NEW FISSION-BARRIER CALCULATION

P. Möller and A. J. Sierk (LANL)

T. Ichikawa (RIKEN)

A. Iwamoto (JAEA)

R. Bengtsson, Henrik Uhrenholt, and Sven Åberg (LUND)

Fission Calculation Details

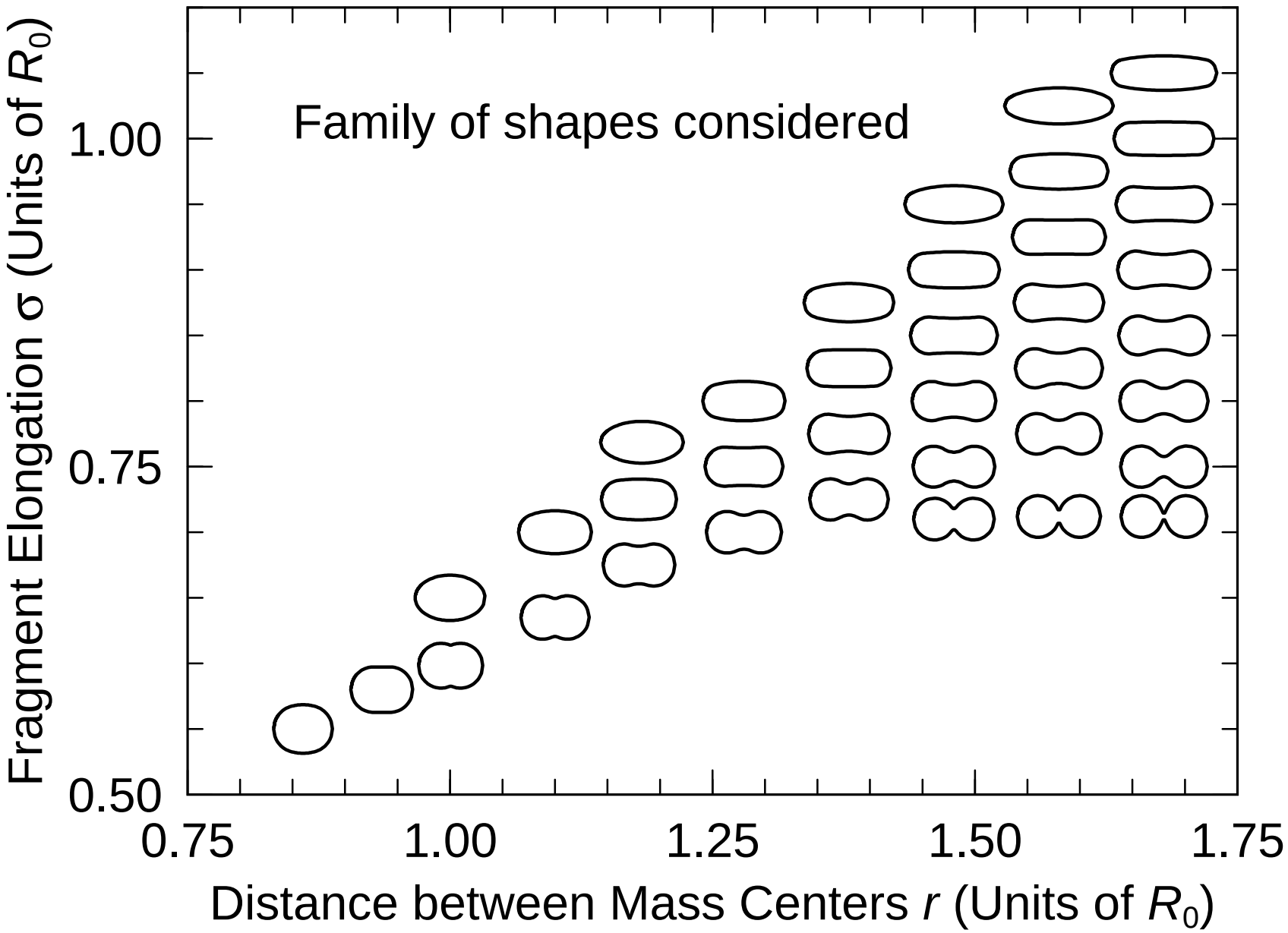
1. Fission Barriers of 5254 nuclei calculated for
   $170 < A \leq 330$
   Several different parameterizations are used
2. 5D parameterization, energy for 5 000 000 different shapes are calculated for each nucleus
3. For small deformations a 3D parameterization is used
   Elongation, neck and axial-asymmetry shape degrees of freedom.
4. An improved determination of the ground-state energy and shape is done in a 4D space
5. When multiple minima are present a special strategy is used to establish which minimum and saddle define the "barrier".
   (In practice this technique cannot be implemented in HFB)

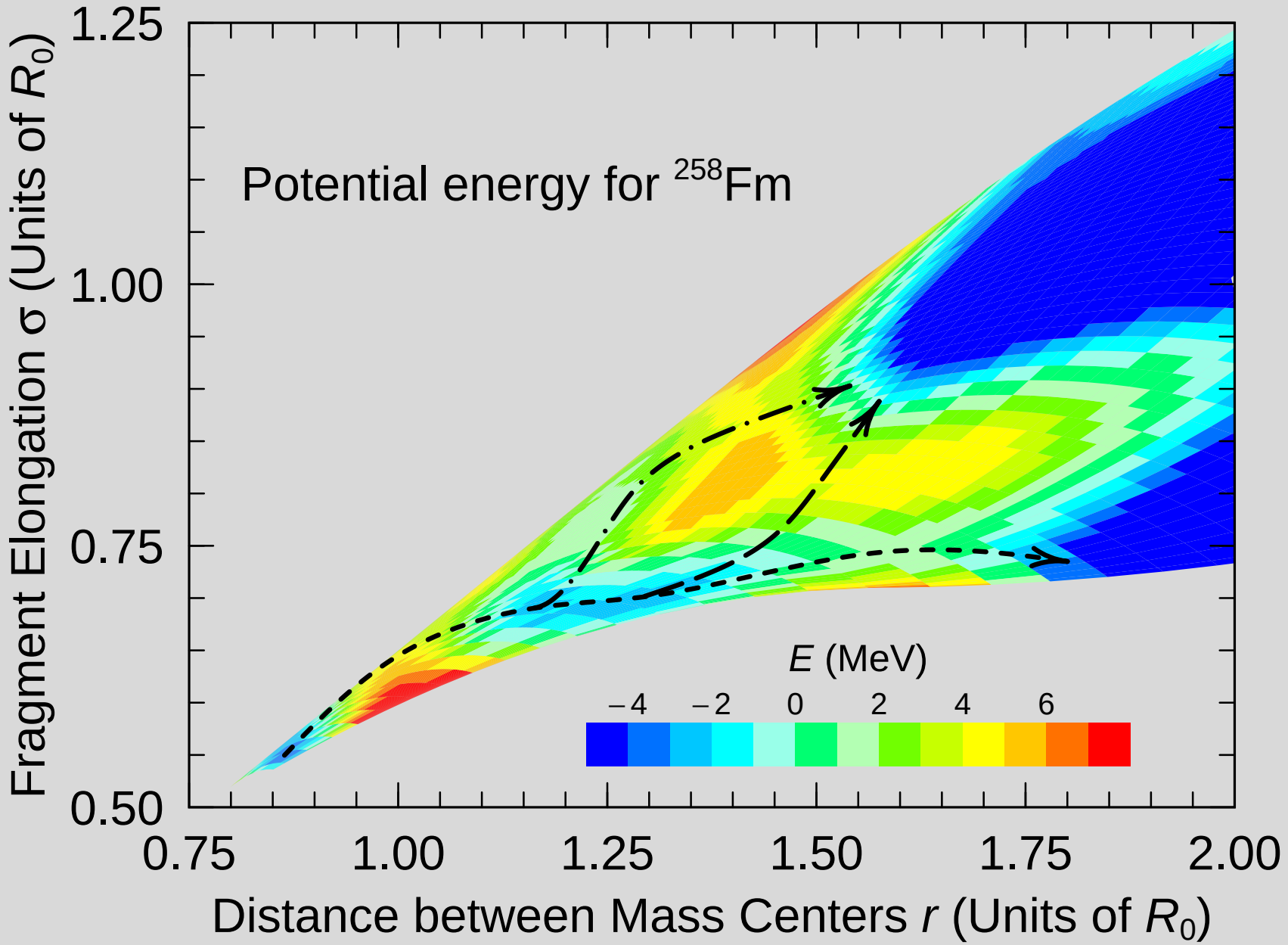
6. Just the potential energies correspond to more than 250 Gb of information.

