PTRAC to PoliMi

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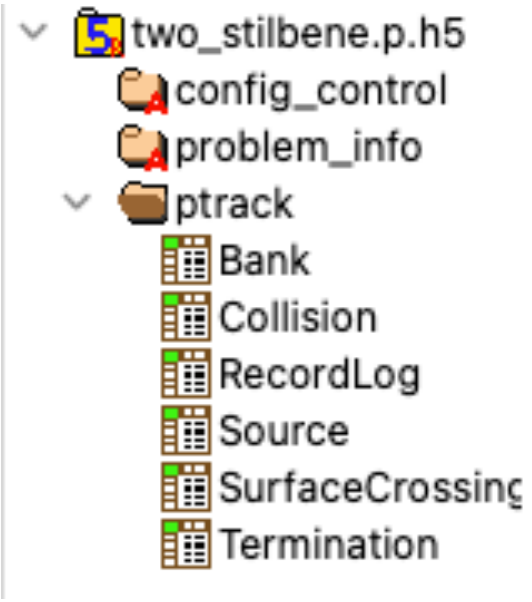
PTRAC Output – All Events in Histories w/ Collision

```
PTRAC FLUSHNPS=1e5 FILE=HDF5 CELL=901,902 $ All events for histories with collisions in cells specified
```

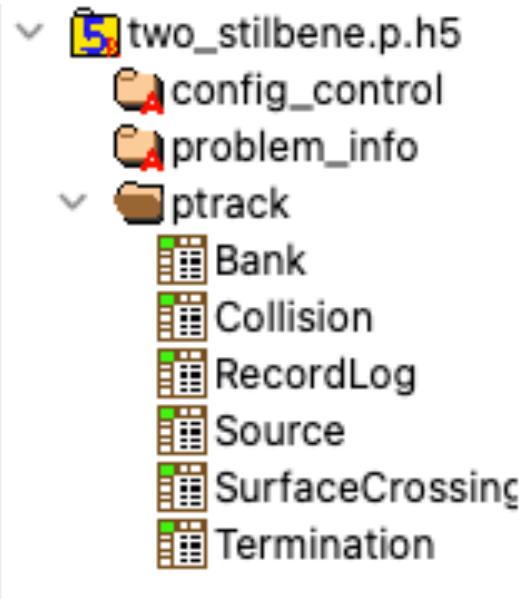
- Outputs all events related to random sampling
  - CELL filter limits outputs to all particle tracking for histories with collisions in cells specified
- Source
  - Initiation event for each history, for IPOL or par=sf, first sf particle
- Bank
  - Secondary particle generation
    - Includes remaining sf particles, induced fission particles, other secondary particles (i.e. n,2n, inelastic gammas)
- Collision
  - Outputs very similar data to PoliMi data file, missing:
    - **Energy deposition** (outputs outgoing energy)
    - **Particle number**
    - **Generation number**



PTRAC Output – All Events in Histories w/ Collision Cont.

```
PTRAC FLUSHNPS=1e5 FILE=HDF5 CELL=901,902 $ All events for histories with collisions in cells specified
```

- Outputs all events related to random sampling
  - CELL filter limits outputs to all particle tracking for histories with collisions in cells specified
- SurfaceCrossing
  - Outputs any particle surface crossing event
  - Important for calculating energy deposition in analog mode
- Termination
  - Final event for each particle
- RecordLog
  - An index for all the other branches of the HDF5 output
  - 1000 = Source, 2000 = Bank, 3000 = SurfaceCrossing, 4000 = Collision, 5000 = Termination
  - Outputs events in **exact order** MCNP does particle simulation



PTRAC to PoliMi

- Collision
  - Outputs very similar data to PoliMi data file, missing:
    - **Energy deposition** (outputs outgoing energy)
    - **Particle number**
    - **Generation number**

Collision at /ptrack/ [single_stilbene.p.h5 in /Users/fdarby/Documents/Git/basic_u235_oscar_response/single_stilbene]

0-based

MCNP6.3 HDF5 Collision Branch Output

	0																
	x	y	z	u	v	w	energy	weight	time	nps	node	material_id	cell_id	particle_type	num_collisions_this_branch	zaid	reaction_type
0	-1.7040...	2.79766...	0.3984...	0.73070...	0.6540...	0.19580...	0.2640...	1.0	4.78304...	123	6	1	901	1	1	1001	2
1	1.29496...	5.48183...	1.20206...	0.38154...	-0.8483...	0.36704...	0.21554...	1.0	5.3606...	123	6	1	901	1	2	6012	2
2	1.32389...	5.41751...	1.22989...	0.8489...	-0.3608...	-0.3861...	0.05129...	1.0	5.37241...	123	6	1	901	1	3	1001	2

MCNPX-PoliMi Collision File Output (Polimi 2.0.0)

nps	pnum	pid	rxn	zaid	cell	energy dep.	time (shakes)	x	y	z	weight	gen	#_coll	code	incident energy
123	1	1	-99	6012	901	0.148116	4.75	-1.69	2.40	0.40	1.000E+00	0	0	0	6.612E-01
123	1	1	-99	6012	901	0.060509	4.83	-1.63	2.00	1.07	1.000E+00	0	1	0	5.131E-01

Flynn's MCNP6.3 HDF5 PTRAC → PoliMi Collision File

nps	pnum	pid	rxn	zaid	cell	energy dep.	time (shakes)	x	y	z	weight	gen	#_coll	code	incident energy
123	3	1	-99	1001	901	0.397134	4.78	-1.70	2.80	0.40	1.000e+00	0	1	0	2.641e-01
123	3	1	-99	6012	901	0.048516	5.36	1.29	5.48	1.20	1.000e+00	0	2	0	2.155e-01

PTRAC to PoliMi

Flynn's MCNP6.3 HDF5 PTRAC → PoliMi Collision File

nps	pnum	pid	rxn	zaid	cell	energy dep.	time (shakes)	x	y	z	weight	gen	#_coll	code	incident energy
123	2	1	-99	1001	901	0.397134	4.78	-1.70	2.80	0.40	1.000E+00	0	1	0	2.641E-01
123	2	1	-99	6012	901	0.048516	5.36	1.29	5.48	1.20	1.000E+00	0	2	0	2.155E-01
123	2	1	-99	1001	901	0.164248	5.37	1.32	5.42	1.23	1.000E+00	0	3	0	5.130E-02
123	2	1	-99	1001	901	0.010257	5.46	1.57	5.32	1.12	1.000E+00	0	4	0	4.104E-02
500	1	1	-99	1001	901	0.655608	3.80	1.71	3.47	-1.83	1.000E+00	0	1	0	4.204E-01
500	1	1	-99	1001	901	0.045248	4.03	0.37	4.81	-1.10	1.000E+00	0	2	0	3.751E-01
500	1	1	-99	6012	901	0.055912	4.07	0.23	5.07	-0.91	1.000E+00	0	3	0	3.192E-01
702	3	1	-99	6012	901	0.150581	4.68	0.59	4.48	1.16	1.000E+00	0	1	0	5.828E-01
1237	4	1	-99	1001	901	0.074093	13.08	1.60	1.26	0.22	1.000E+00	0	1	0	9.245E-03
1237	4	1	-99	6012	901	0.002467	13.50	2.13	1.43	0.31	1.000E+00	0	2	0	6.778E-03

PTRAC to PoliMi, Energy Deposited, One Stilbene Cf-252

Flynn's MCNP6.3 HDF5 PTRAC → PoliMi Collision File

Record Log

	nps	node	type	event_array_index
0	123	4	1000	0
1	123	5	3000	0
2	123	6	3000	1
3	123	6	5000	0
4	123	4	2000	0
5	123	5	3000	2
6	123	6	3000	3
7	123	6	4000	0

SurfaceCrossing

	x	y	z	u	v	w	energy
0	-0.0010...	-50.940...	-0.0020...	0.0246...	-0.2809...	-0.9594...	2.33819...
1	0.25623...	-53.867...	-9.9967...	0.0246...	-0.2809...	-0.9594...	2.33819...
2	-0.0012...	-50.938...	9.91360...	-0.0316...	0.99947...	0.00739...	0.66119...
3	-1.65211...	1.16000...	0.3863...	-0.0316...	0.99947...	0.00739...	0.66119...

```
energy dep.
0.397134
```

Collision

	x	y	z	u	v	w	energy	weight	time	nps	node	material_id	cell_id	particle_type	num_collisions_this_branch	zaid	reaction_type
0	-1.7040...	2.79766...	0.3984...	0.73070...	0.6540...	0.19580...	0.2640...	1.0	4.78304...	123	6	1	901	1	1	1001	2

- Use prior event energy, collision outgoing energy, and collision type to calculate energy deposited
- Below example is simple elastic scattering, so energy is conserved

- RecordLog
  - An index for all the other branches of the HDF5 output
  - 1000 = Source, 2000 = Bank, 3000 = SurfaceCrossing, 4000 = Collision, 5000 = Termination
  - Outputs events in **exact order** MCNP does particle simulation, **one particle at a time from birth to termination**

PTRAC to PoliMi, Energy Deposited Special Cases, Michael Rising [https://www.osti.gov/servlets/purl/1371662]

- Michael Rising did this with PTRAC in MCNP6.2 in 2017 (with our group!)
- Kind enough to share code
- Handles non elastic scatter rxns
- Inelastic scatter
  - Calculates deposition from non conserved momentum
  - Depends on nucleus mass
- Radiative capture
  - Depends on nucleus mass
- Alpha production
  - Depends on q-value of reaction that is nucleus dependent

```
    # Inelastic scatter: calculated from kinematics
    elif (51 <= rxn) and (rxn <=91):
        d1 = prev_vec
        d2 = vec
        mu = np.dot(d1,d2) / (np.dot(d1,d1)*np.dot(d2,d2))**0.5
        try:
            dep = (prev_erg + erg - 2*mu*(prev_erg*erg)**0.5)/masses[za]
        except KeyError:
            stdout.write(f"WARNING: Inelastic Collision Missing Mass, {nps} {za}\n")
            dep = prev_erg
```

```
    # Radiative capture
    elif (rxn == 102) | (rxn == 101):
        try:
            dep = prev_erg/(masses[za]+1)
        except KeyError:
            stdout.write(f"WARNING: Capture Collision Missing Mass, {nps} {za}\n")
            dep = prev_erg
```

```
    # Alpha production
    elif rxn == 107:
        try:
            dep = prev_erg + qvals[za][rxn]
        except KeyError:
            stdout.write(f"WARNING: Alpha Production Missing Q-value, {nps} {za} {rxn}\n")
            dep = prev_erg
```

```
masses = {1001:0.99916733,
          6012:11.9078563}
```

```
qvals = {6012:
         {107:-5.70205}}
```

PTRAC to PoliMi, Particle Number, One Stilbene Cf-252

Flynn's MCNP6.3 HDF5 PTRAC → PoliMi Collision File

Record Log

	0			
	nps	node	type	event_array_index
0	123	4	1000	0
1	123	5	3000	0
2	123	6	3000	1
3	123	6	5000	0
4	123	4	2000	0
5	123	5	3000	2
6	123	6	3000	3
7	123	6	4000	0
8	123	6	4000	1
9	123	6	4000	2
10	123	6	4000	3
11	123	7	3000	4
12	123	8	3000	5
13	123	8	5000	1
14	123	3	2000	1

- First particle in history is always generated as a source event (type 1000)
- Secondary particles are always generated from bank events for the same history (type 2000)
- Update particle number for all type 1000 and type 2000 events

