TOPAS-nBio-dev (TOPAS v4.0) Regression testing (cf. TOPAS-nBio-dev (TOPAS v4.0))

José Ramos-Méndez, Naoki D. Kondo, and Thongchai A.M. Masilela

University of California San Francisco

April 4, 2024

Table of Contents I

DBSCAN - TsEmDNAPhysics

DBSCAN - g4em-dna_opt2

DBSCAN - g4em-dna_opt4

DBSCAN - g4em-dna_opt6

LET I

LET II

Fricke: IRT

G-value: step-by-step

G-value vs. LET: step-by-step

G-value: IRT

G-value vs. LET: IRT

G-value of H₂O₂: IRT

Table of Contents II

G-value of H: IRT

G-value and Temperature I: IRT

G-value and Temperature II: IRT

Nanodosimetry I: TsEmDNAPhysics and g4em-dna_opt2

Nanodosimetry I: g4em-dna_opt4 and g4em-dna_opt6

Nanodosimetry II: TsEmDNAPhysics and g4em-dna_opt2

Nanodosimetry II: g4em-dna_opt4 and g4em-dna_opt6

Nanodosimetry III: TsEmDNAPhysics

Nanodosimetry III: g4em-dna_opt2

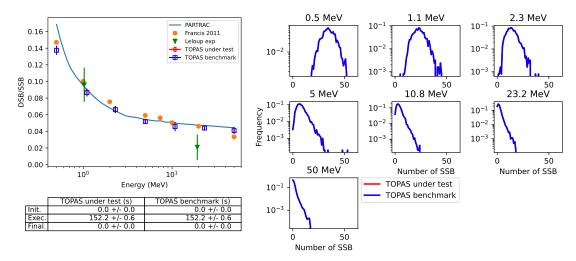
Nanodosimetry III: g4em-dna_opt4

Nanodosimetry III: g4em-dna_opt6

SSBs as a function of DMSO: single pulse, low dose rate

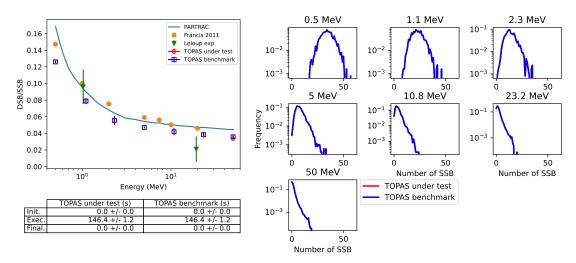


DBSCAN - TsEmDNAPhysics



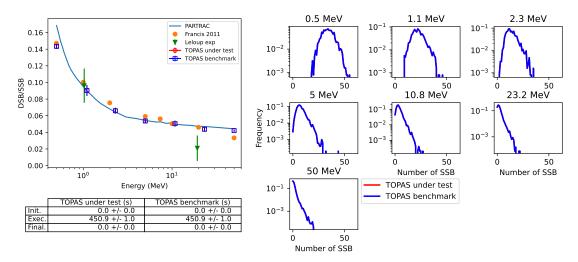
Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. Comput Methods Programs Biomed. 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

DBSCAN - g4em-dna_opt2



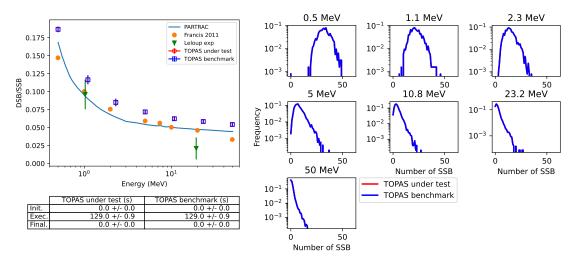
Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. Comput Methods Programs Biomed. 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

DBSCAN - g4em-dna_opt4



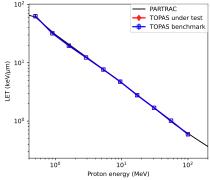
Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. Comput Methods Programs Biomed. 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

DBSCAN - g4em-dna_opt6



Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. Comput Methods Programs Biomed. 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