7. Saddles, minima, valleys are determined in a completely automated fashion. Compact result files are generated for each nucleus

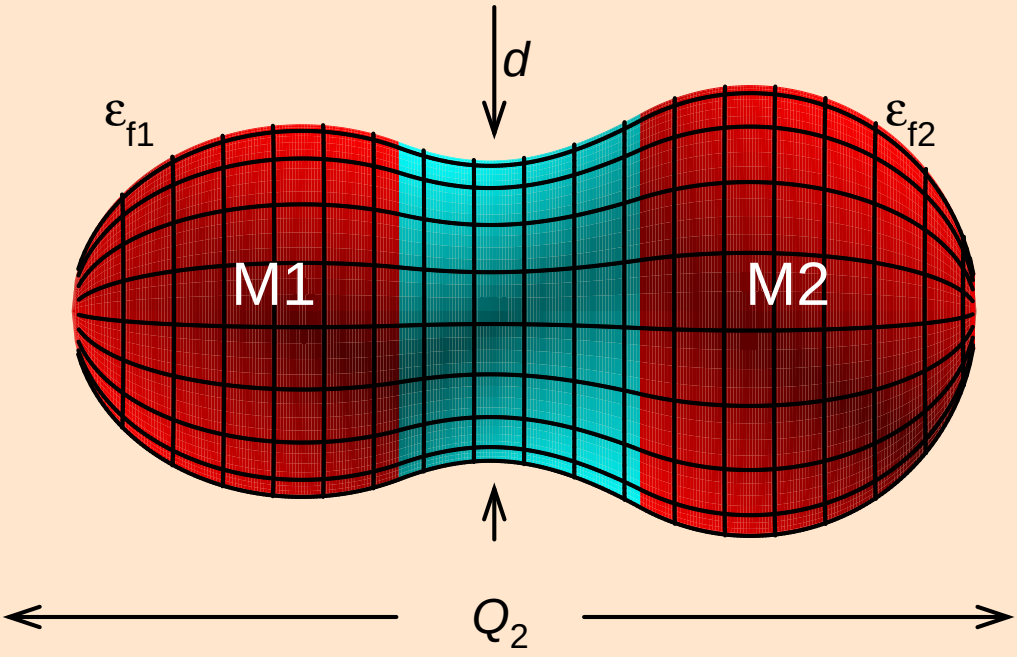
8. Data sets, such as tables of barrier heights (Z, N, A, E_{f}) are generated, also by automated scripts.

Results will be made available at URL
http://t16web.lanl.gov/Moller/abstracts.html
(Capital M is essential)
Results more complete than can be published will be available here in due course.


Family of shapes considered
Fragment Elongation σ (Units of R_0)
1.00
0.75
0.50
0.75
1.00
1.25
1.50
1.75
Distance between Mass Centers r (Units of R_0)


Potential energy for ^{258}Fm
Fragment Elongation σ (Units of R_0)
1.25
1.00
0.75
0.50
0.75
1.00
1.25
1.50
1.75
2.00
Distance between Mass Centers r (Units of R_0)
E (MeV)
−4
−2
0
2
4
6

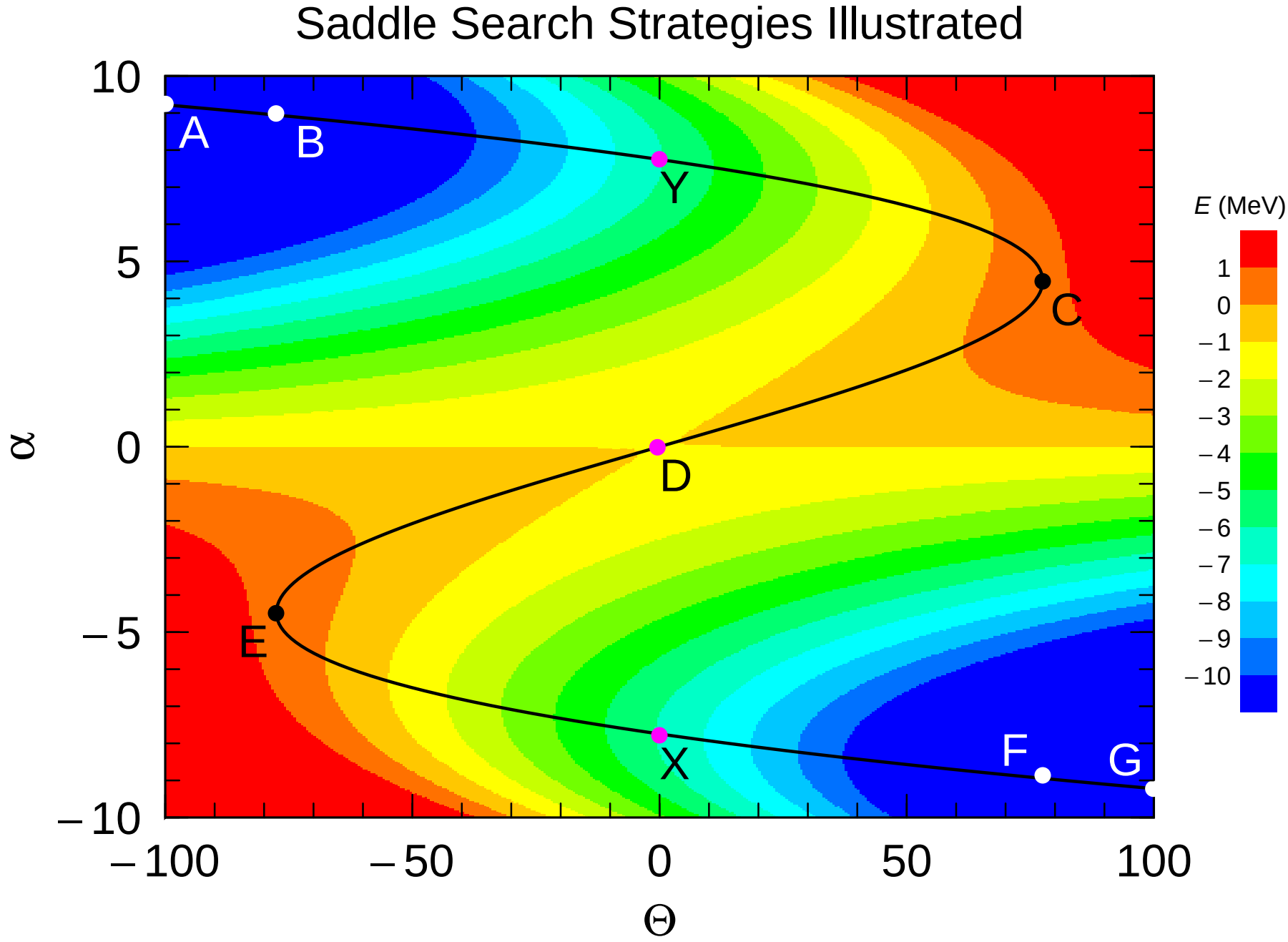
Five Essential Fission Shape Coordinates

