TOPAS-nBio v3.0 (OpenTOPAS v4.0)
Regression testing (cf. TOPAS-nBio v2.0 (TOPAS v3.9))

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

University of California San Francisco

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Introduction

Welcome to the TOPAS-nBio regression test results!

This document depicts the results for 13 separate regression tests, comparing TOPAS-nBio v3.0 (the latest release which works with OpenTOPAS v4.0) to TOPAS-nBio v2.0.

Given the substantial changes to the code (see release notes), certain regression tests are not able to be performed in TOPAS-nBio v2.0. In these cases TOPAS-nBio v3.0 is simply compared against itself. The affected tests are as follows:

- ▶ Fricke: IRT
- ▶ G-value of H_2O_2/H
- ▶ G-value and Temperature
- ▶ Nanodosimetry I/III

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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

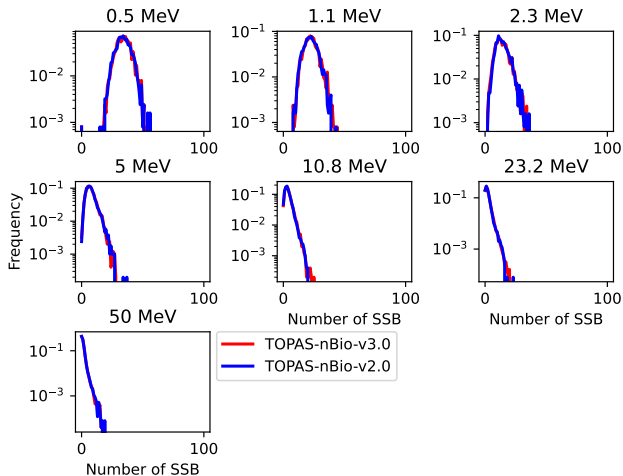|	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	407.4 +/- 103.5	642.5 +/- 137.4
Final.	0.0 +/- 0.0	0.0 +/- 0.0

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

	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	1812.7 +/- 478.4	2244.2 +/- 181.3
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ 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
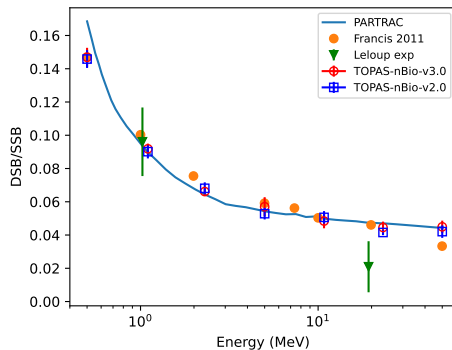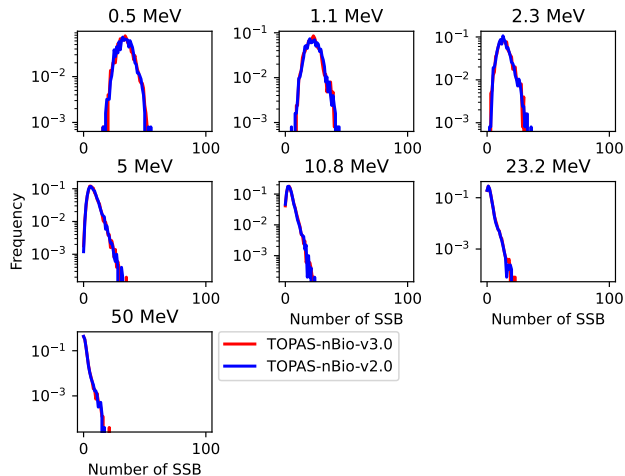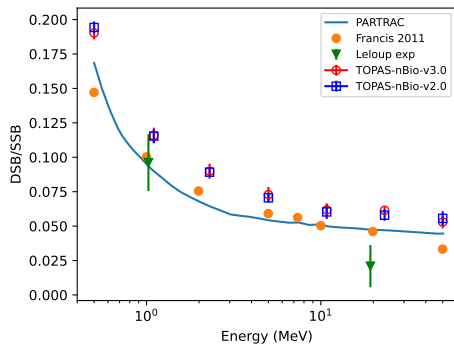
DBSCAN - g4em-dna_opt6