PTRAC to PoliMi, Par. Num., One Stilbene Cf-252, **SUR/COL**

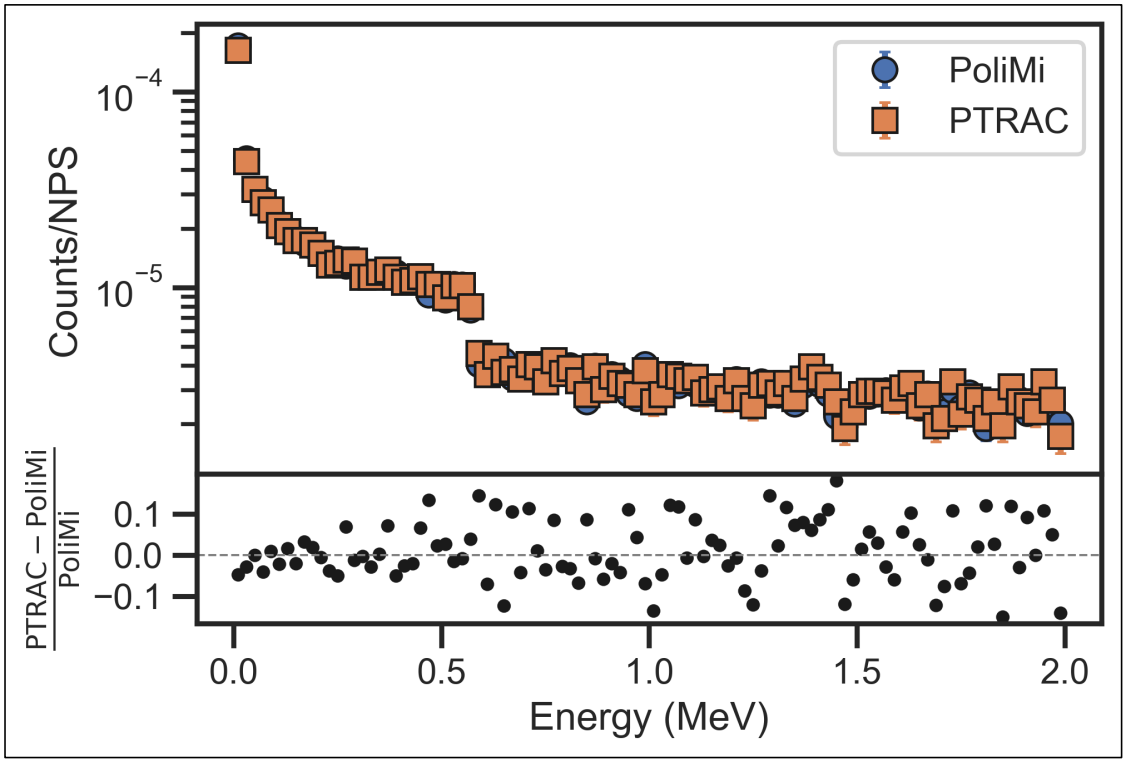
Flynn's MCNP6.3 HDF5 PTRAC → PoliMi Collision File

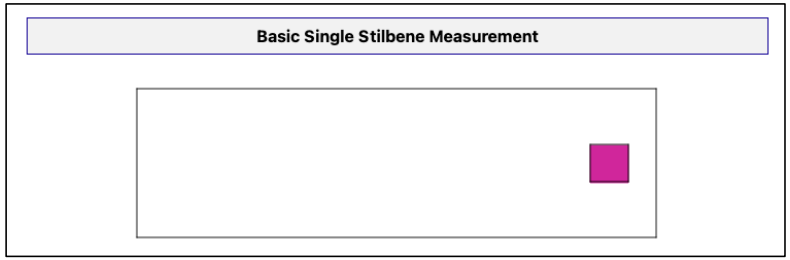
- No output source or bank events (saves memory)
- Cannot calculate the true particle number
- Use surface crossing logic to update particle number when a new particle is detected
- SurfaceCrossing includes "time" and "num_collisions"

- Update particle number if either the time or number of collisions value decreases
- It's possible to not update the number when you should if:
  a new particle takes longer and more collisions to interact from birth
- Misclassification should be rare, but it is possible

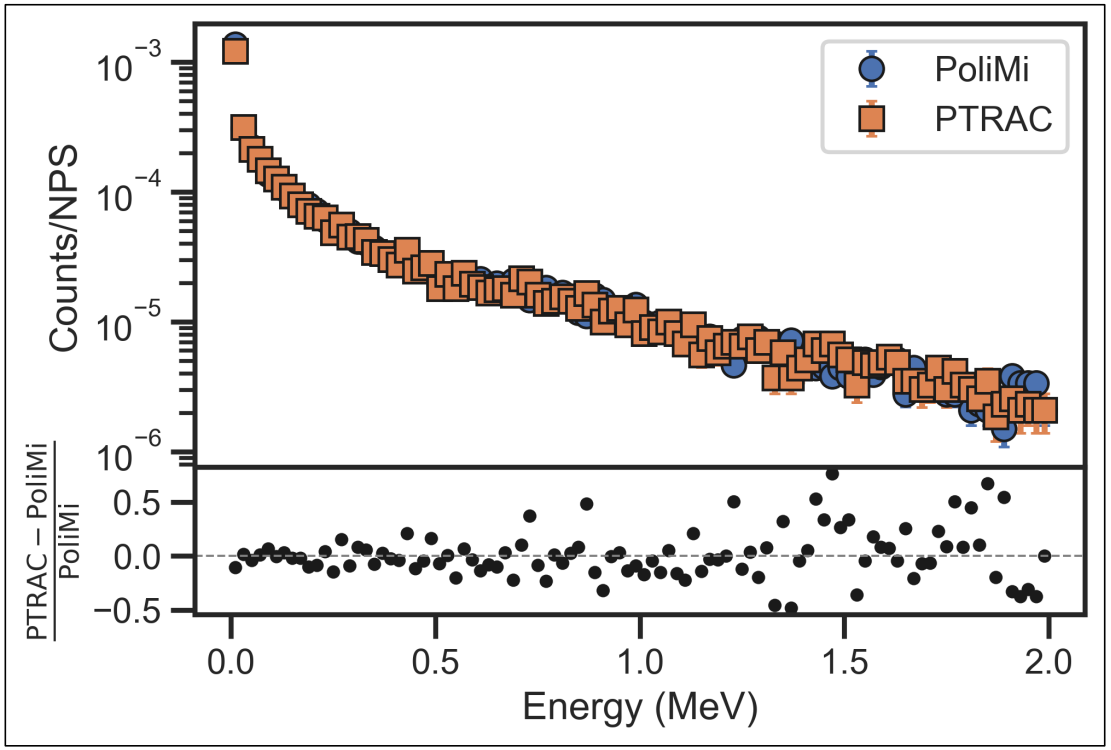
```
def surface_crossing_par_number_update(event_type, current_particle_num, current_event_data,
                                       prev_event_data, prev_surface_crossing):
    """Updates particle number based on surface crossing events."""
    if event_type == 3000: # Surface crossing
        if prev_event_data is None or prev_surface_crossing is None:
            prev_surface_crossing = current_event_data
            return current_particle_num + 1, prev_surface_crossing

        time_increased = current_event_data['time'] > prev_surface_crossing['time']
        collisions_increased = current_event_data['num_collisions_this_branch']
                               > prev_surface_crossing['num_collisions_this_branch']

        if not (time_increased and collisions_increased):
            prev_surface_crossing = current_event_data
            return current_particle_num + 1, prev_surface_crossing

    return current_particle_num, prev_surface_crossing
```

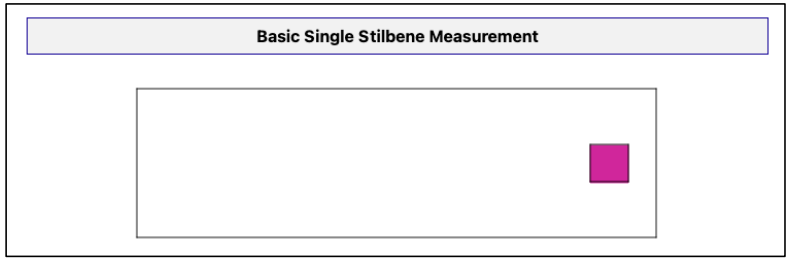
Example 1: Single Stilbene, 2 MeV Isotropic Neutrons



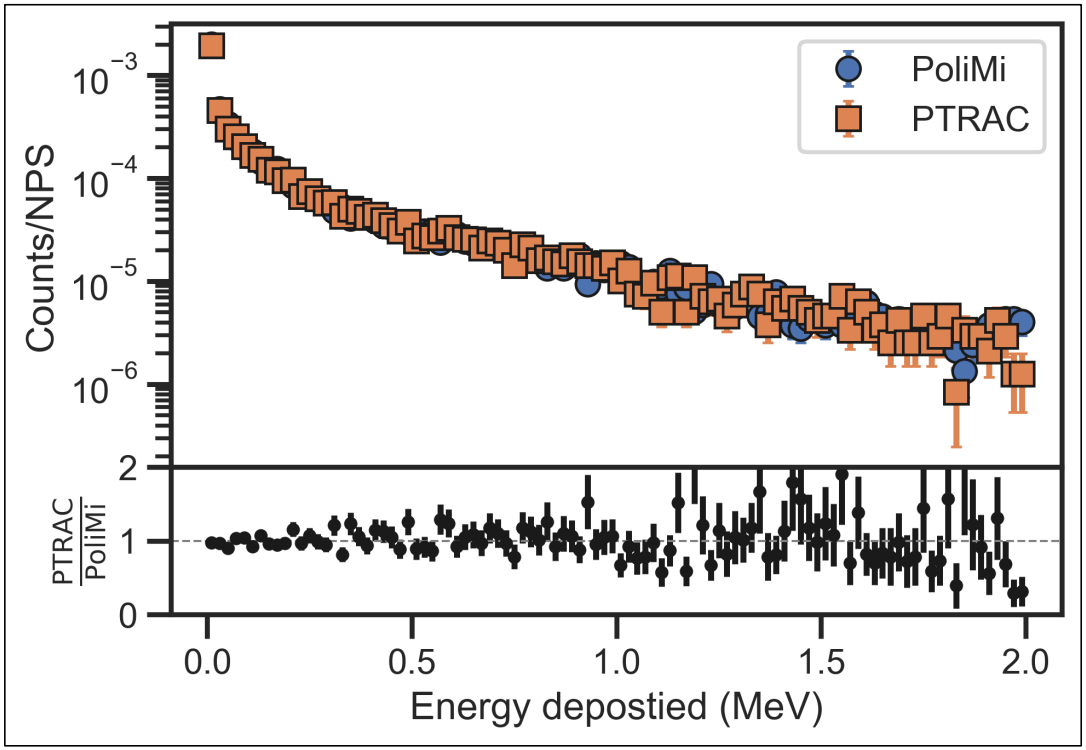


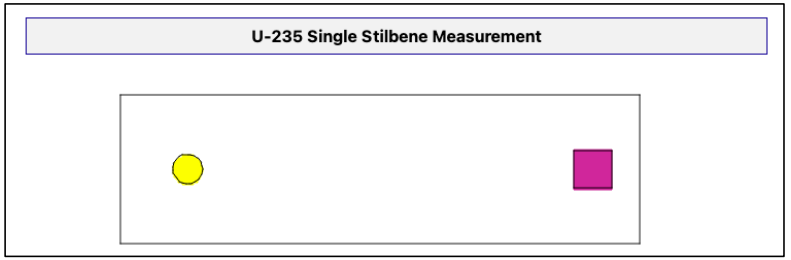
Example 2: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1