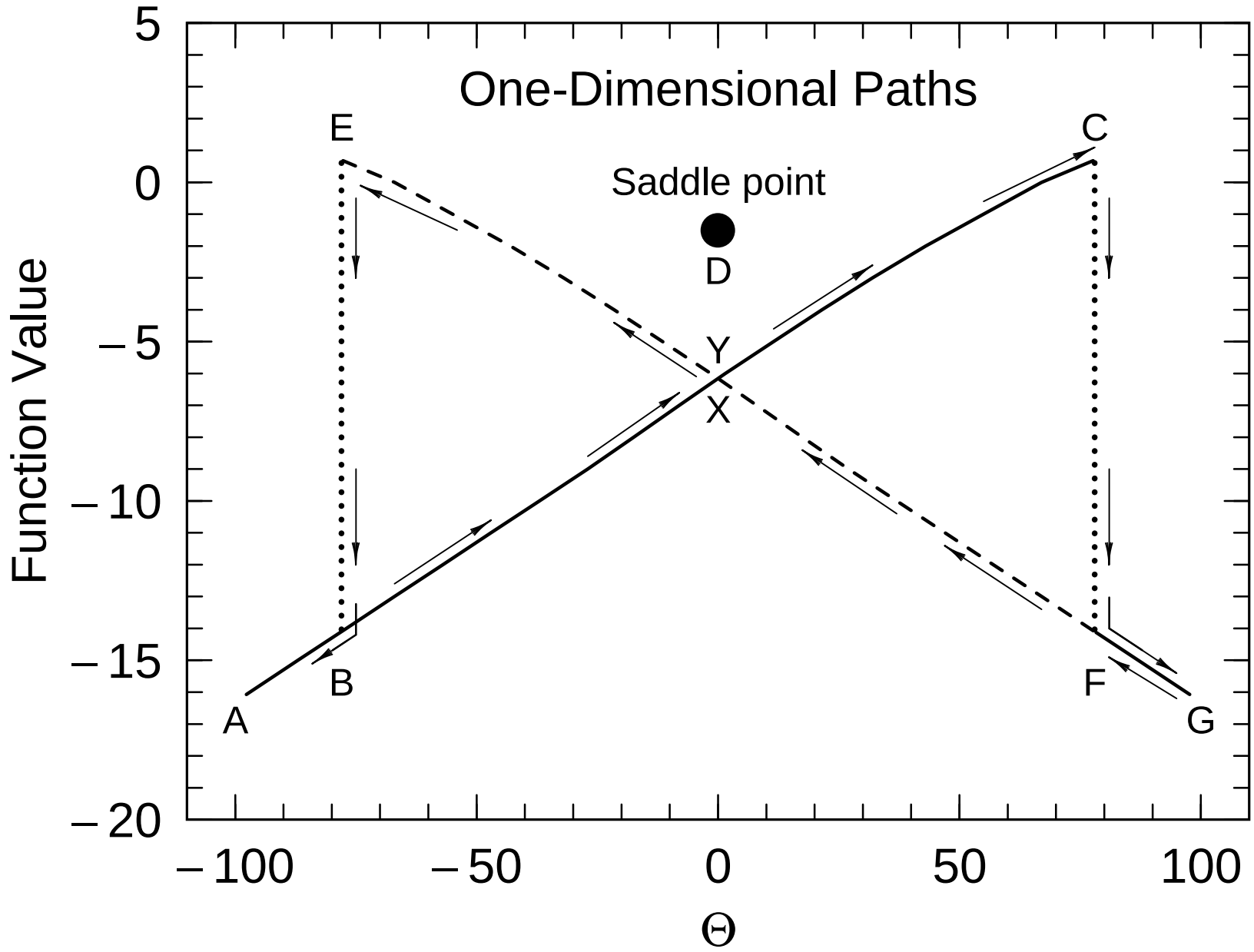


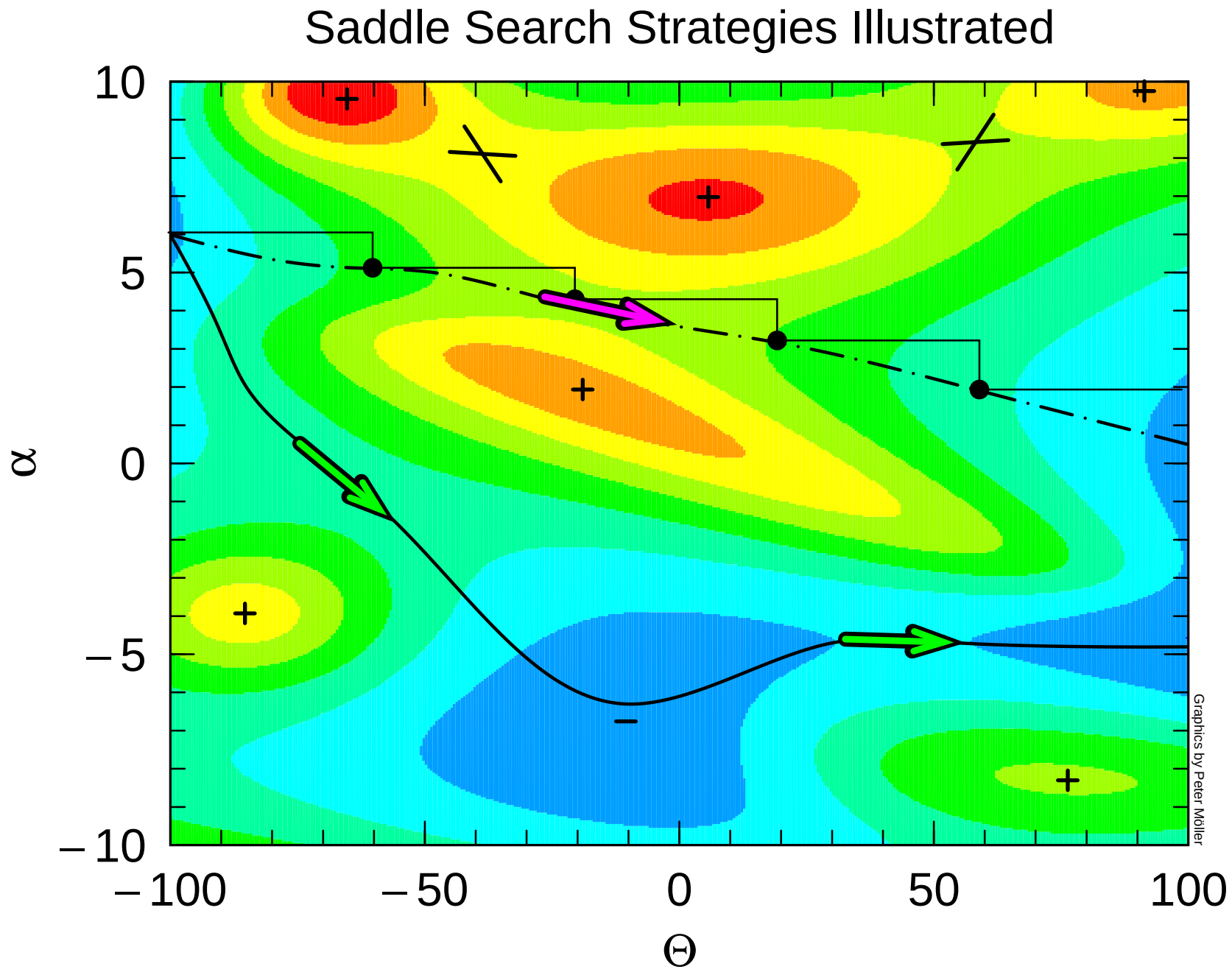
45	Q_2 ~	Elongation (fission direction)
⊗		
35	α_g ~	(M1-M2)/(M1+M2) Mass asymmetry
⊗		
15	ε_{f1} ~	Left fragment deformation
⊗		
15	ε_{f2} ~	Right fragment deformation
⊗		
15	d ~	Neck