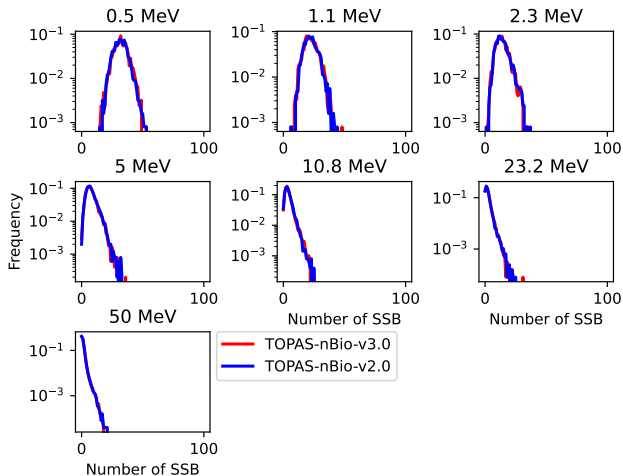|	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	481.9 +/- 54.7	2108.6 +/- 247.8
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ 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

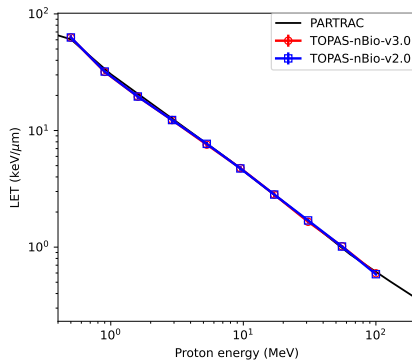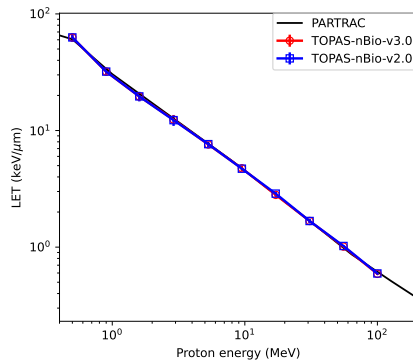|	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	717.5 +/- 89.6	1192.6 +/- 183.2
Final.	0.0 +/- 0.0	0.0 +/- 0.0

	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	650.2 +/- 212.9	773.9 +/- 211.8
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
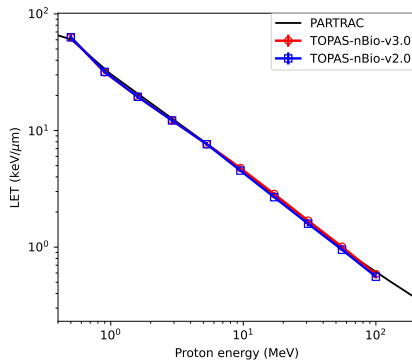
	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	2811.8 +/- 334.0	2544.5 +/- 803.2
Final.	0.0 +/- 0.0	0.0 +/- 0.0
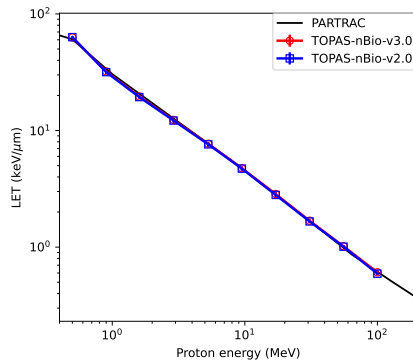
	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	596.7 +/- 137.6	2763.6 +/- 384.7
Final.	0.0 +/- 0.0	0.0 +/- 0.0