LET I



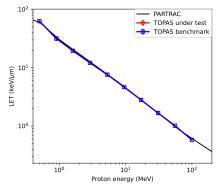
	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	264.0 +/- 1.4	264.0 +/- 1.4
Final.	0.0 +/- 0.0	0.0 +/- 0.0

102			AC under test benchmark
LET (keV/µm)			8
<u> </u>	10 ⁰ Protoi	10 ¹ n energy (MeV)	10 ²

	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	253.6 +/- 0.5	253.6 +/- 0.5
Final.	0.0 +/- 0.0	0.0 +/- 0.0

LET as a function of proton energy for TsEmDNAPhysics (left) and g4em-dna_opt2 (right).

LET II



1	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	724.3 +/- 1.0	724.3 +/- 1.0
Final.	0.0 +/- 0.0	0.0 +/- 0.0

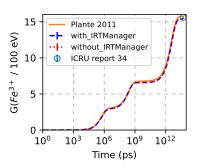
102			PARTRAC TOPAS under test TOPAS benchmark
LET (keV/μm)			
Ь	100	10 ¹ Proton energy (Me	10 ²

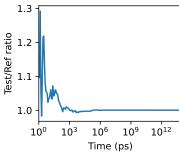
	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	234.9 +/- 0.9	234.9 +/- 0.9
Final.	0.0 +/- 0.0	0.0 +/- 0.0

LET as a function of proton energy for g4em-dna_opt4 (left) and g4em-dna_opt6 (right).

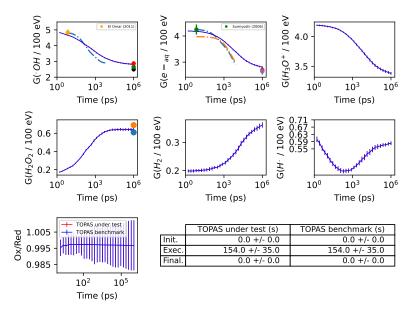
Fricke: IRT

	with_IRTManager	without_IRTManager	
Init. (s)	0.010 +/- 0.000	0.010 +/- 0.000	
Exec. (s)	1262.560 +/- 22.274	1281.648 +/- 28.085	
Final. (s)	0.006 +/- 0.005	0.006 +/- 0.005	
Value (/100eV)	15.393 +/- 0.005	15.387 +/- 0.005	

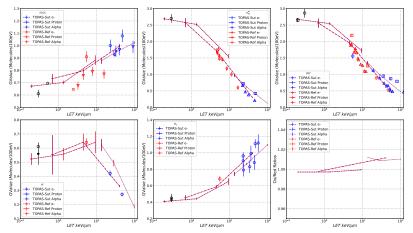




G-value: step-by-step

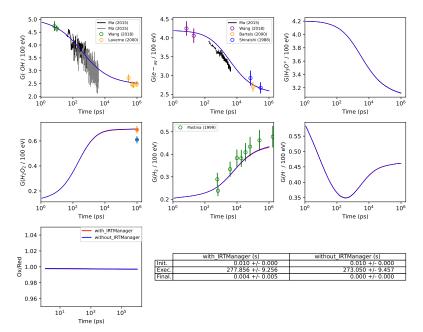


G-value vs. LET: step-by-step

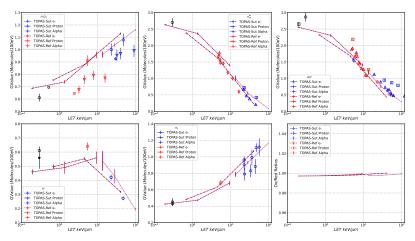


	TOPAS-Ref	TOPAS-Sut
Real	35918.750 +/- 564.408	35918.750 +/- 564.408
User	35895.032 +/- 564.205	35895.032 +/- 564.205
Sys	16.572 +/- 0.227	16.572 +/- 0.227