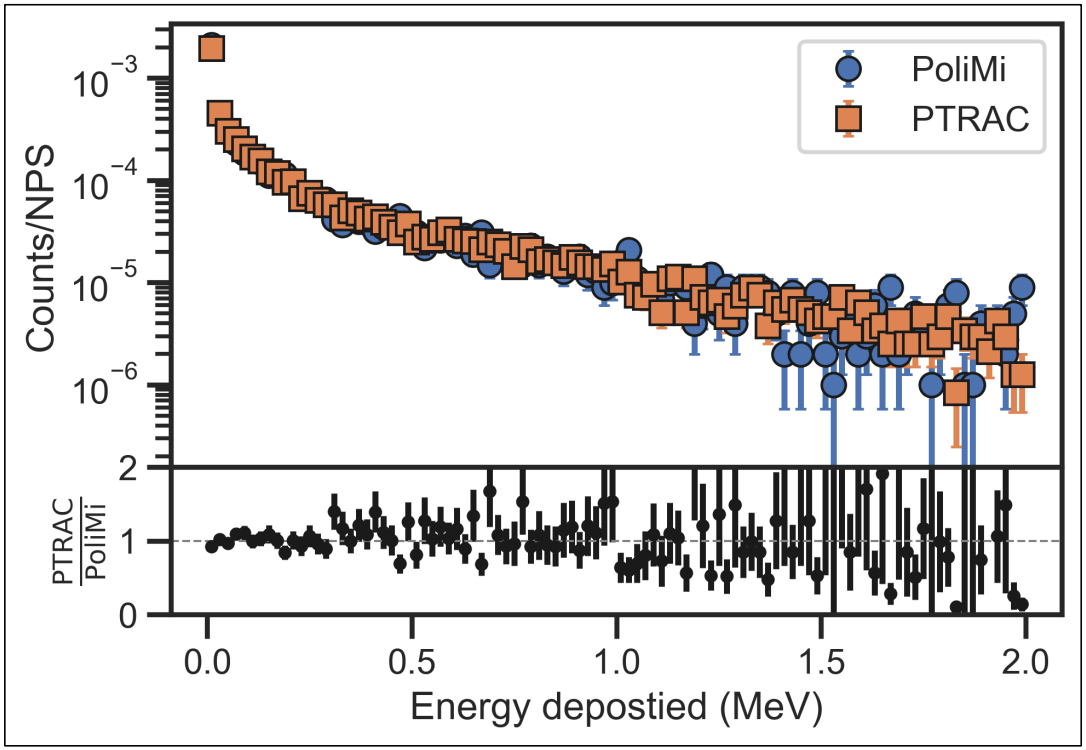


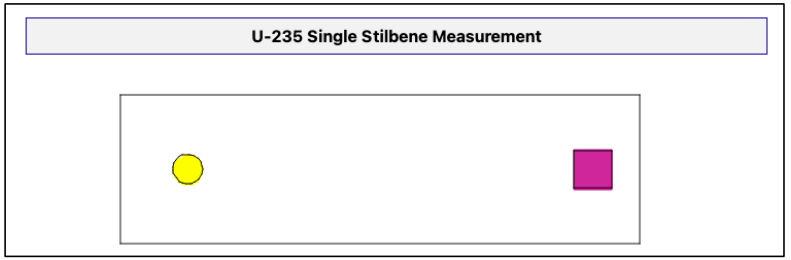
Example 3: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1
U-235 spherical shell, IPOL(2-5) = 0 (no IPOL if params)



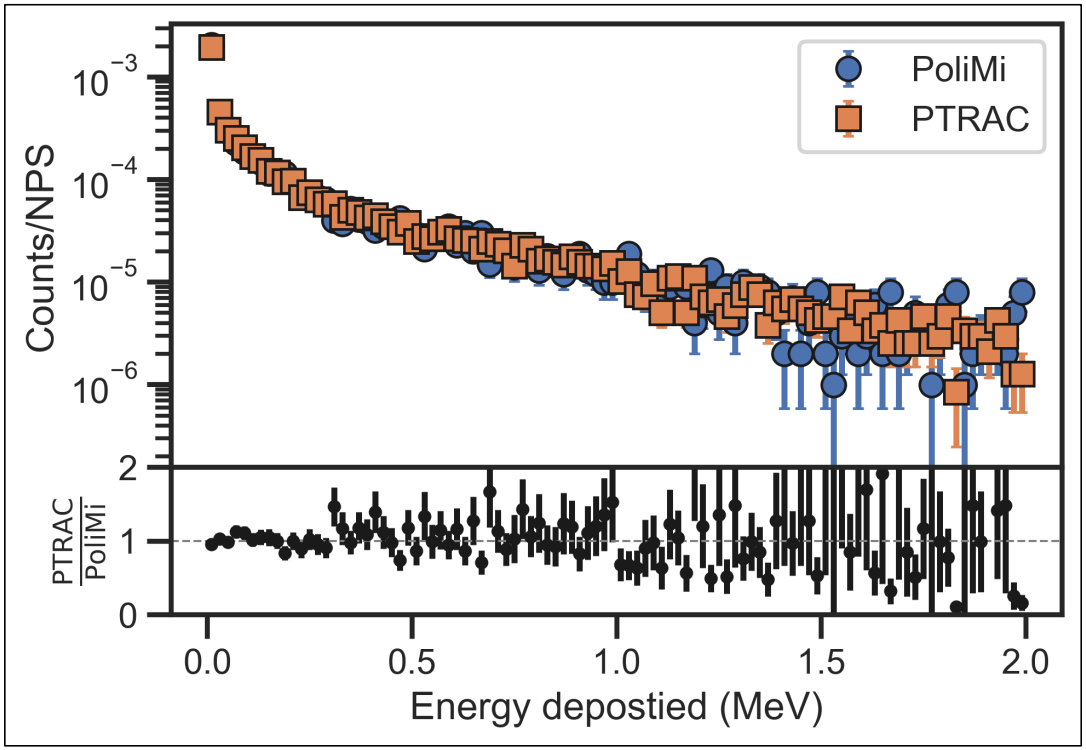


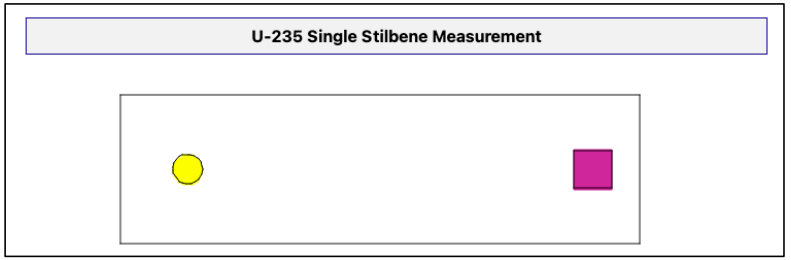
Example 4: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1
U-235 spherical shell, IPOL(2) = 1 (Terrell mult., X nubar)



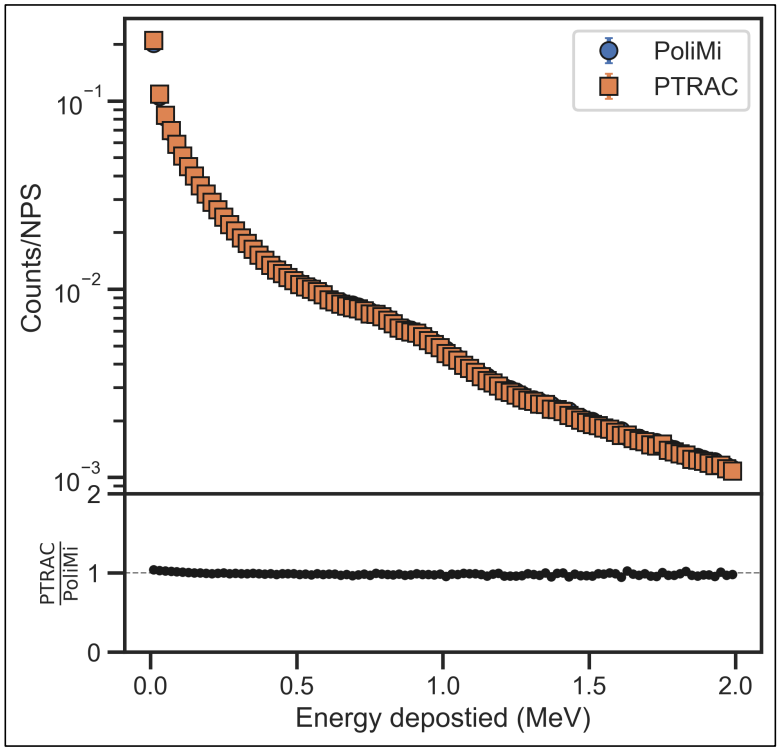


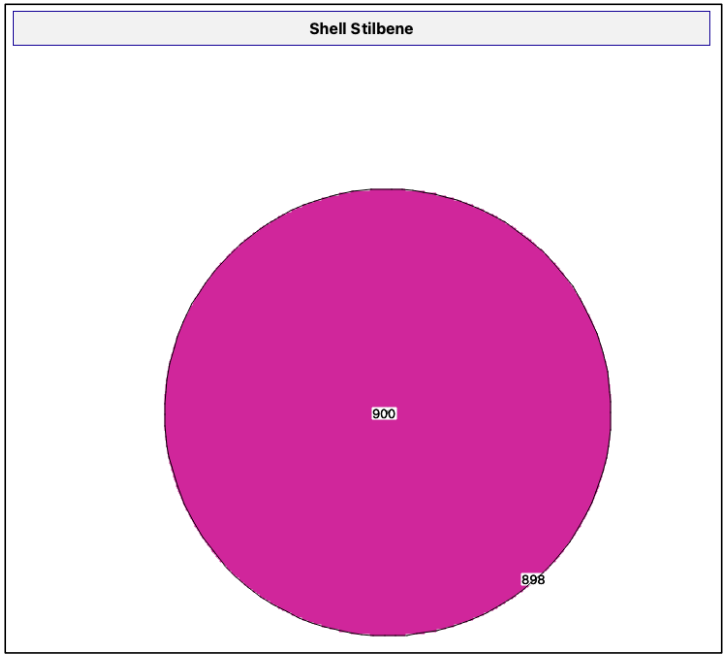
Example 5: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1
U-235 spherical shell, IPOL(2) = 2 (Zucker&Holden)