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

Fricke: IRT

	TOPAS-nBio-v3.0	TOPAS-nBio-v3.0
Init. (s)	0.024 +/- 0.005	0.024 +/- 0.005
Exec. (s)	16.564 +/- 4.157	16.564 +/- 4.157
Final. (s)	0.030 +/- 0.016	0.030 +/- 0.016
Value (/100eV)	15.466 +/- 0.053	15.466 +/- 0.053
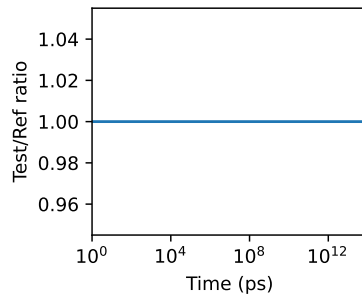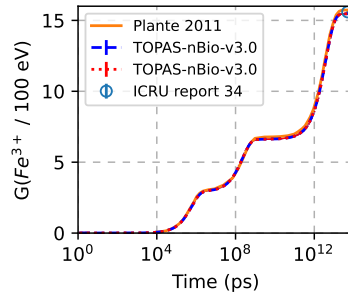
G-value: step-by-step

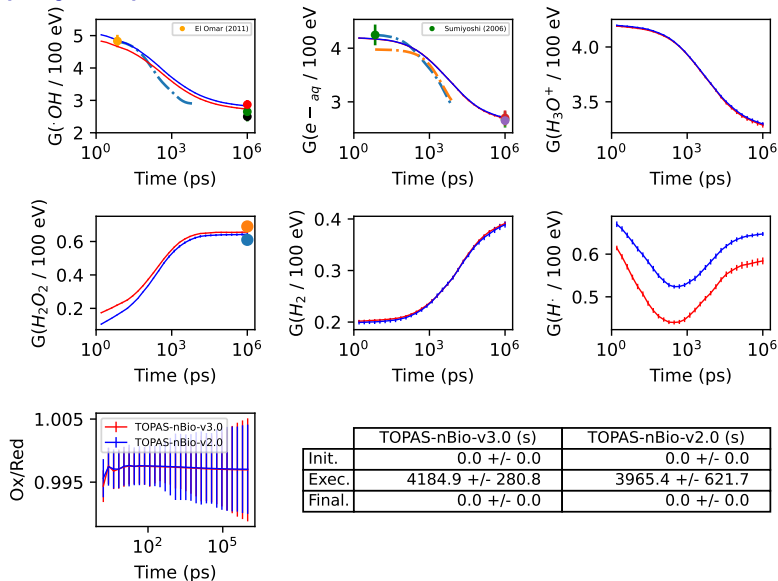The discrepancy between H yields can be attributed to a change that was made to the H_2O^+ and H_2O^* dissociation displacements. There is a lack of experimental data in pure liquid water to conclude which graph is correct, correspondingly the H yield behavior was validated with a scavenging system, as shown in the "G-value of H: IRT" regression test.

G-value vs. LET: step-by-step
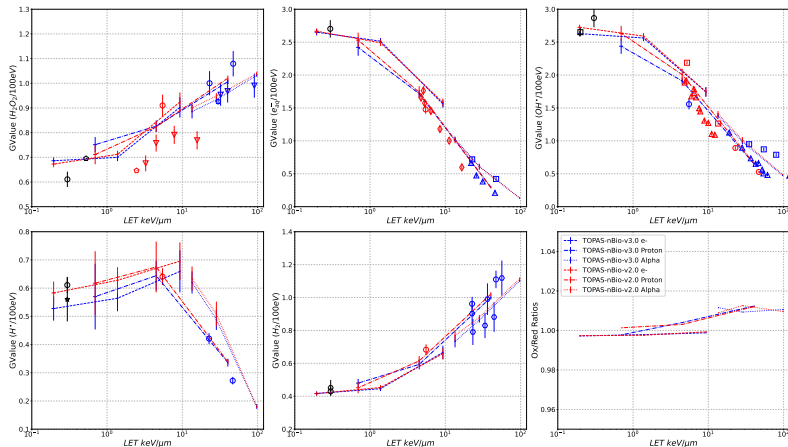
	TOPAS-nBio-v2.0	TOPAS-nBio-v3.0
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	3218.36 +- 390.17	3041.16 +- 688.34
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value: IRT