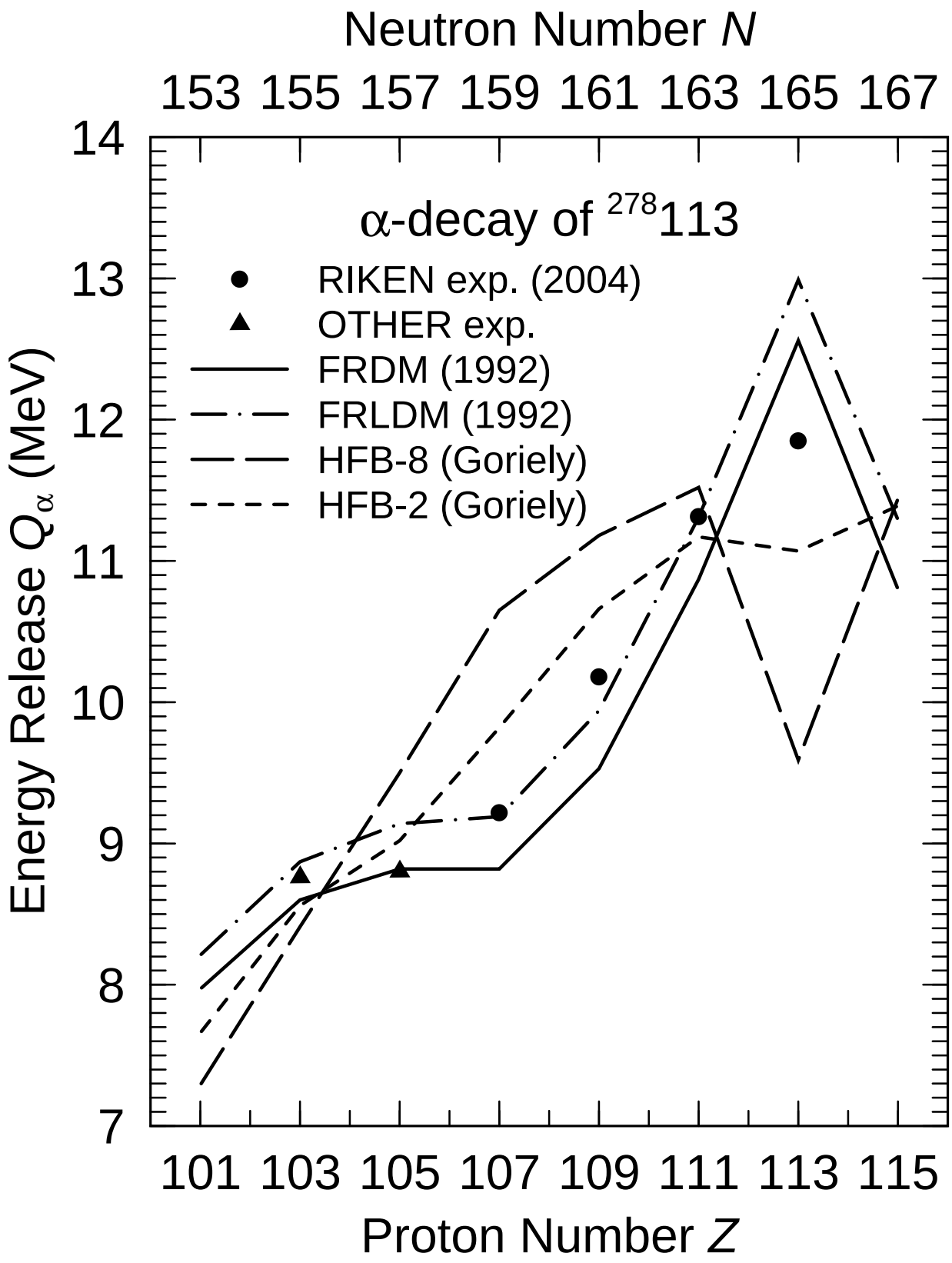
⇒ 5 315 625 grid points – 306 300 unphysical points