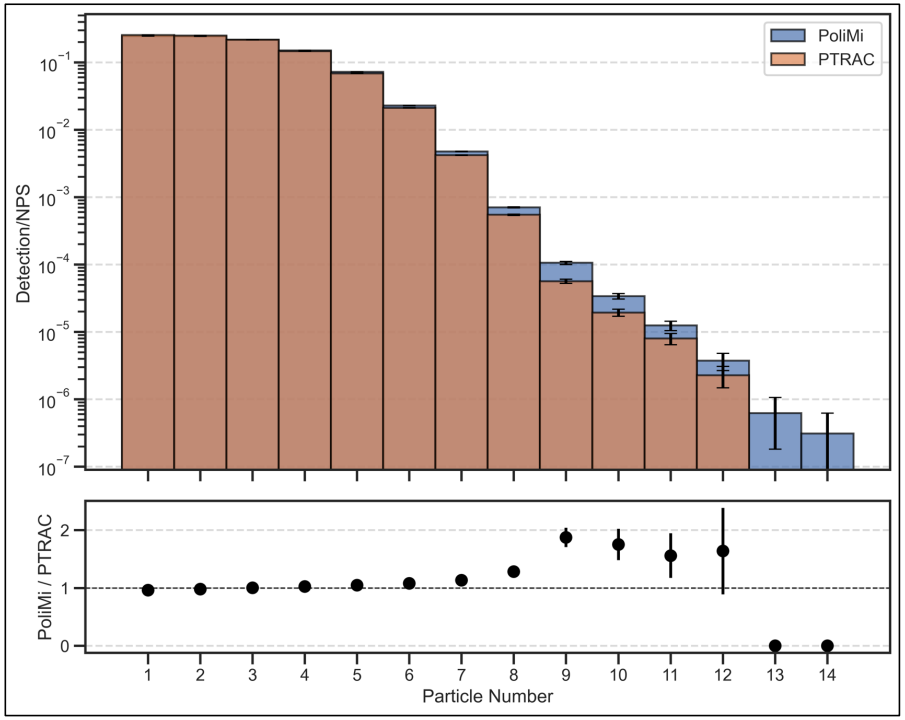


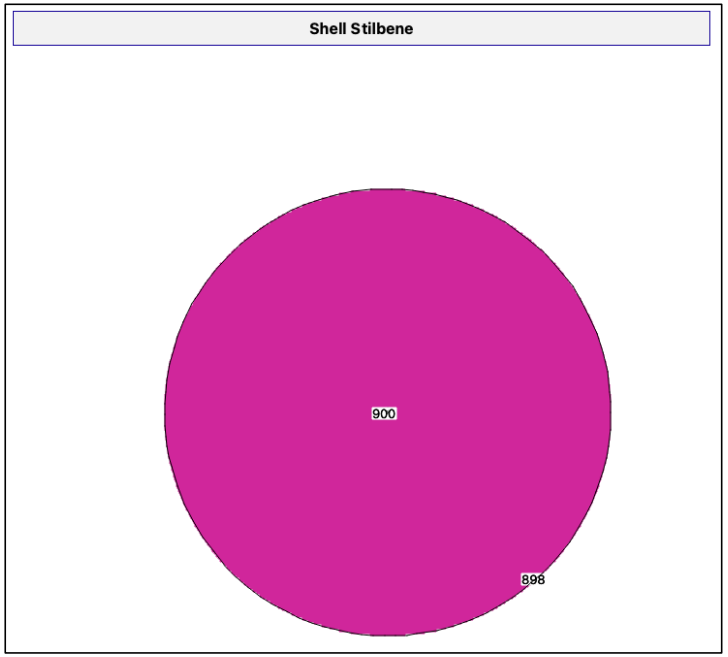
Example 6: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1, stilbene shell



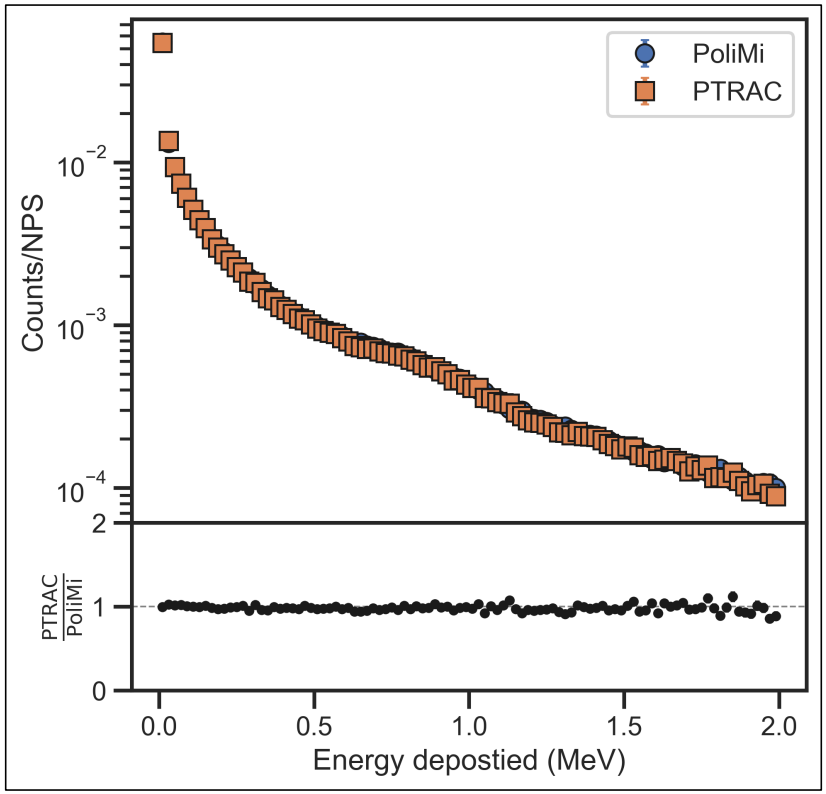


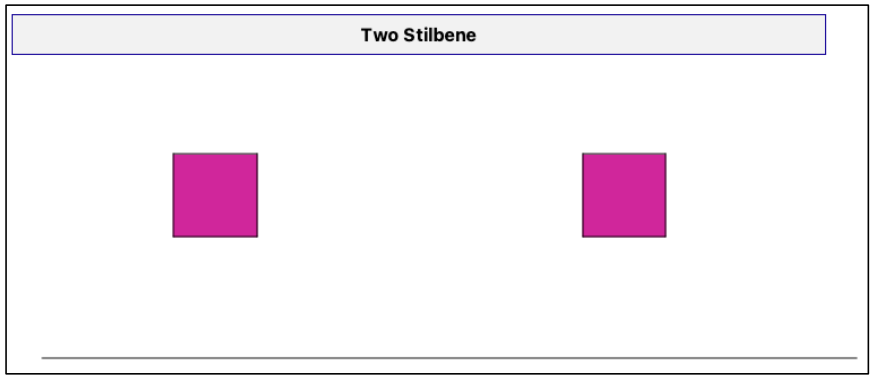
Example 6: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1, stilbene shell





Example 7: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1, two stilbenes, each 10 cm from source, all PTRAC





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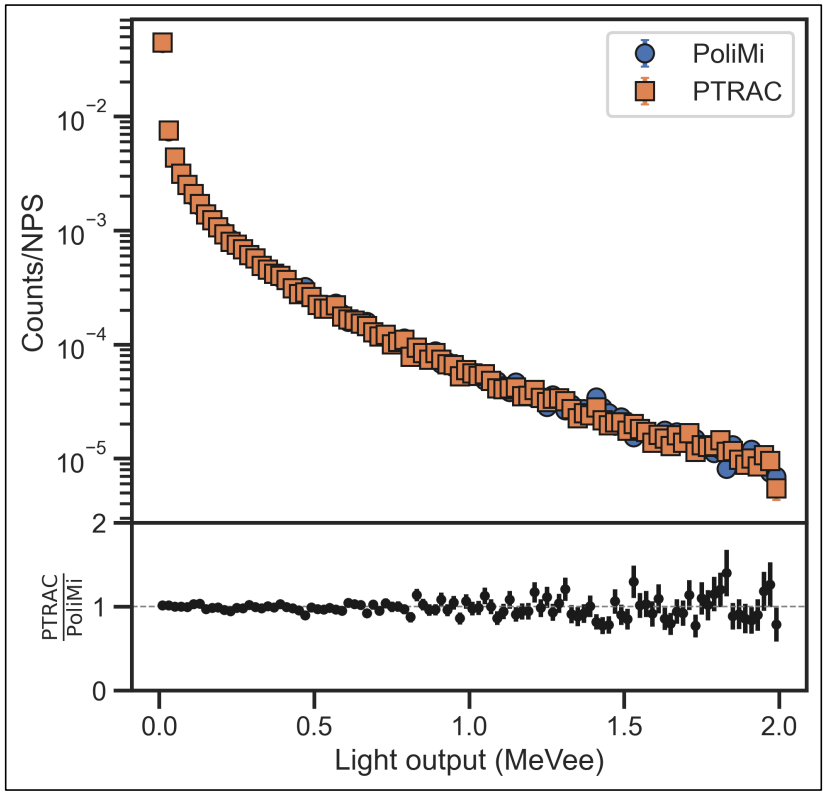

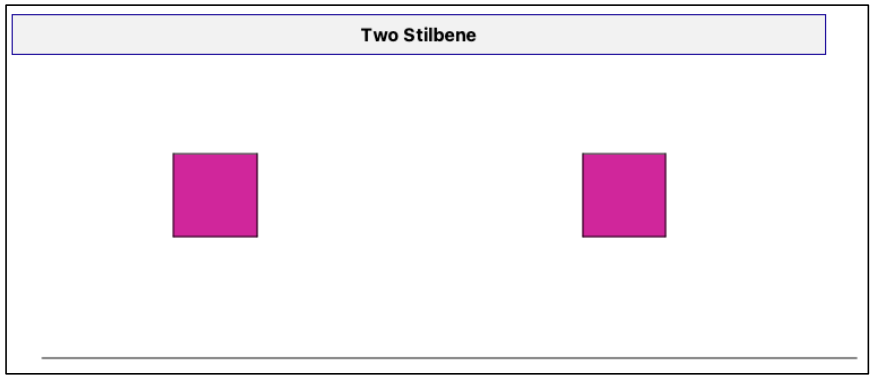

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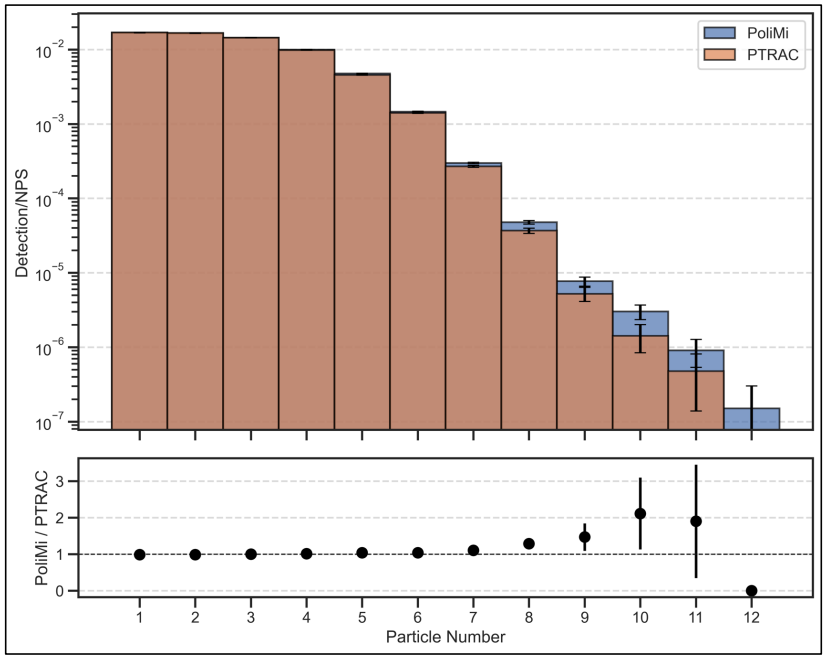