	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.028 +/- 0.008	0.018 +/- 0.004
Exec.	584.560 +/- 52.509	824.994 +/- 380.845
Final.	0.014 +/- 0.011	0.014 +/- 0.009
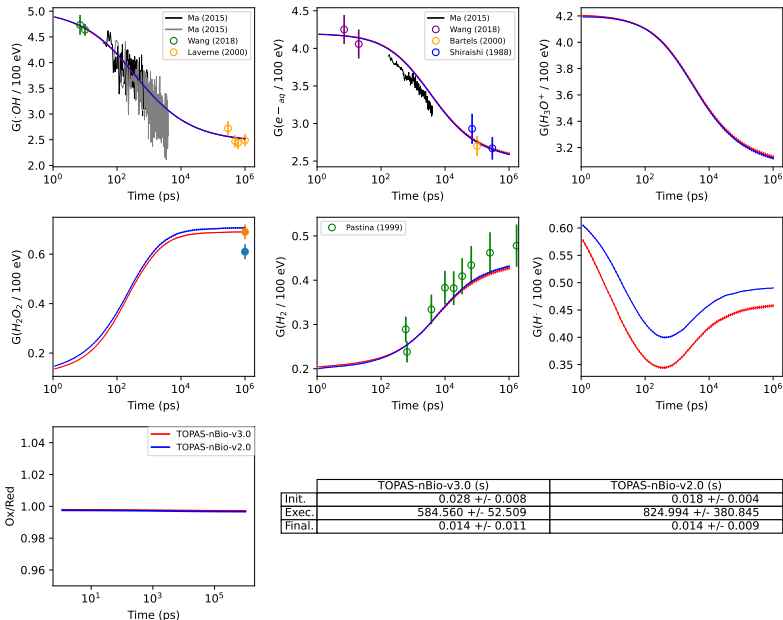
▶ See footnote on page 12 for an explanation of the H yield discrepancy

G-value vs. LET: IRT
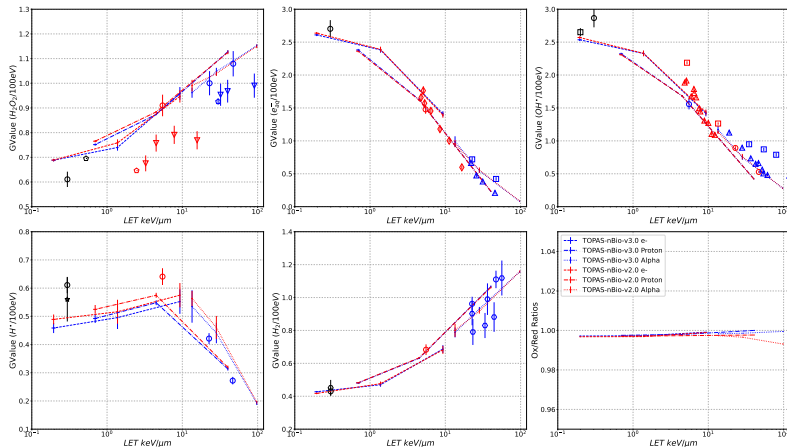
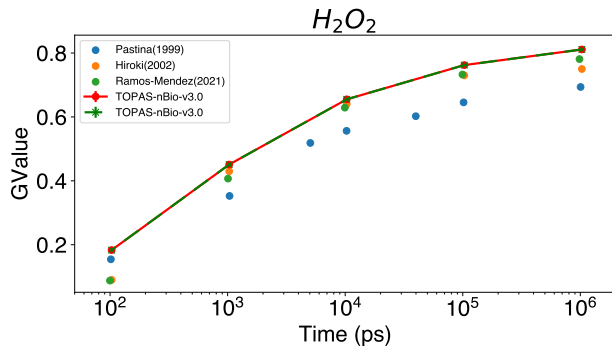|	TOPAS-nBio-v2.0	TOPAS-nBio-v3.0
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	194.56 +- 14.74	146.19 +- 16.05
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value of H$_2$O$_2$: IRT