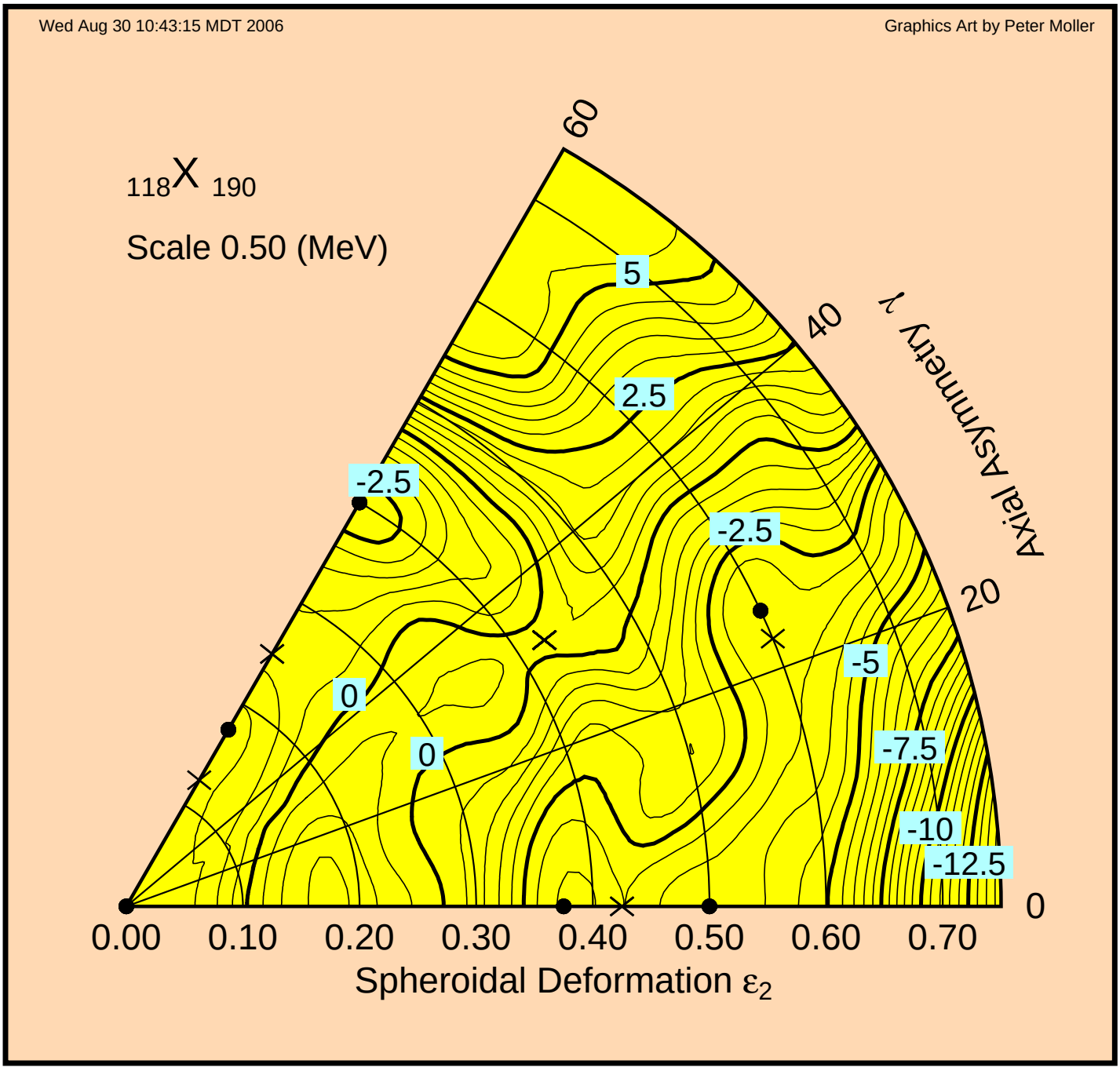
⇒ 5 009 325 physical grid points

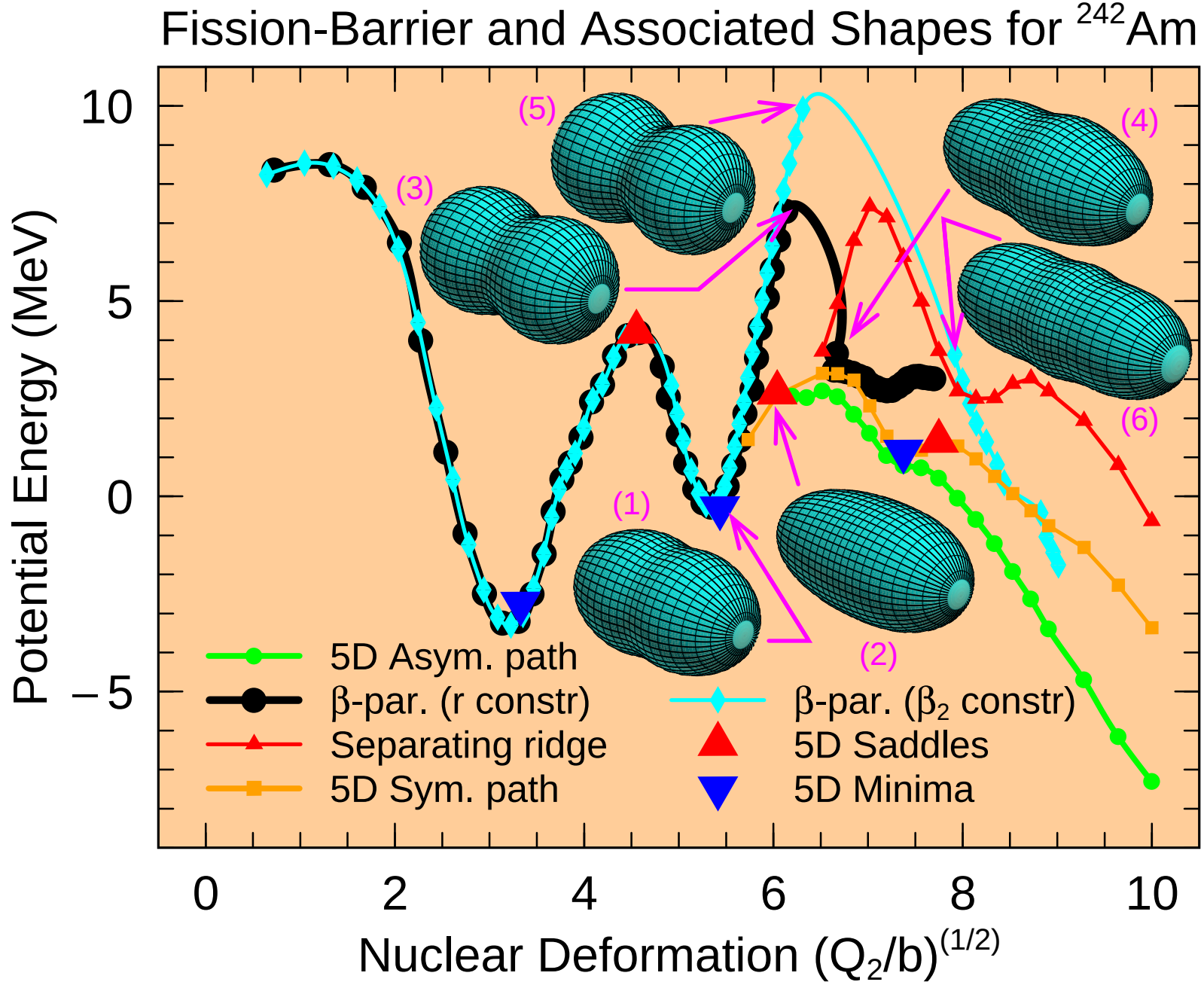

Saddle Search Strategies Illustrated
10
5
0
−5
−10
α
−100
−50
0
50
100
Θ
A
B
Y
C
D
E
X
F
G
E (MeV)
1
0
−1
−2
−3
−4
−5
−6
−7
−8
−9
−10

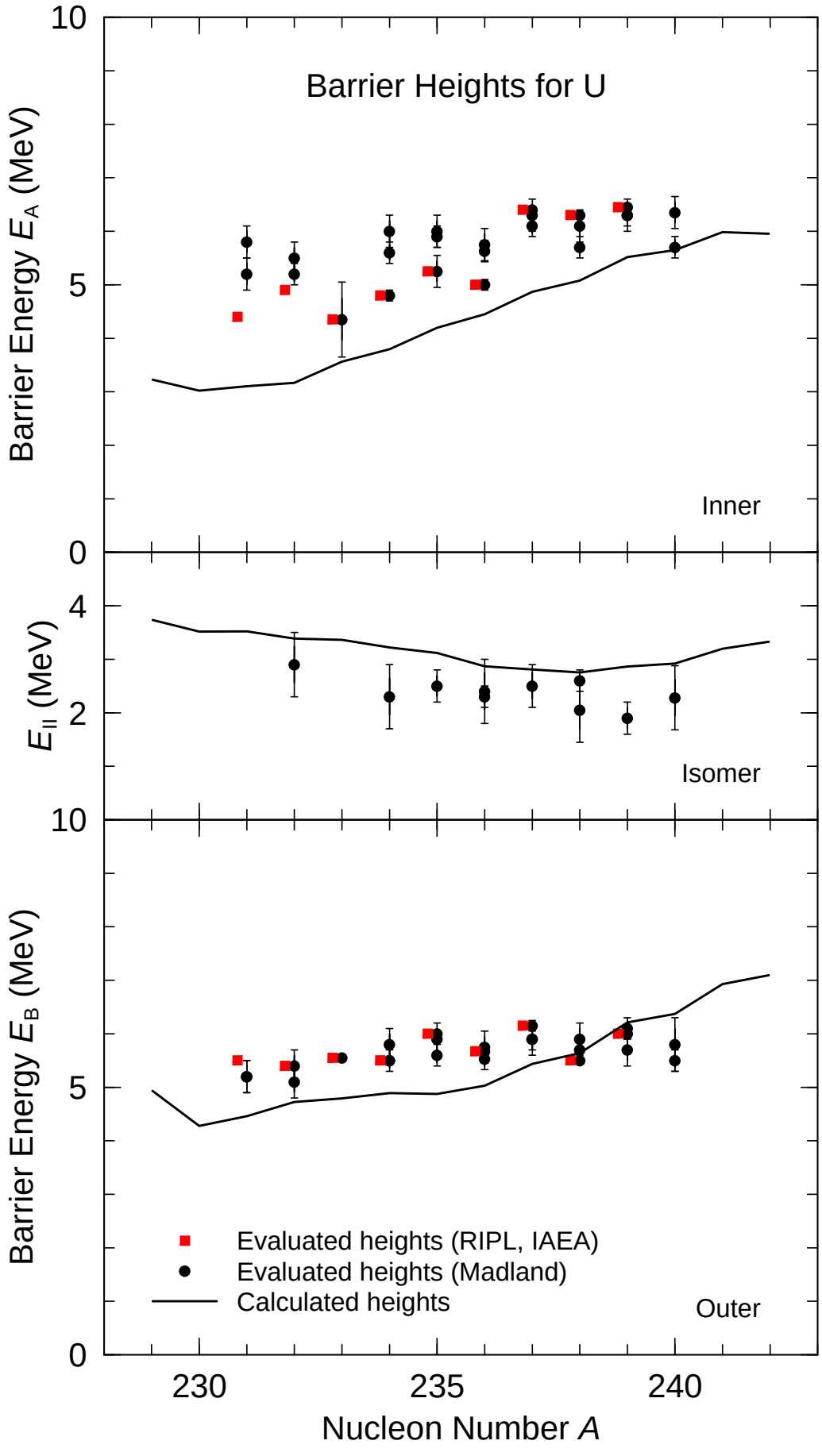

One-Dimensional Paths
Saddle point
E
C
D
Y
X
A
B
F
G
5
0
– 5
– 10
– 15
– 20
– 100
– 50
0
50
100
Function Value
Θ