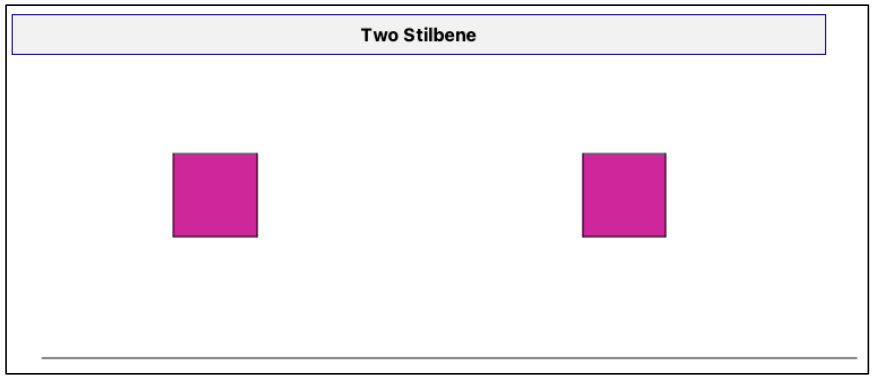

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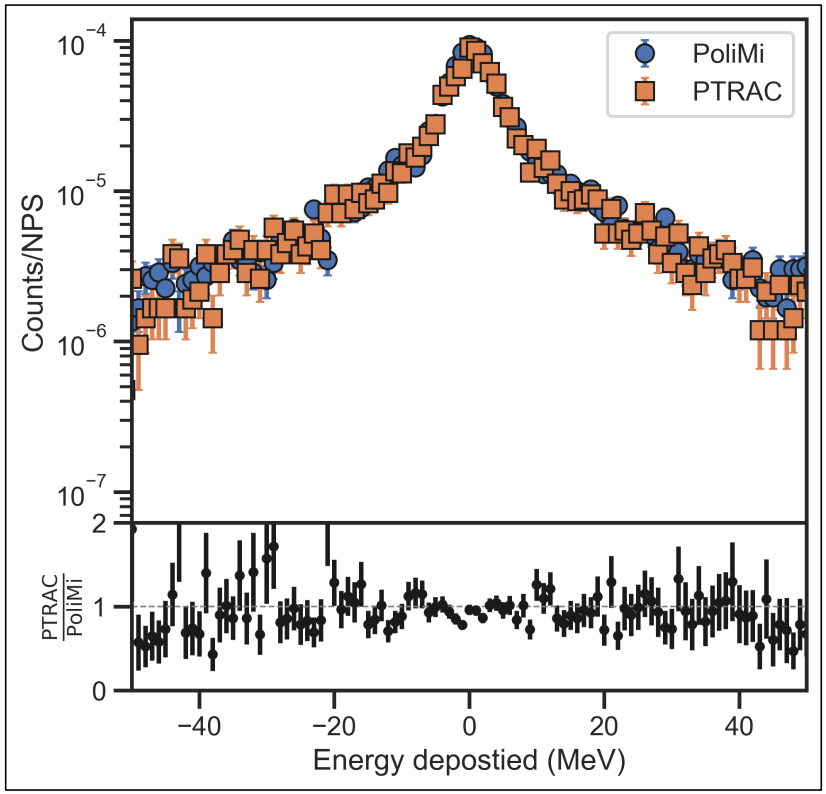
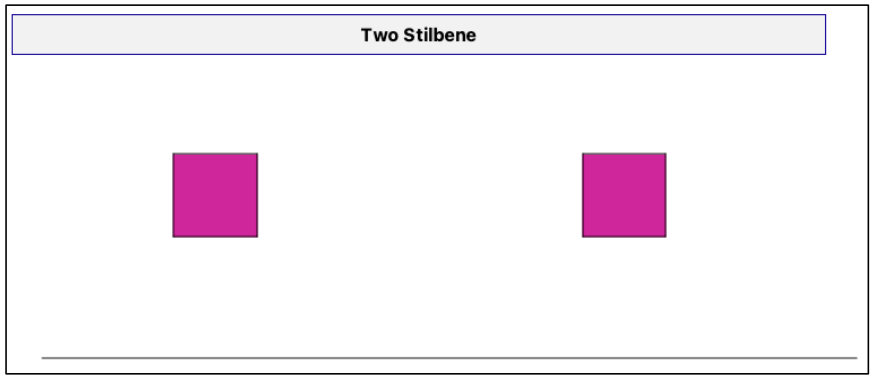
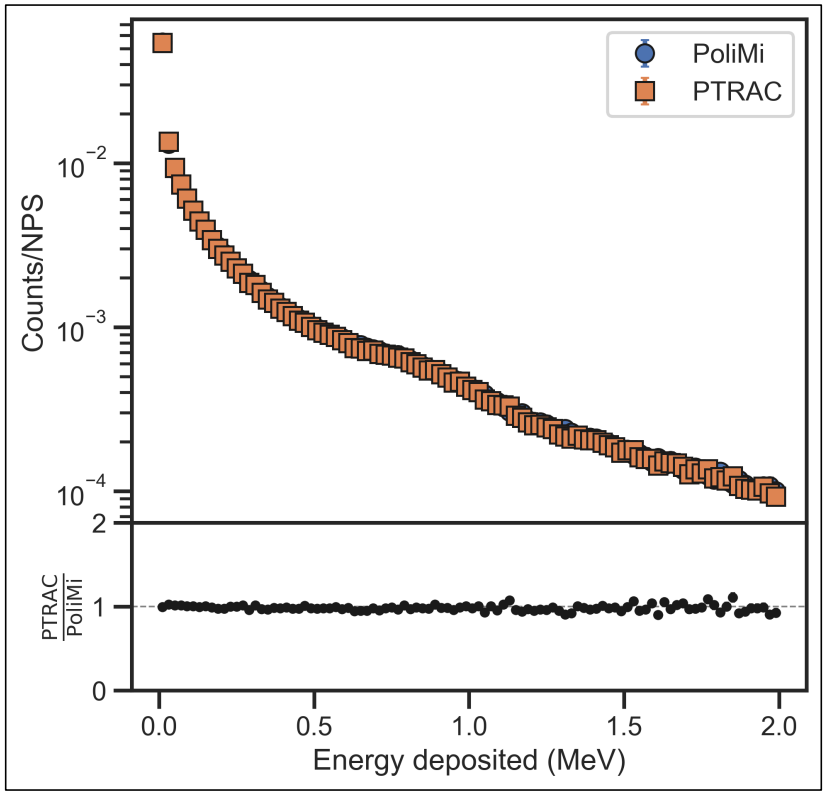
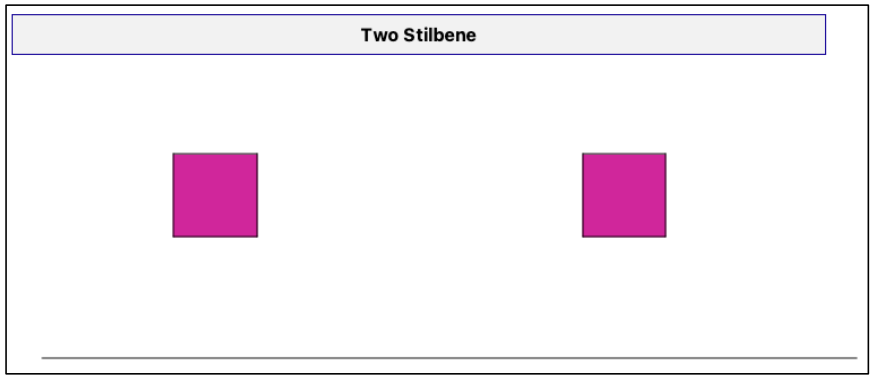




Example 7: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1, two stilbenes, each 10 cm from source, SUR/COL





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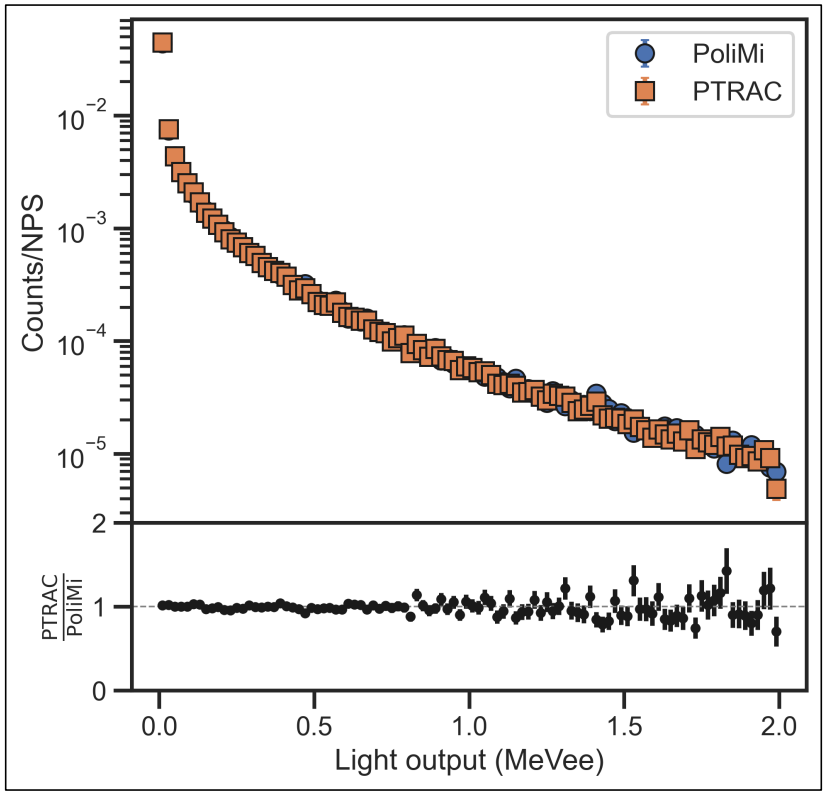
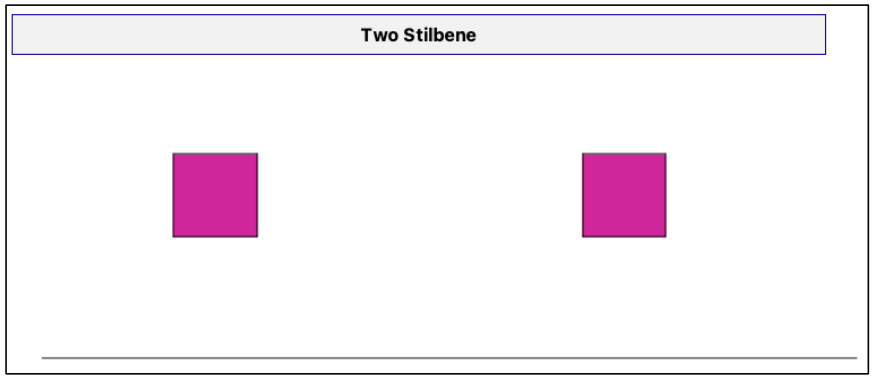
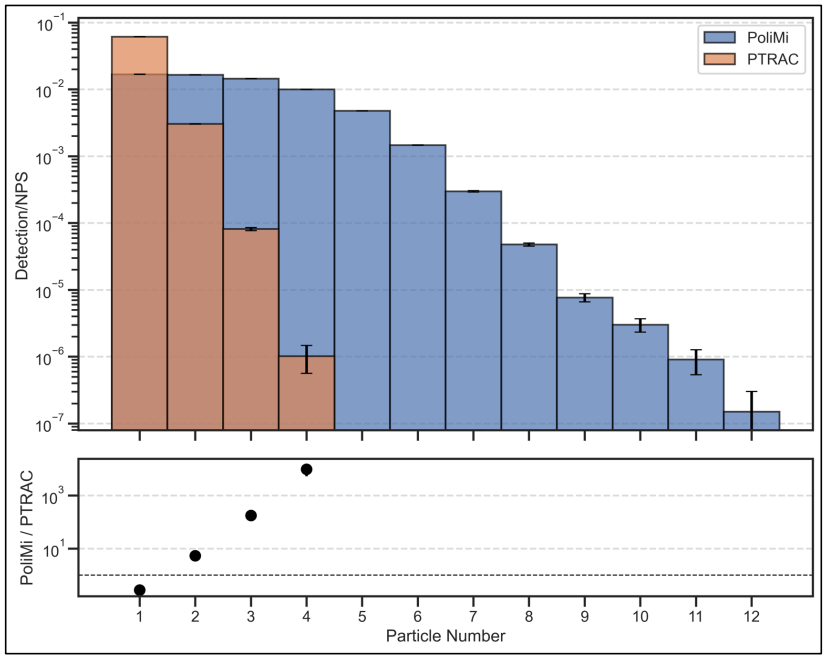
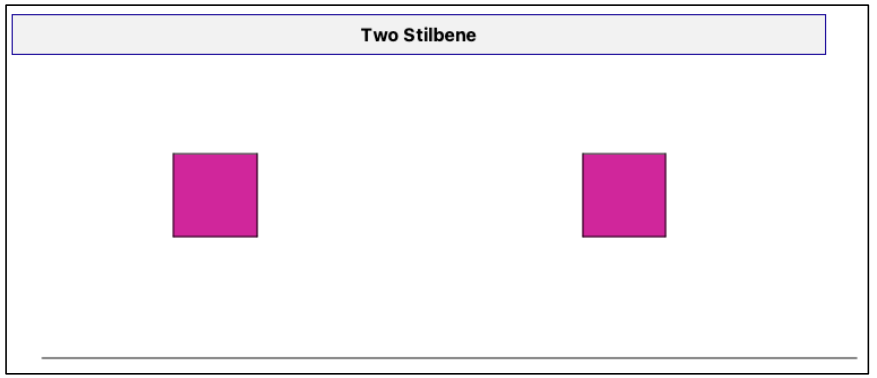