H_2O_2

Legend:
- Pastina(1999)
- Hiroki(2002)
- Ramos-Mendez(2021)
- TOPAS-nBio-v3.0
- TOPAS-nBio-v3.0

GValue vs Time (ps)

	Reference	Under Test
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	2442.34 +- 1003.79	2442.34 +- 1003.79
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value of H: IRT
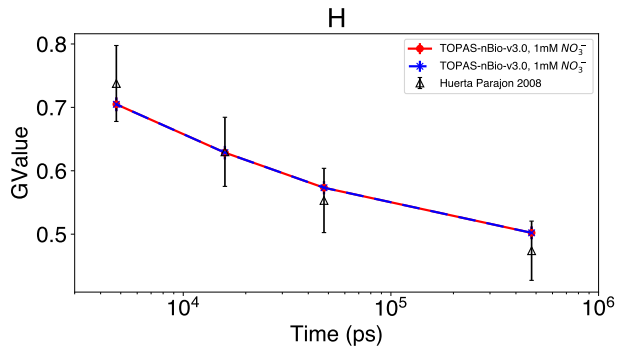
	Reference	Under Test
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	441.61 +- 165.61	441.61 +- 165.61
Sys (s)	0.0 +- 0.0	0.0 +- 0.0
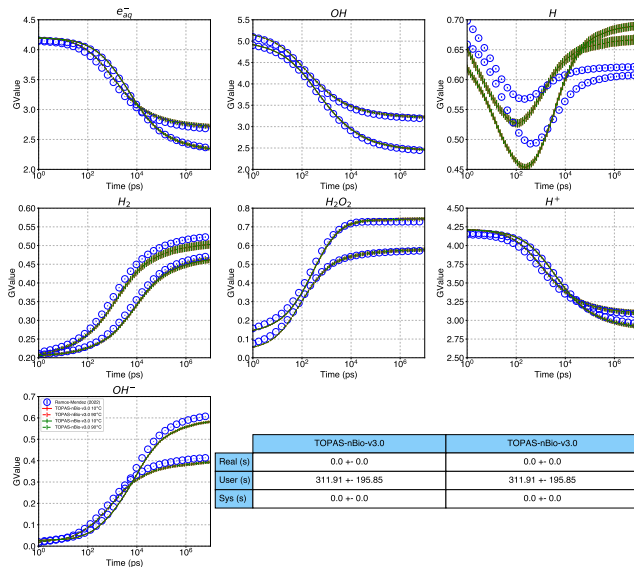
▶ See footnote on page 12 for an explanation of the H yield discrepancy

G-value and Temperature II: IRT
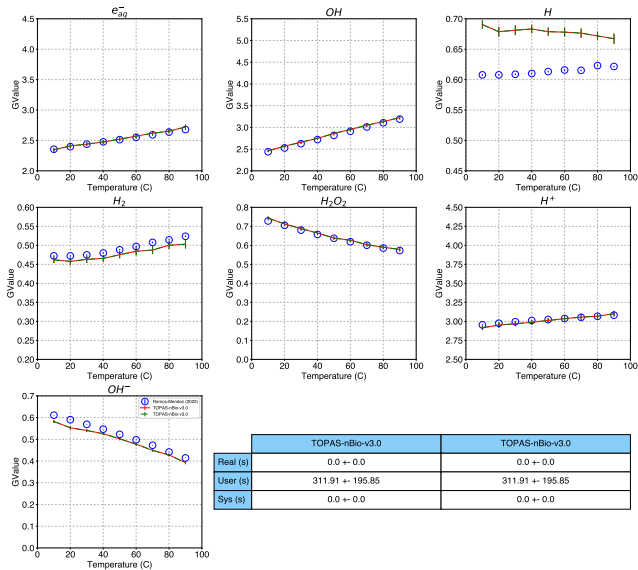
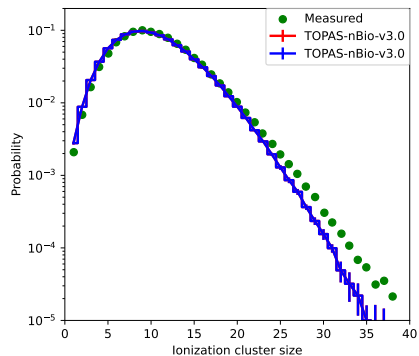# Nanodosimetry I: TsEmDNAPhysics and g4em-dna_opt2
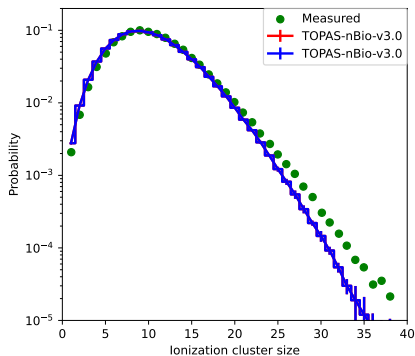
	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	24655.5 +/- 5903.8	24655.5 +/- 5903.8
Final.	0.0 +/- 0.0	0.0 +/- 0.0