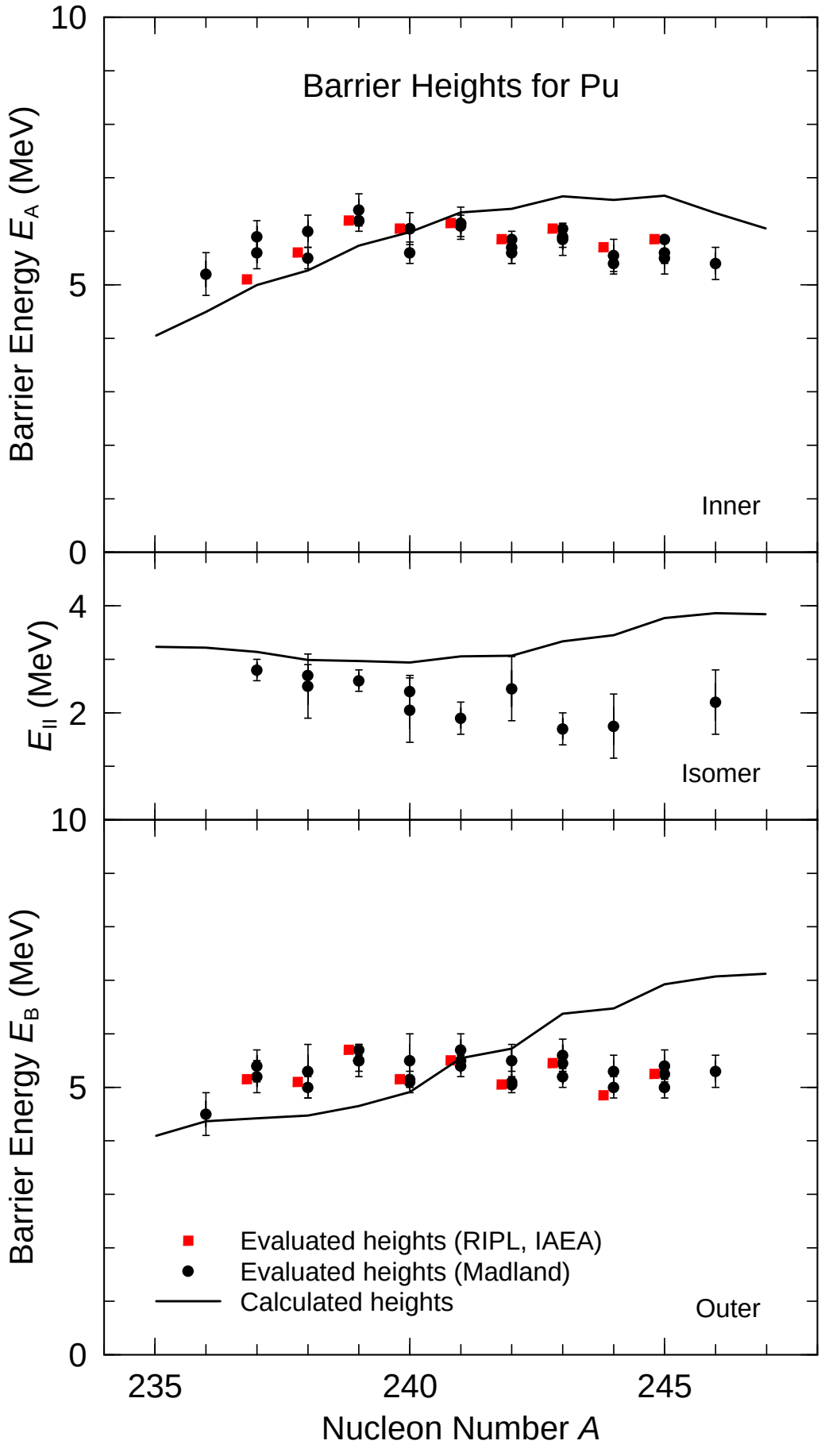

Saddle Search Strategies Illustrated
10
5
0
−5
−10
α
−100
−50
0
50
100
Θ
Graphics by Peter Möller

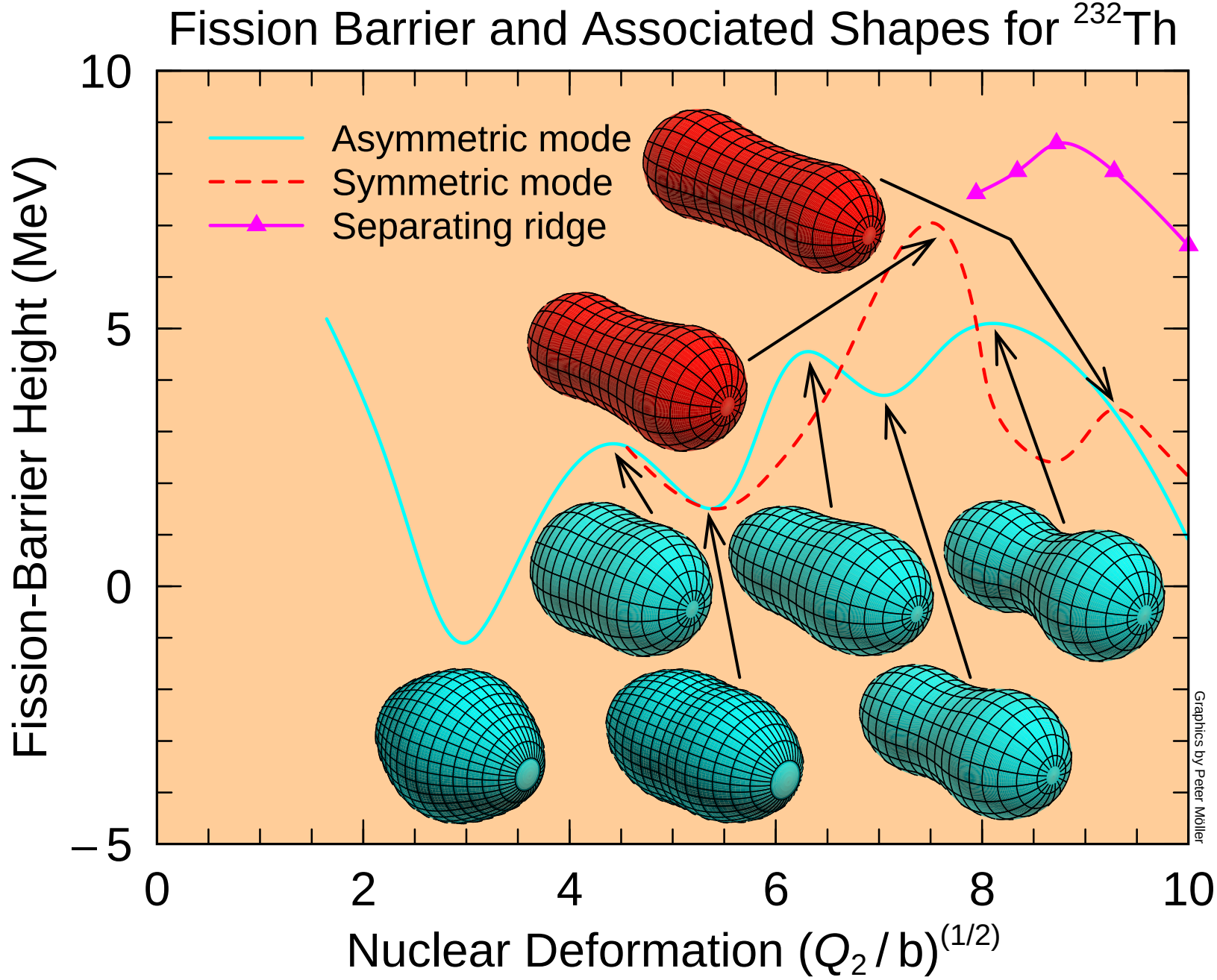

Neutron Number N
153 155 157 159 161 163 165 167
α-decay of 278113
RIKEN exp. (2004)
OTHER exp.
FRDM (1992)
FRLDM (1992)
HFB-8 (Goriely)
HFB-2 (Goriely)
Energy Release Qα (MeV)
14
13
12
11
10
9
8
7
101 103 105 107 109 111 113 115
Proton Number Z


Wed Aug 30 10:43:15 MDT 2006
Graphics Art by Peter Moller
118X 190
Scale 0.50 (MeV)
60
40
20
0
Axial Asymmetry γ
5
2.5
-2.5
-2.5
0
0
-5
-7.5
-10
-12.5
0.00
0.10
0.20
0.30
0.40
0.50
0.60
0.70
Spheroidal Deformation ε2


Fission-Barrier and Associated Shapes for ^{242}Am
Potential Energy (MeV)
10
5
0
–5
0
2
4
6
8
10
Nuclear Deformation $(Q_2/b)^{(1/2)}$
(1)
(2)
(3)
(4)
(5)
(6)
5D Asym. path
β-par. (r constr)
Separating ridge
5D Sym. path
β-par. (β_2 constr)
5D Saddles
5D Minima


Barrier Heights for U
Barrier Energy E_A (MeV)
Inner
E_{II} (MeV)
Isomer
Barrier Energy E_B (MeV)
Outer
Evaluated heights (RIPL, IAEA)
Evaluated heights (Madland)
Calculated heights
Nucleon Number A
0
2
4
5
10
230
235
240


Barrier Heights for Pu
Barrier Energy E_A (MeV)
Inner
E_{II} (MeV)
Isomer
Barrier Energy E_B (MeV)
Outer
Evaluated heights (RIPL, IAEA)
Evaluated heights (Madland)
Calculated heights
Nucleon Number A
0
2
4
5
10
235
240
245