G-value: IRT

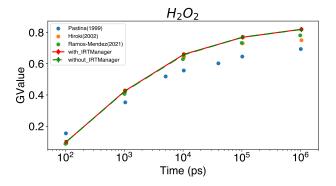


G-value vs. LET: IRT



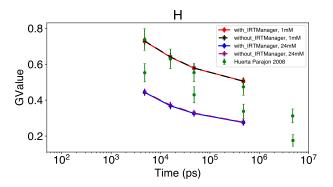
	TOPAS-Ref	TOPAS-Sut
Real	1365.454 +/- 23.439	1365.454 +/- 23.439
User	1090.800 +/- 23.443	1090.800 +/- 23.443
Sys	10.438 +/- 0.247	10.438 +/- 0.247

G-value of H_2O_2 : IRT



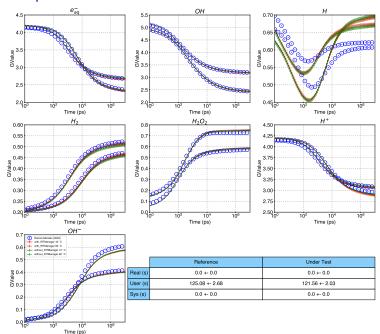
	Reference	Under Test
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	213.47 +- 1.17	182.19 +- 1.1
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value of H: IRT

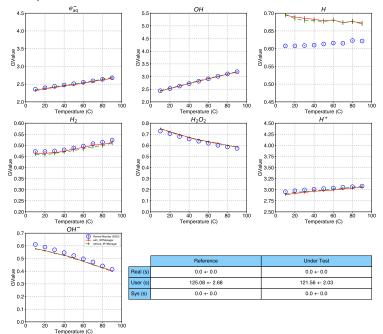


	Reference	Under Test	
Real (s)	0.0 +- 0.0	0.0 +- 0.0	
User (s)	572.38 +- 11.45	543.03 +- 21.58	
Sys (s)	0.0 +- 0.0	0.0 +- 0.0	

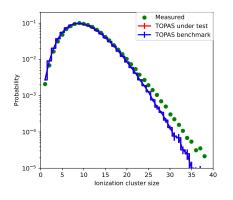
G-value and Temperature I: IRT



G-value and Temperature II: IRT



Nanodosimetry I: TsEmDNAPhysics and g4em-dna_opt2

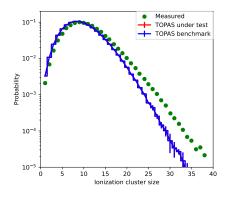


10-1	B	~~	‡	Measured TOPAS un TOPAS be	
10-2	f		1		
Probability	•		*E		
10-4				X	
10-5 0	5	10 15 Ionizat	20 2		35 40

	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	10342.3 +/- 25.4	10342.3 +/- 25.4
Final.	0.0 +/- 0.0	0.0 +/- 0.0

	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	10082.1 +/- 49.3	10082.1 +/- 49.3
Final.	0.0 +/- 0.0	0.0 +/- 0.0

Nanodosimetry I: g4em-dna_opt4 and g4em-dna_opt6

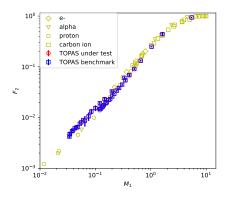


10-1 -	A PROPERTY OF	1	→ т	easured OPAS un OPAS be	der tes	
10-2		•	*			
Probability	4		*	<u> </u>		
10-4				1	M.	
10 ⁻⁵ -					4	¥
	5 10		20 25 cluster size	30	35	40

[TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	8531.7 +/- 11.6	8531.7 +/- 11.6
Final.	0.0 +/- 0.0	0.0 +/- 0.0

	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	7789.4 +/- 37.9	7789.4 +/- 37.9
Final.	0.0 +/- 0.0	0.0 +/- 0.0

Nanodosimetry II: TsEmDNAPhysics and g4em-dna_opt2

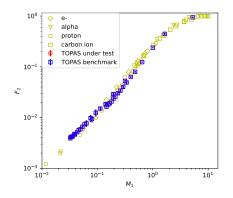


	10° -	◇ ✓ O Φ Φ	e- alpha proton carbon ion TOPAS under test TOPAS benchmark		B. C.
F ₂	10-2				
	10 ⁻³ -	<u>O</u>	10-1	10°	101