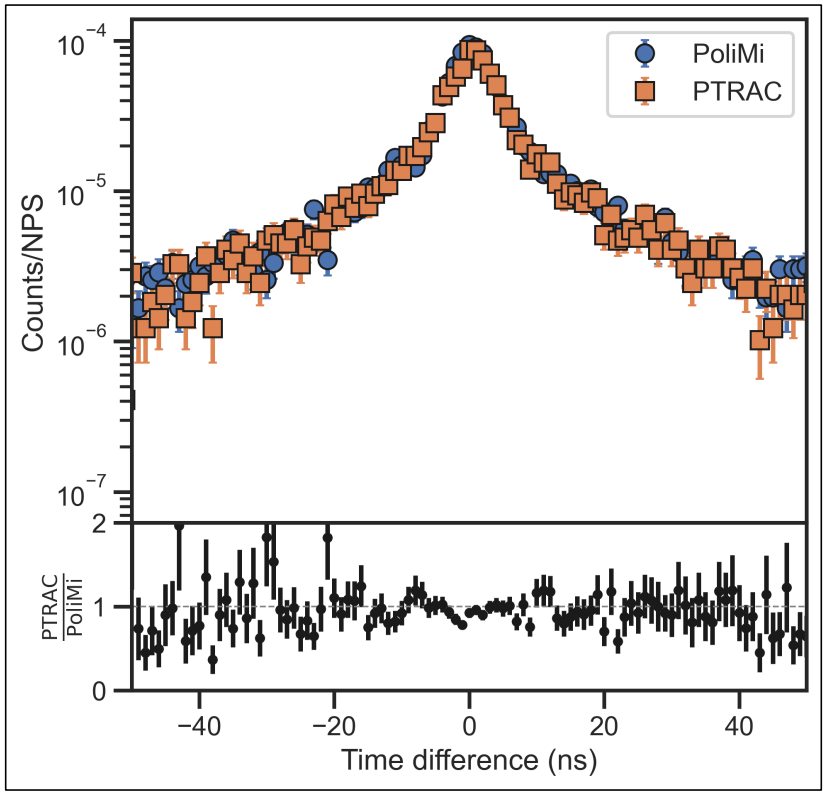


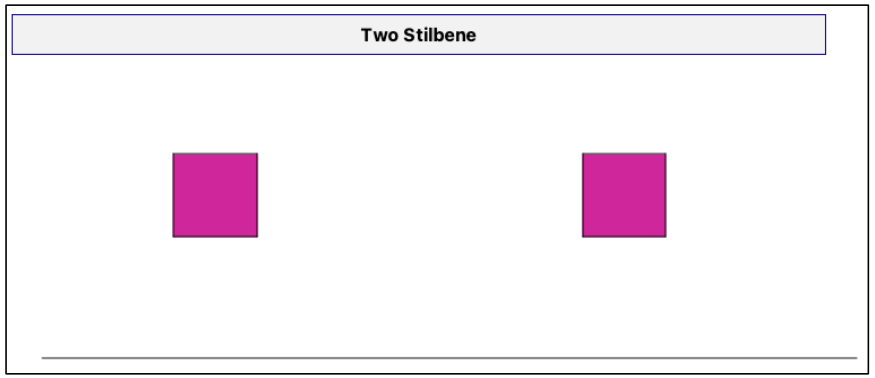
Example 7: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1, two stilbenes, each 10 cm from source, all SUR/COL



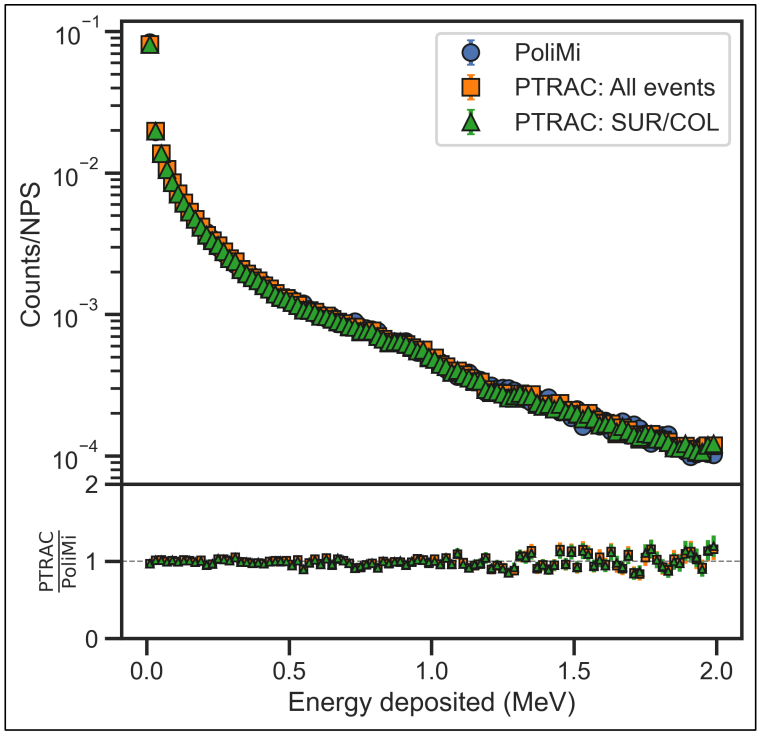


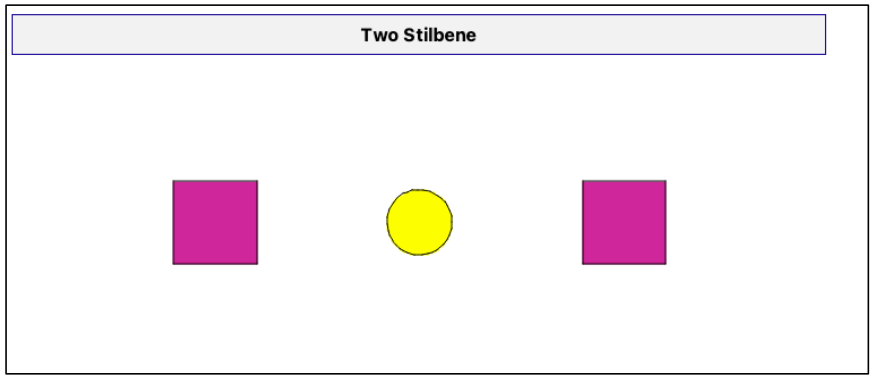
Example 7: Cf-252, MCNP6 par=sf, PoliMi IPOL(1)=1, two stilbenes, each 10 cm from source, all SUR/COL





Example 8: Cf-252, U-235 (2 cm diameter, 18.7 g/cc, keff ~ 0.2), MCNP6 par=sf, PoliMi IPOL(1)=1, IPOL(2) = 1 two stilbenes, each 10 cm from source





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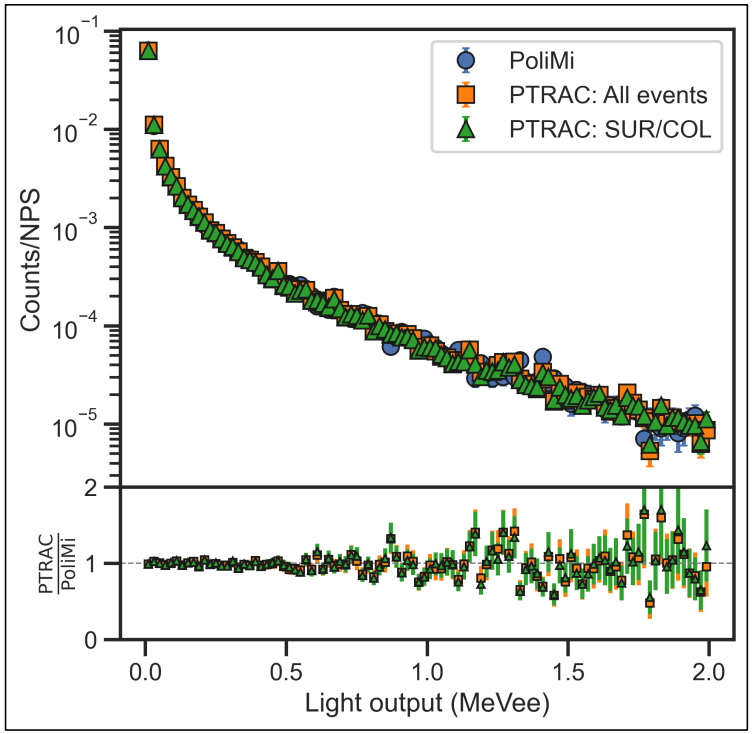

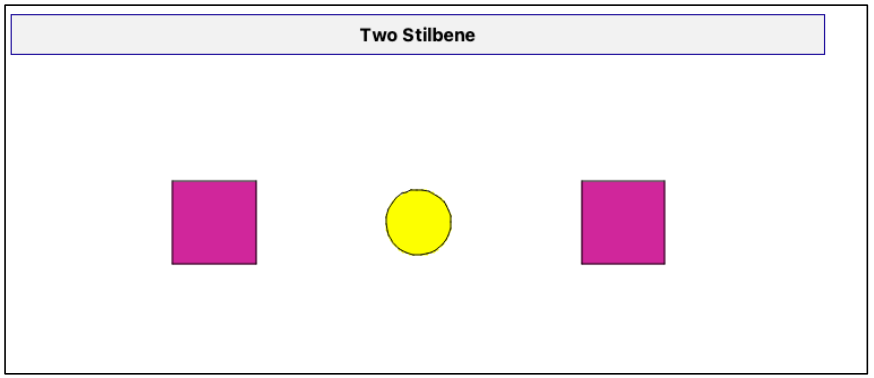

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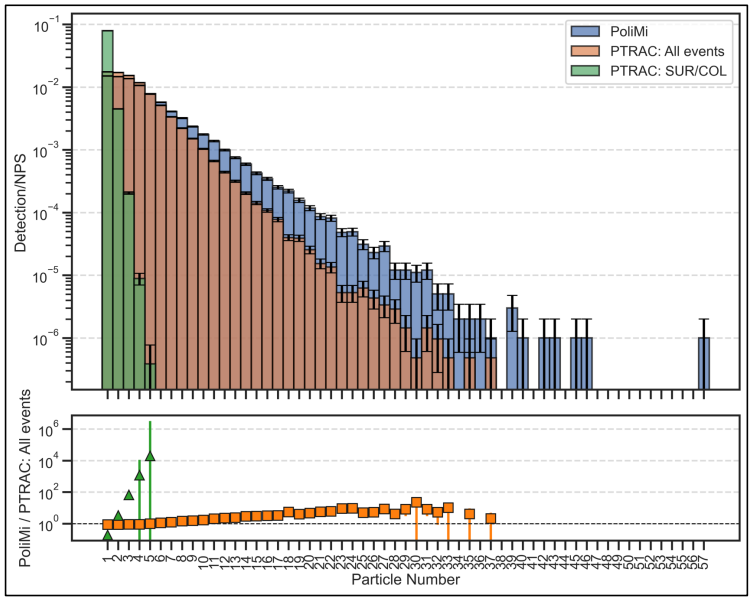