Fission Barrier and Associated Shapes for ^{232}Th
Asymmetric mode
Symmetric mode
Separating ridge
Fission-Barrier Height (MeV)
10
5
0
−5
0
2
4
6
8
10
Nuclear Deformation $(Q_2 / b)^{(1/2)}$
Graphics by Peter Möller

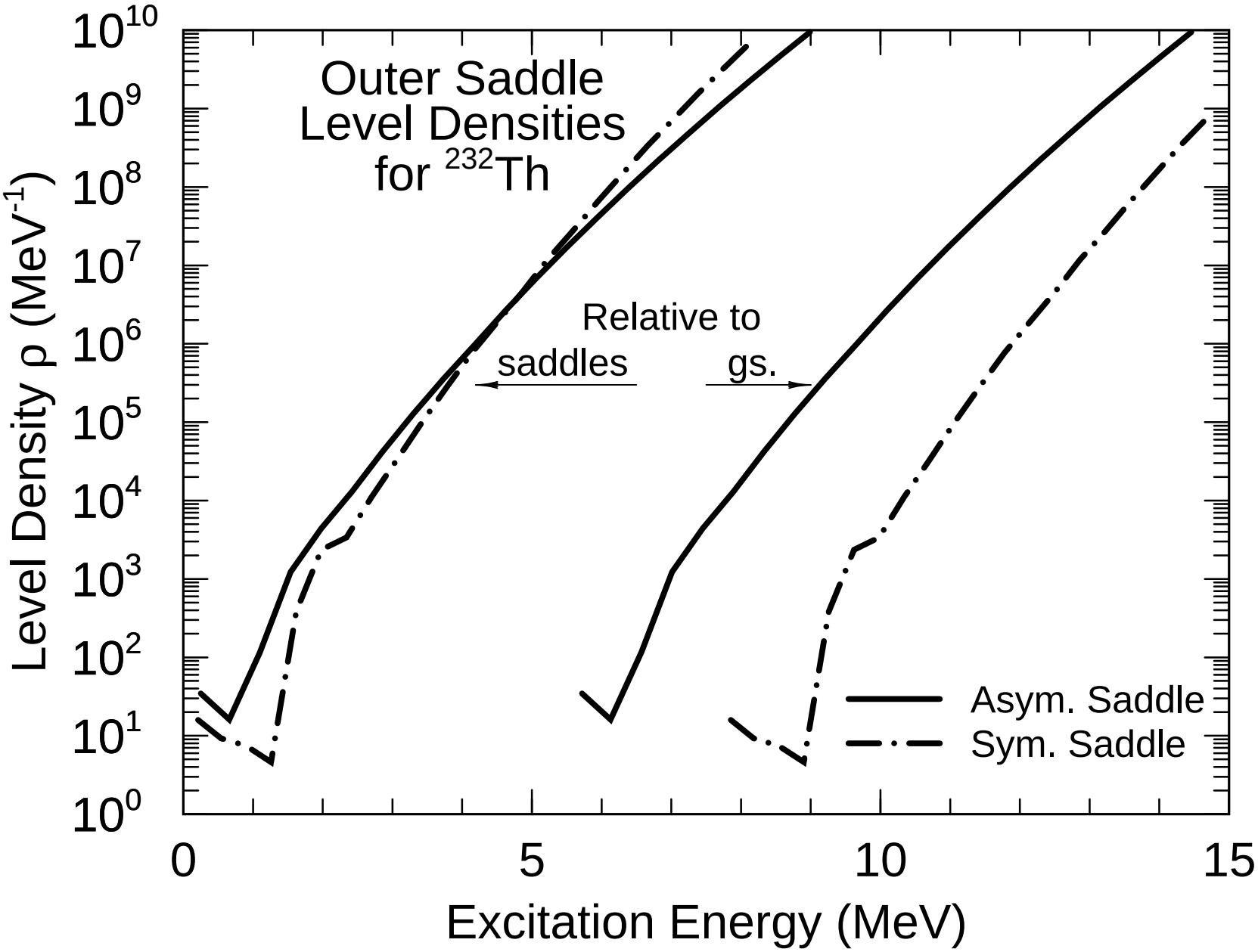

Outer Saddle
Level Densities
for 232Th
Relative to
saddles
gs.
Asym. Saddle
Sym. Saddle
Level Density ρ (MeV-1)
Excitation Energy (MeV)
10^10
10^9
10^8
10^7
10^6
10^5
10^4
10^3
10^2
10^1
10^0
0
5
10
15

TABLE I: Fermi-gas level-density parameters determined from adjustments of parameters of the Fermi-gas model to microscopic calculations of intrinsic level densities. The numbers in parentheses are (1) for an asymmetric saddle, and (2) for a symmetric saddle. B and C refer to the second and third saddle, respectively, for a triple-humped barrier, see Fig. **??**.

Nucleus		$Q_2^{1/2}$ (barn$^{1/2}$)	Density Fit a (MeV)$^{-1}$	Density Fit $E_{\rm shift}$ (MeV)	Log Fit a (MeV)$^{-1}$	Log Fit $E_{\rm shift}$ (MeV)
		even-even systems				
^{232}Th	(1)	7.75	17.708	2.483	15.403	1.177
^{232}Th	(2)	7.56	20.538	2.492	18.963	1.898
		odd-even systems				
^{239}Am	(1)	6.04	19.369	1.275	16.906	0.607
^{241}Am	(1)	6.04	19.879	1.232	19.156	0.980
^{243}Am	(1)	6.04	20.281	1.097	17.828	0.470
		odd-odd systems				
^{238}Am	(1B)	6.20	19.041	0.810	19.125	0.700
^{238}Am	(1C)	7.56	17.259	0.232	17.814	0.420
^{242}Am	(1)	6.04	19.740	0.618	21.961	0.980