	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	119.6 +/- 0.6	119.6 +/- 0.6
Final.	0.0 +/- 0.0	0.0 +/- 0.0

ĺ	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	93.8 +/- 0.2	93.8 +/- 0.2
Final.	0.0 +/- 0.0	0.0 +/- 0.0

Nanodosimetry II: g4em-dna_opt4 and g4em-dna_opt6

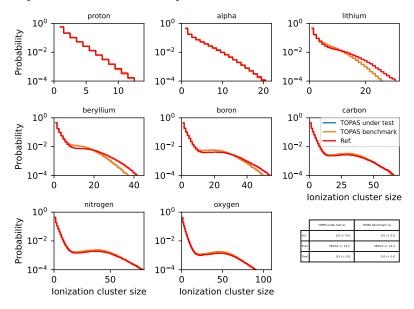


	100 -	♦	e-		ra\Z <mark>ro</mark> v	
	- 1	▽	alpha			
		0	proton		400	
			carbon ion		r 💆	
		Φ	TOPAS under test			
	10-1 -	Ф	TOPAS benchmark	rain ()	
	10 -			go	S GARDEN	
			0	90		
F_2			qui ^e	,		
	10-2		•			
	- 1		∞ * ▽			
			0			
			8			
	10-3 -	0				
	10	-2	10-1		100	10 ¹
				M_1		

	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	1796.0 +/- 3.7	1796.0 +/- 3.7
Final.	0.0 +/- 0.0	0.0 +/- 0.0

ĺ	TOPAS under test (s)	TOPAS benchmark (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	1312.8 +/- 5.1	1312.8 +/- 5.1
Final.	0.0 +/- 0.0	0.0 +/- 0.0

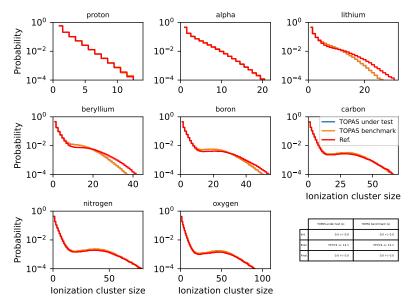
Nanodosimetry III: TsEmDNAPhysics



Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. Phys Med Biol. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee



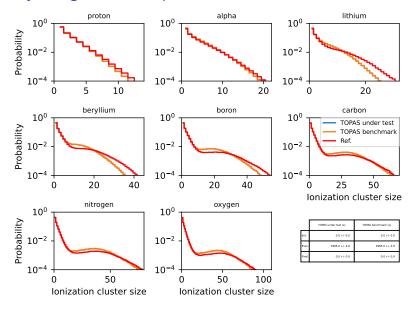
Nanodosimetry III: g4em-dna_opt2



Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. Phys Med Biol. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee



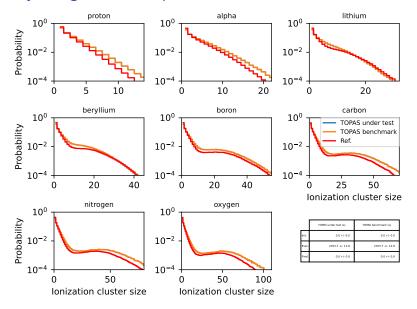
Nanodosimetry III: g4em-dna_opt4



Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. Phys Med Biol. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee



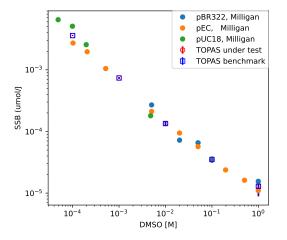
Nanodosimetry III: g4em-dna_opt6



Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. Phys Med Biol. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee



SSBs as a function of DMSO: single pulse, low dose rate



	TOPAS under test (s)	TOPAS benchmark (s)
Init.	1.0 +/- 0.0	1.0 +/- 0.0
Exec.	23787.1 +/- 176.4	23787.1 +/- 176.4
Final.	0.0 +/- 0.0	0.0 +/- 0.0