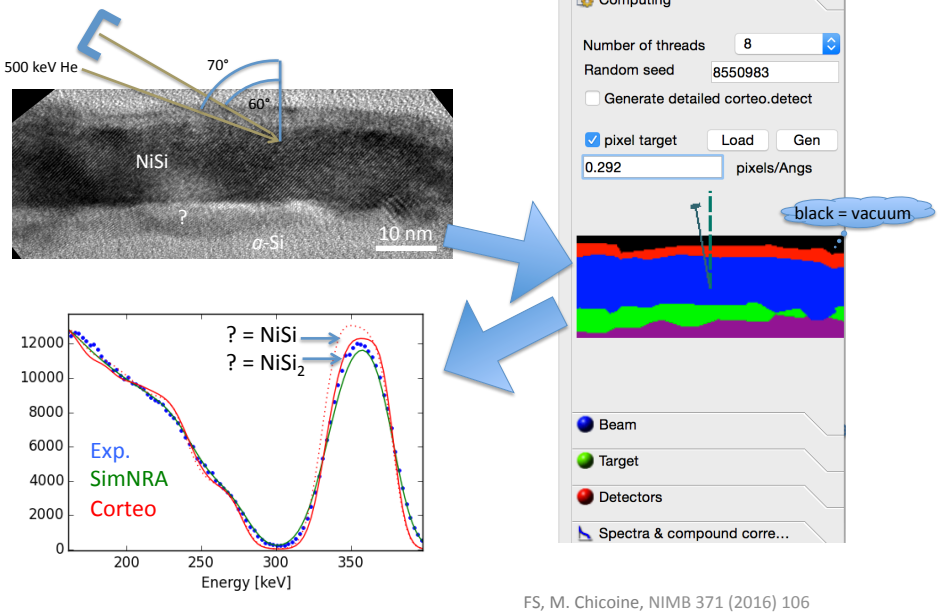




90 min @ 6x3.8 GHz, much shorter if, e.g., E_{min} =20 MeV

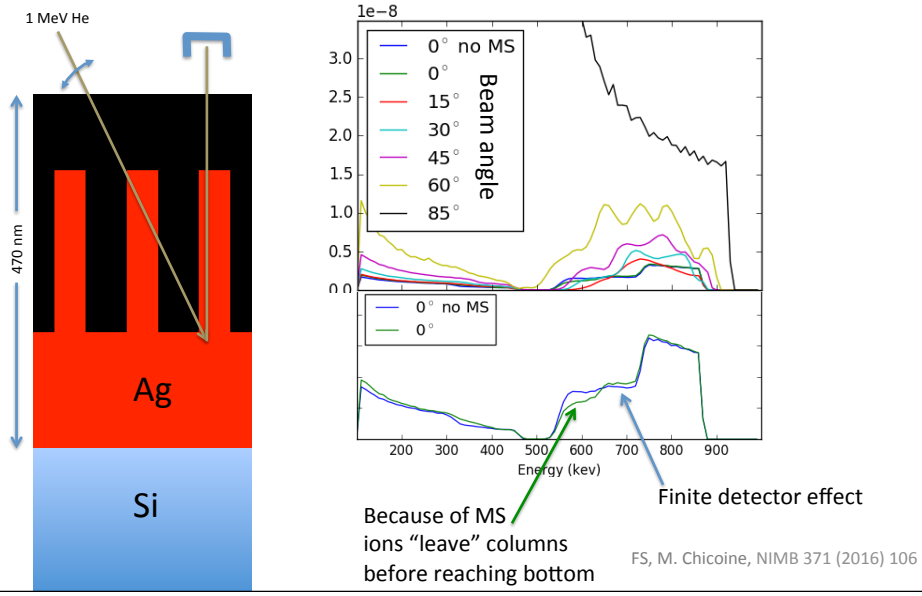
FS, NIMB 332 (2014) 404

2D or 3D pixel targets



FS, M. Chicoine, NIMB 371 (2016) 106

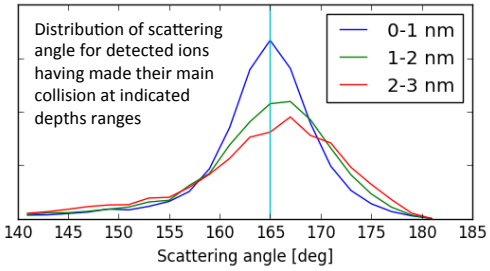
Feature replication with increasing angle in periodic structures

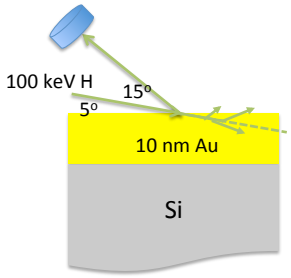


FS, M. Chicoine, NIMB 371 (2016) 106

MS induces asymmetric broadening at grazing incidence

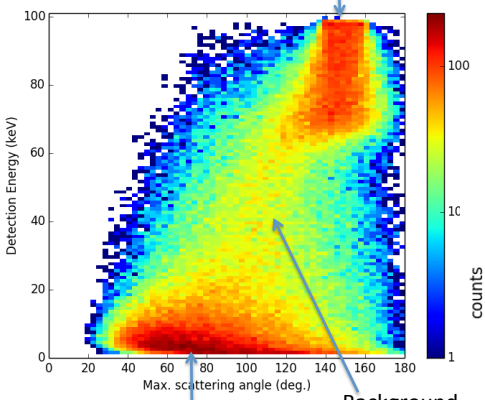
ions deflected towards the surface may escape the sample