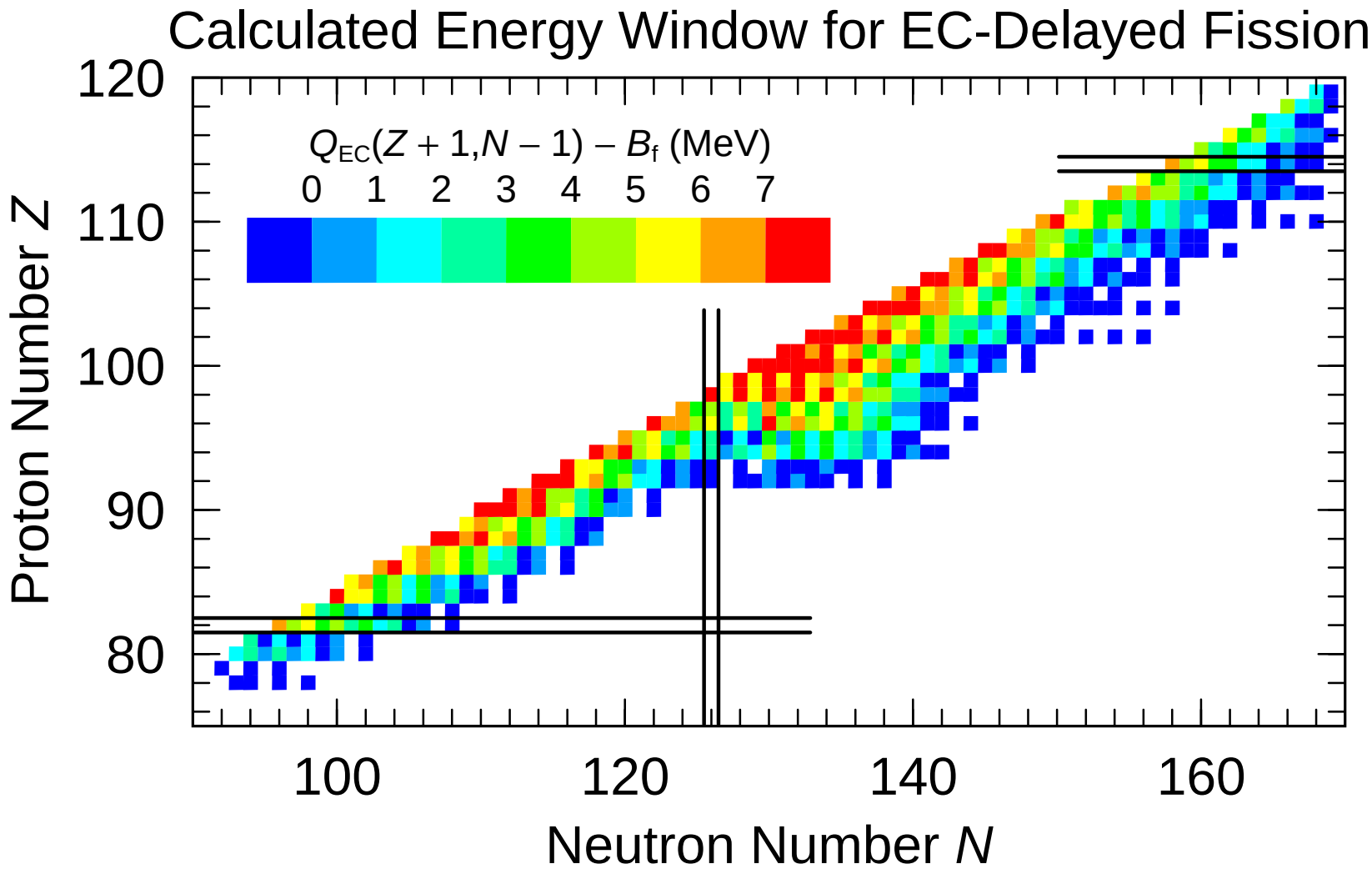
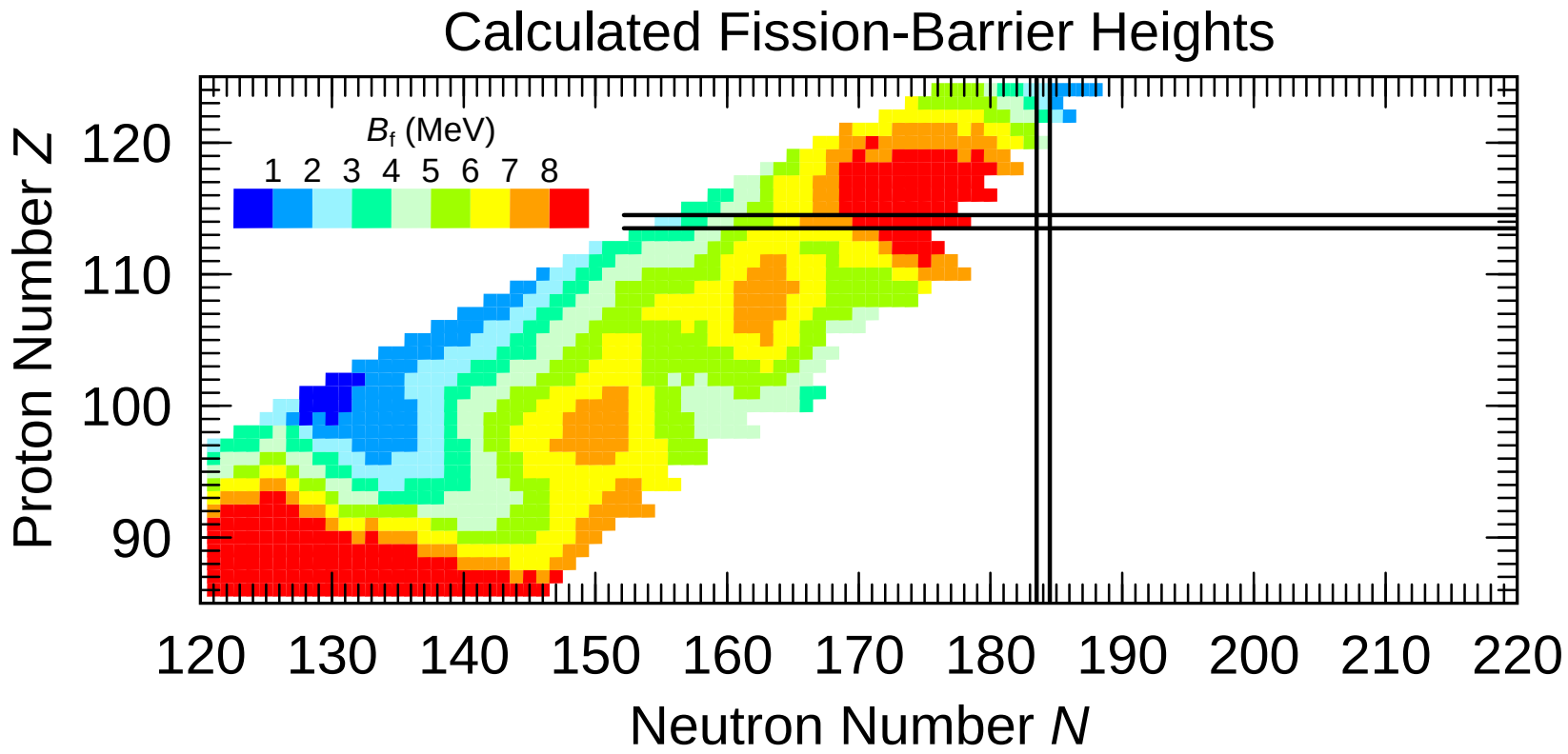

Calculated Energy Window for EC-Delayed Fission
$Q_{EC}(Z+1,N-1) - B_f$ (MeV)
0 1 2 3 4 5 6 7
Proton Number Z
120
110
100
90
80
100
120
140
160
Neutron Number N

TABLE I: Calculated Q values $Q_{\rm EC}$ for electron capture and calculated fission-barrier heights $B_{\rm f}$ for reactions where EC-delayed fission has been observed experimentally.

Reaction			$Q_{\rm EC}$ (MeV)	$B_{\rm f}$ (MeV)	$Q_{\rm EC} - B_{\rm f}$ (MeV)
$^{180}_{81}$Tl	$\stackrel{EC}{\Longrightarrow}$	$^{180}_{80}$Hg	10.44	9.81	0.63
$^{228}_{93}$Np	$\stackrel{EC}{\Longrightarrow}$	$^{228}_{92}$U	4.26	5.13	−0.87
$^{232}_{95}$Am	$\stackrel{EC}{\Longrightarrow}$	$^{232}_{94}$Pu	4.88	3.23	1.65
$^{234}_{95}$Am	$\stackrel{EC}{\Longrightarrow}$	$^{234}_{94}$Pu	4.12	3.83	0.29
$^{238}_{97}$Bk	$\stackrel{EC}{\Longrightarrow}$	$^{238}_{96}$Cm	4.77	4.92	−0.15
$^{242}_{99}$Es	$\stackrel{EC}{\Longrightarrow}$	$^{242}_{98}$Cf	5.22	6.16	−0.94
$^{244}_{99}$Es	$\stackrel{EC}{\Longrightarrow}$	$^{244}_{98}$Cf	4.45	6.69	−2.24
$^{246}_{99}$Es	$\stackrel{EC}{\Longrightarrow}$	$^{246}_{98}$Cf	3.69	7.16	−3.47
$^{248}_{99}$Es	$\stackrel{EC}{\Longrightarrow}$	$^{248}_{98}$Cf	2.98	7.24	−4.26

TABLE I: Fission and α-decay half-lives for selected nuclei. .

Nuclide			$^{10}\mathrm{Log}(T^{\mathrm{f}}_{1/2}/\mathrm{y})$		$^{10}\mathrm{Log}(T^{\alpha}_{1/2}/\mathrm{y})$	
Z	N	A	Calc.	Exp.	Calc.	Exp.
92	144	236	14.31	16.39	8.18	7.37
94	138	232	−1.29		−3.21	−4.19
94	146	240	9.22	11.05	4.51	3.93
100	152	252	6.06	2.09	−1.14	−2.54
100	158	258	−7.34	−10.91		
96	126	222	9.41		−4.12	
98	126	224	1.65		−4.70	
100	126	226	−3.03		−5.29	
96	128	224	−2.16		−8.35	
96	134	230	−10.76		−1.48	
98	132	230	−15.96		−4.52	
112	165	277	−5.37		−11.91	−11.11


Calculated Fission-Barrier Heights
B_f (MeV)
1 2 3 4 5 6 7 8
Proton Number Z
120
110
100
90
120 130 140 150 160 170 180 190 200 210 220
Neutron Number N