	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	20585.2 +/- 390.6	20585.2 +/- 390.6
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry I: g4em-dna_opt4 and g4em-dna_opt6
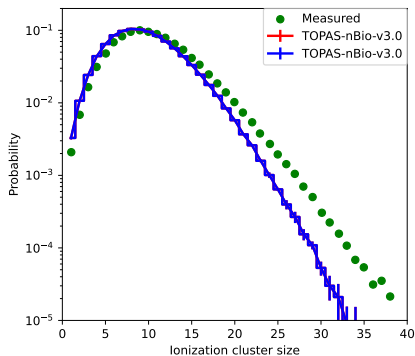
	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	17351.3 +/- 184.3	17351.3 +/- 184.3
Final.	0.0 +/- 0.0	0.0 +/- 0.0

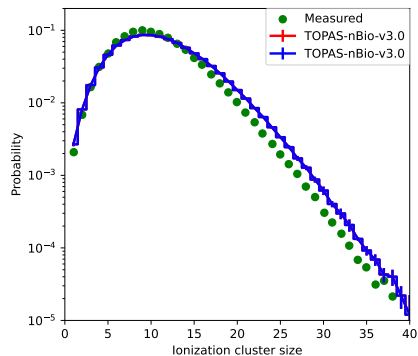|	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	22087.8 +/- 5205.4	22087.8 +/- 5205.4
Final.	0.0 +/- 0.0	0.0 +/- 0.0

► Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry II: TsEmDNAPhysics and g4em-dna_opt2
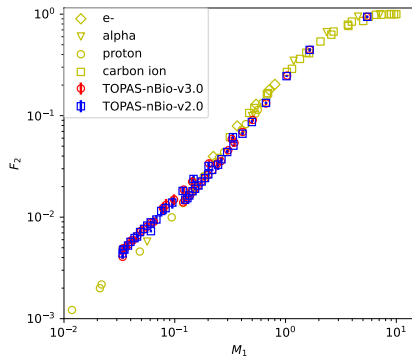
	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	304.6 +/- 76.1	389.8 +/- 37.7
Final.	0.0 +/- 0.0	0.0 +/- 0.0

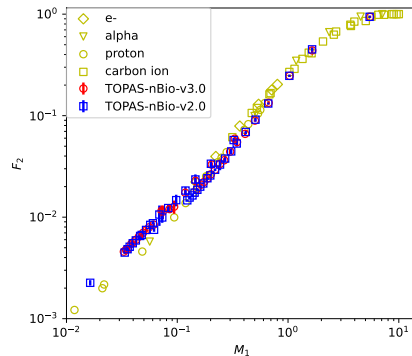|	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	199.6 +/- 18.2	319.9 +/- 33.5
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry II: g4em-dna_opt4 and g4em-dna_opt6
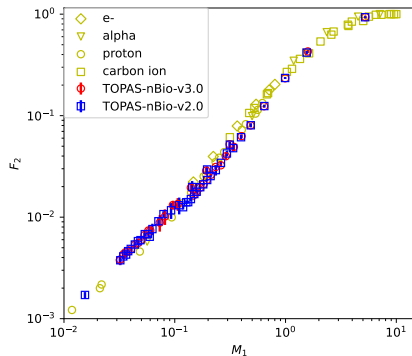
	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	3925.9 +/- 393.2	13221.0 +/- 367.3
Final.	0.0 +/- 0.0	0.0 +/- 0.0