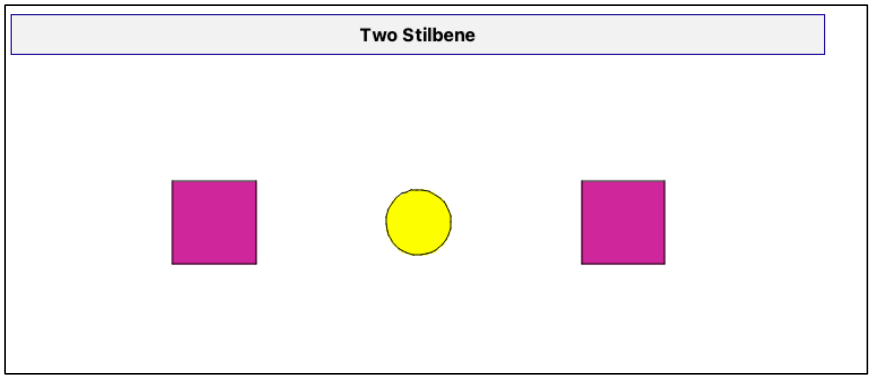

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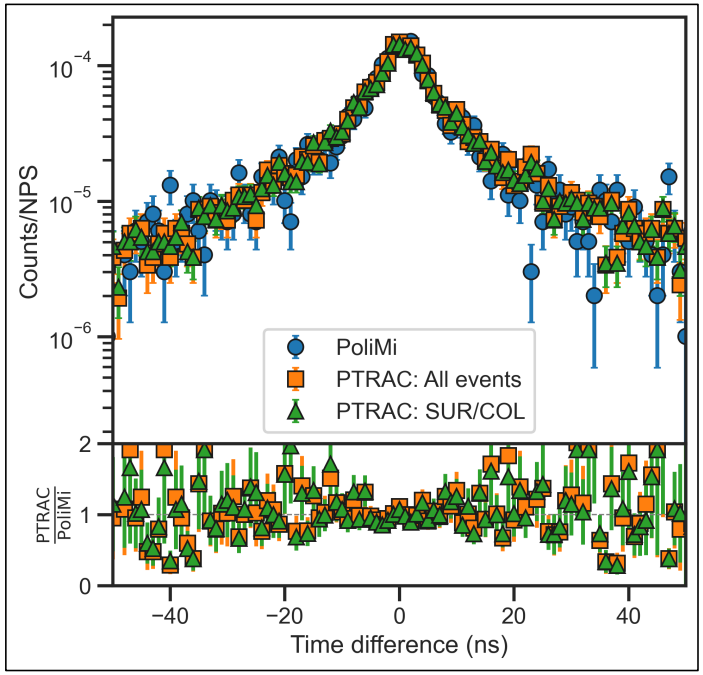
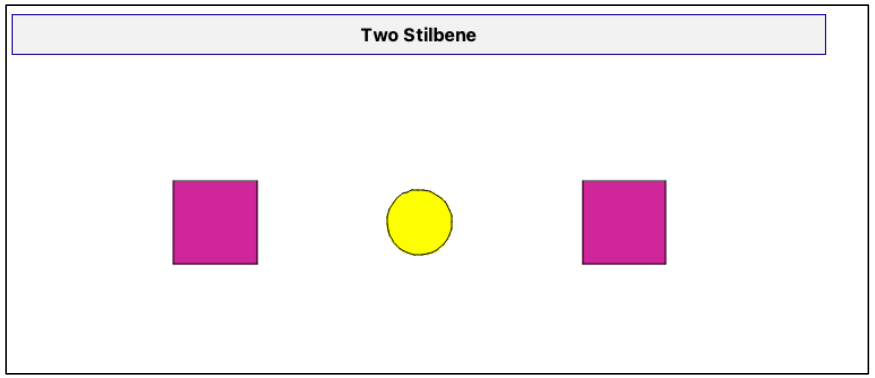
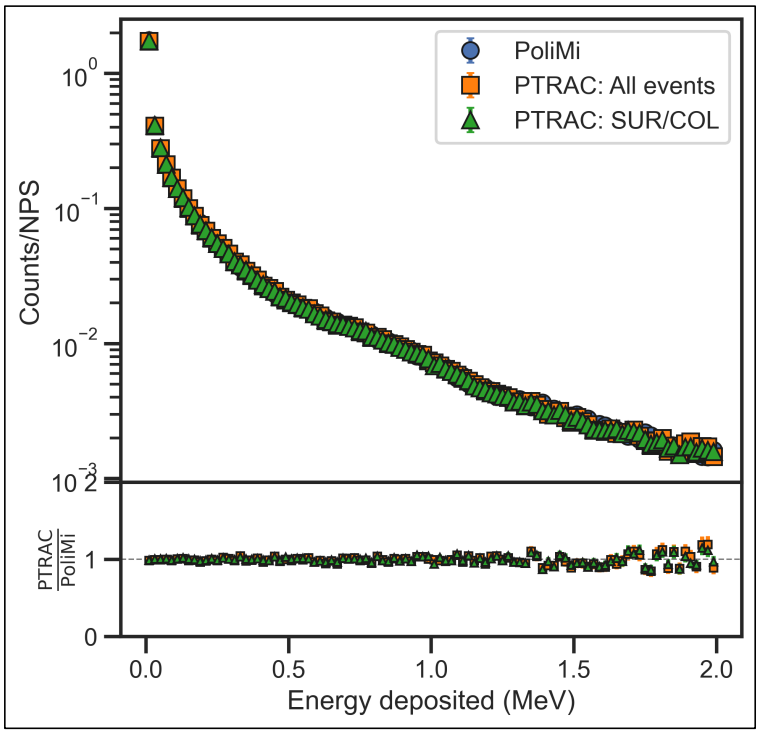
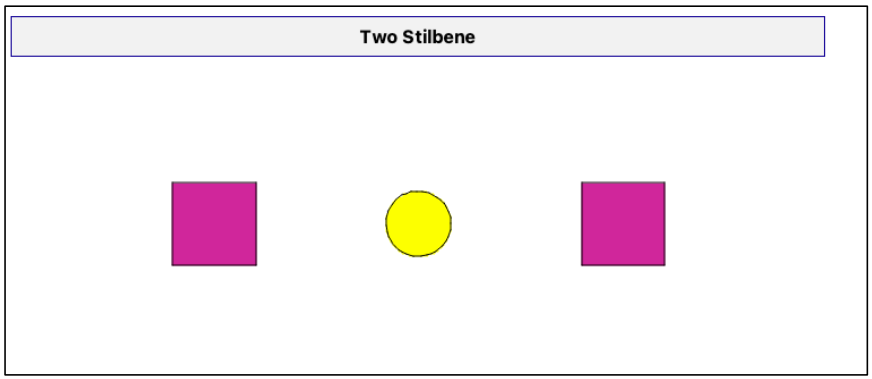




Example 9: Cf-252, U-235 (2 cm diameter, 18.7 g/cc, keff ~ 0.2), MCNP6 par=sf, PoliMi IPOL(1)=1, IPOL(2) = 1 two stilbenes, each 10 cm from source, density U-235 ~ 4 x natural (75 g/cc)





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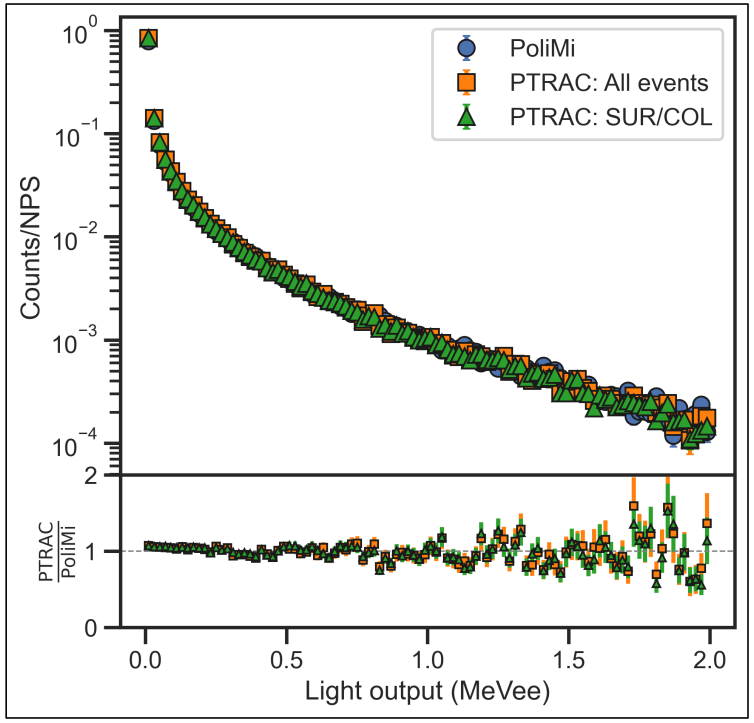

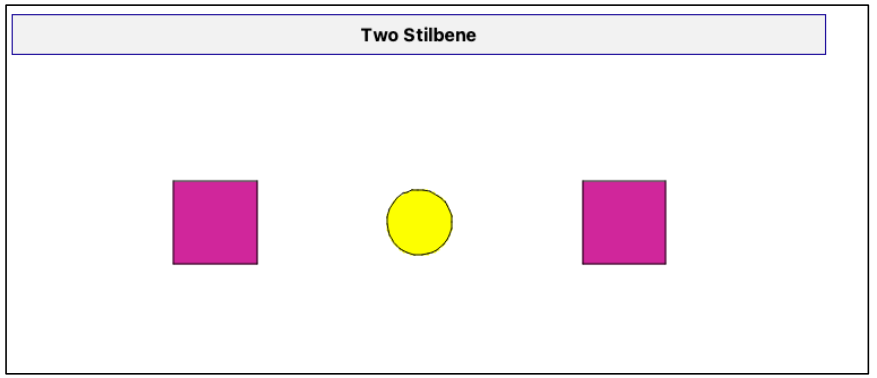

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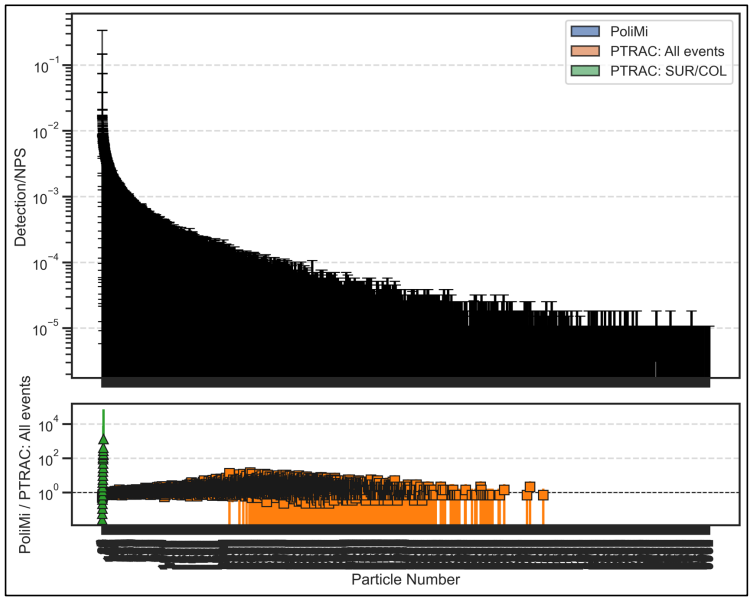