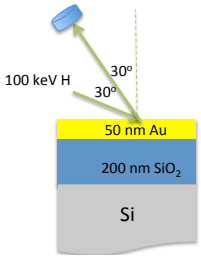
100 keV H -> Au

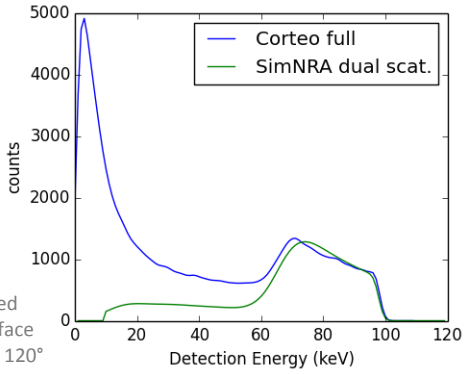
main spectrum
("single" scattering)



Background
Ions first scattered parallel to the surface then second coll. at 120°

Tail
2 wide collisions

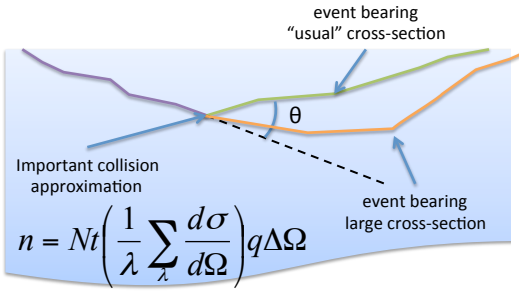




Cut-off angle

Negligible effect in RBS, no effect in ERD

Problem in forward scattering



Peaks = actual background contribution
concentrated in single events

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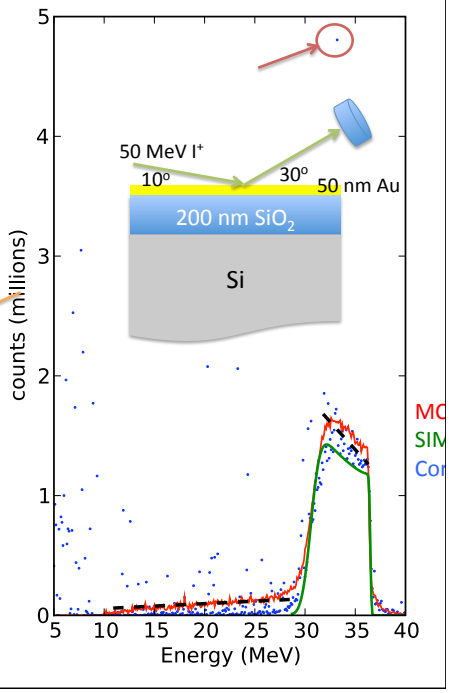
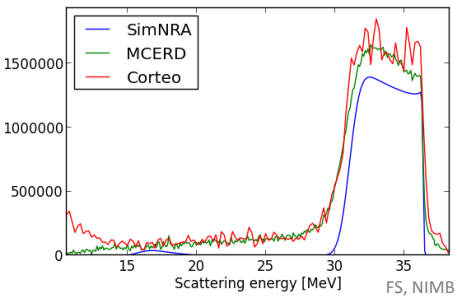


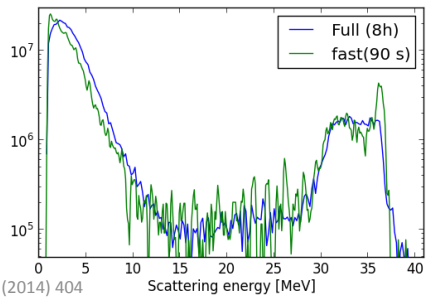
Solution: Hybrid simulations

Important collision approx. gives good results with cut-off on scat. angle ≳10-15°
We need only the ≲10-15° part which results from several large angle collisions:
"incoherent", can be loose on parameters

Full RBS simulations: like running TRIM for 40 years!
spectrum in 1-25 core-days with Corteo

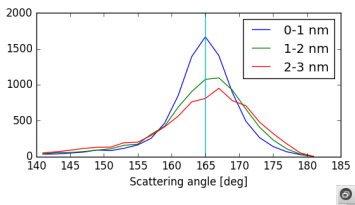
Background simulation possible in 10-100 core-minutes with
mean free path x 50-100
detector area x 25-100
keep only trajectories with max scattering angle <15° & combine it to normal simulation





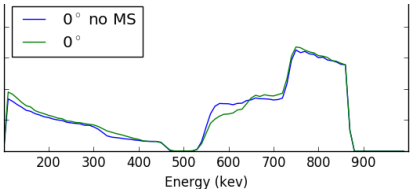
FS, NIMB 332 (2014) 404

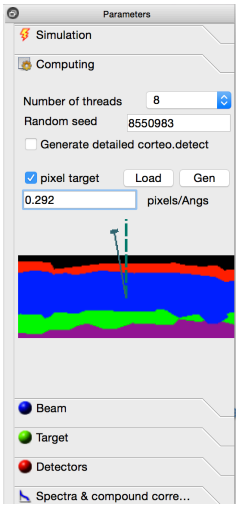
Summary



MS results in many effects
- Broadening
- Background
- Low energy tails
- Asymmetry at grazing angle as particles escape surface
- Particles escaping wall

Fortunately, MC:
- reproduces MS effects in details
- considers real space detectors and geometrical effects
- considers detailed target descriptions
- is fast enough even on a PC thanks to several optimisations





Thanks to:

Martin Chicoine for ERD-TOF spectra and other contributions
Mikko Laitinen & Timo Sajavaara @ Jyväskylä for providing wonderful TOF units!

Louis Godbout for accelerator maintenance and operation

Kai Arstila, Matej Mayer and Nuno Barradas for fruitful discussions

NSERC CRSNG

Fonds de recherche Nature et technologies Québec

RQMP
Le regroupement québécois sur les matériaux de pointe

Calcul Québec