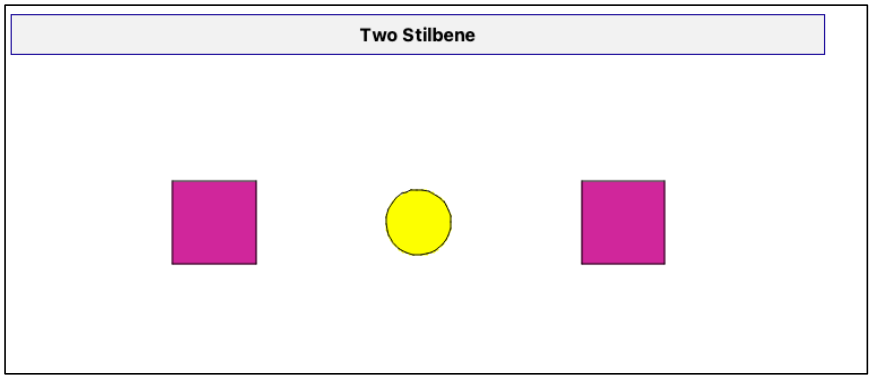

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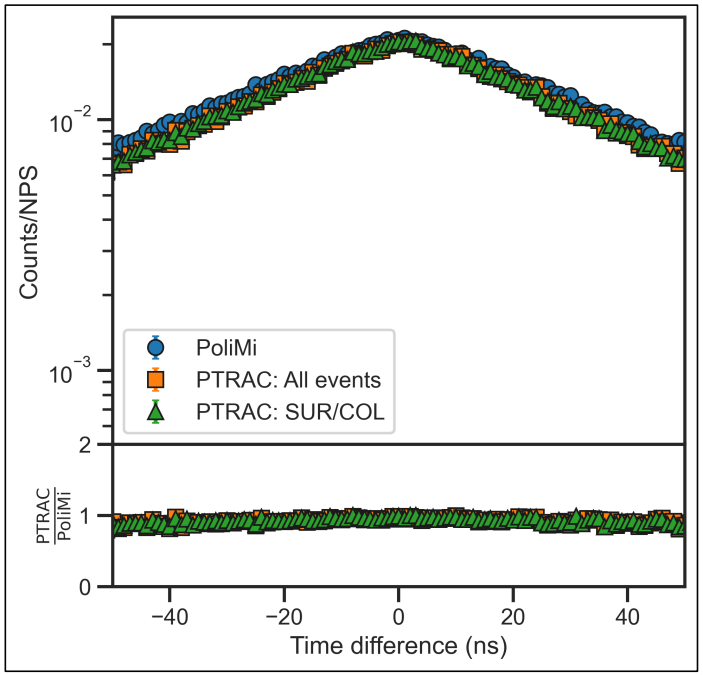
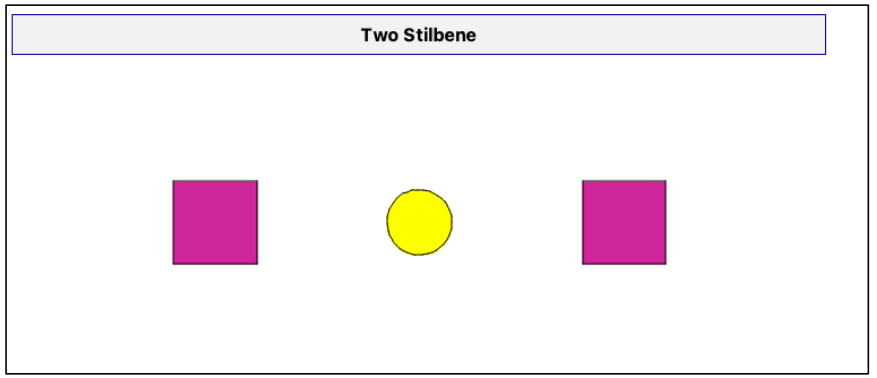
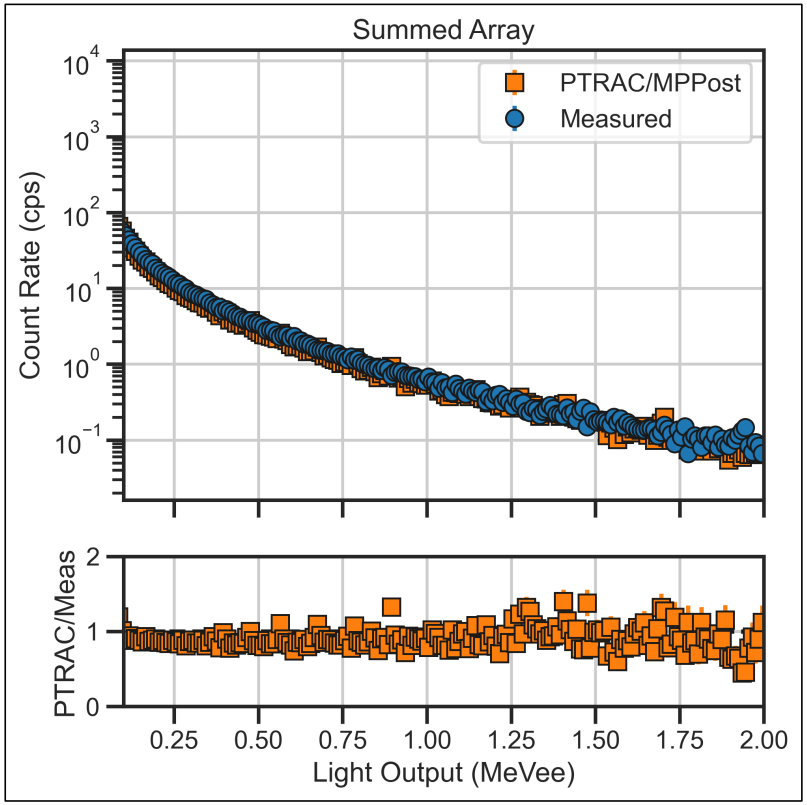
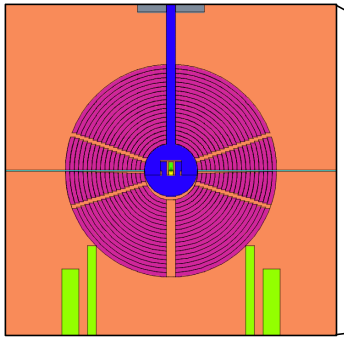




PTRAC to PoliMi MUSIC – Configuration 4 – k-eff ~ 0.88





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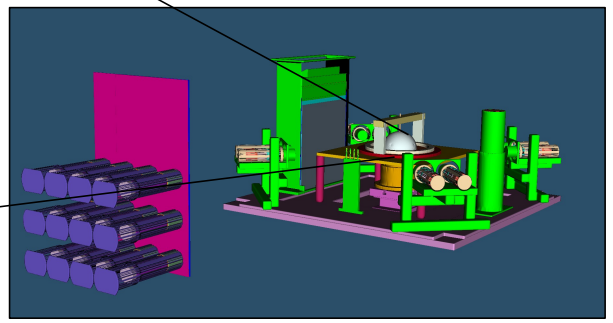
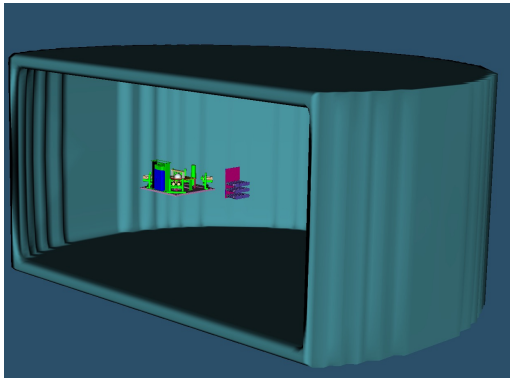
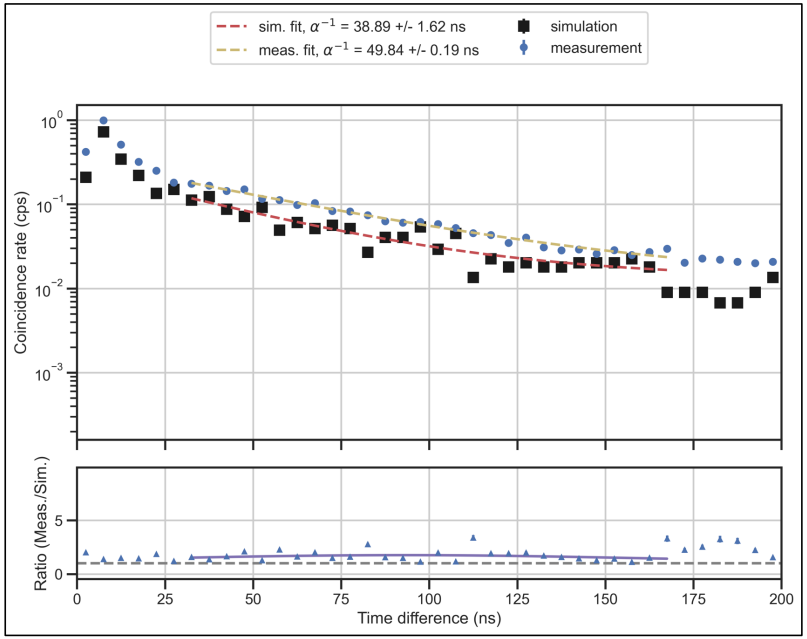
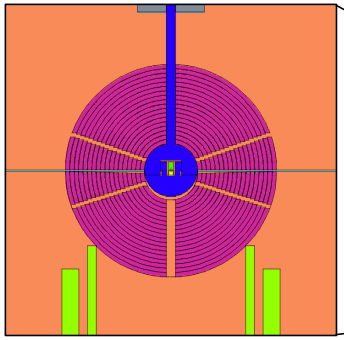




Concrete room included

PTRAC to PoliMi MUSIC – Configuration 4 – k-eff ~ 0.88





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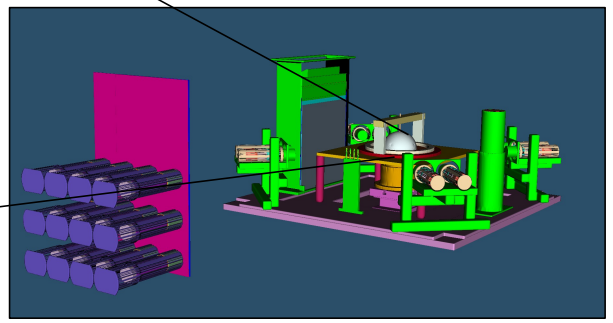

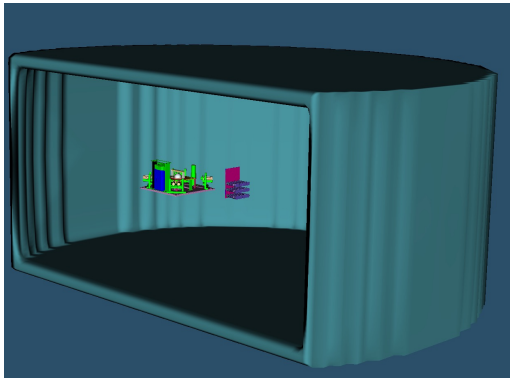

Concrete room included