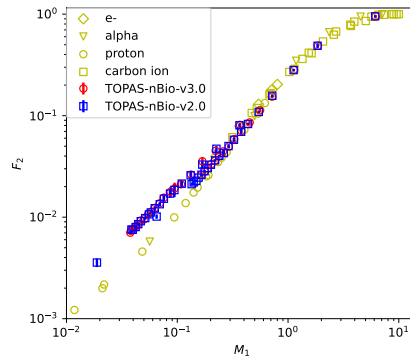|	TOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	2659.4 +/- 302.8	14181.3 +/- 1124.3
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry III: TsEmDNAPhysics
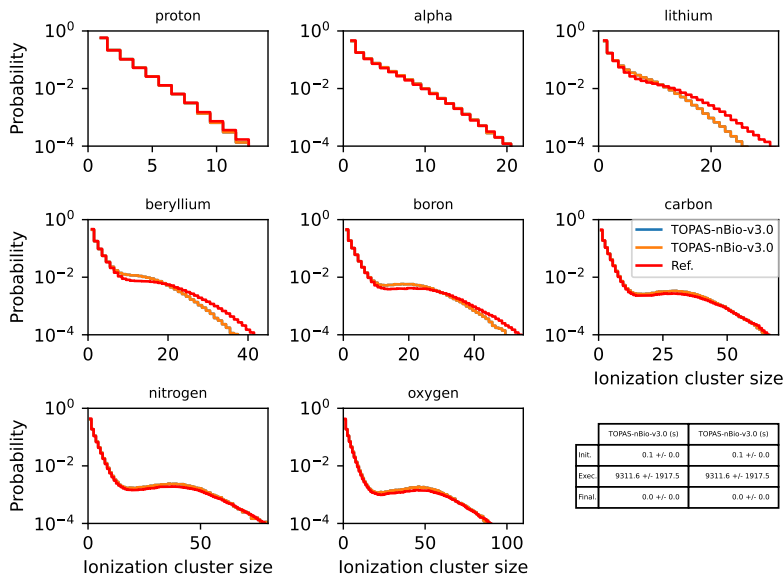
▶ Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol*. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee
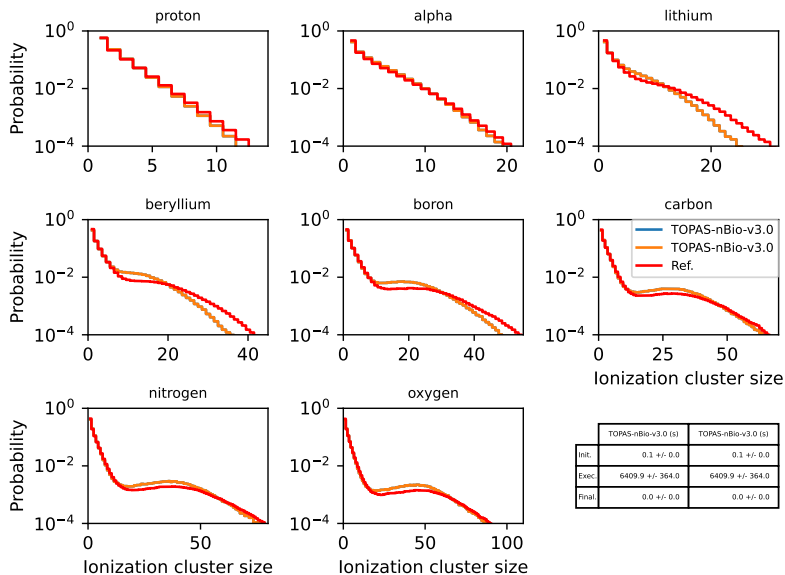
Nanodosimetry III: g4em-dna_opt2
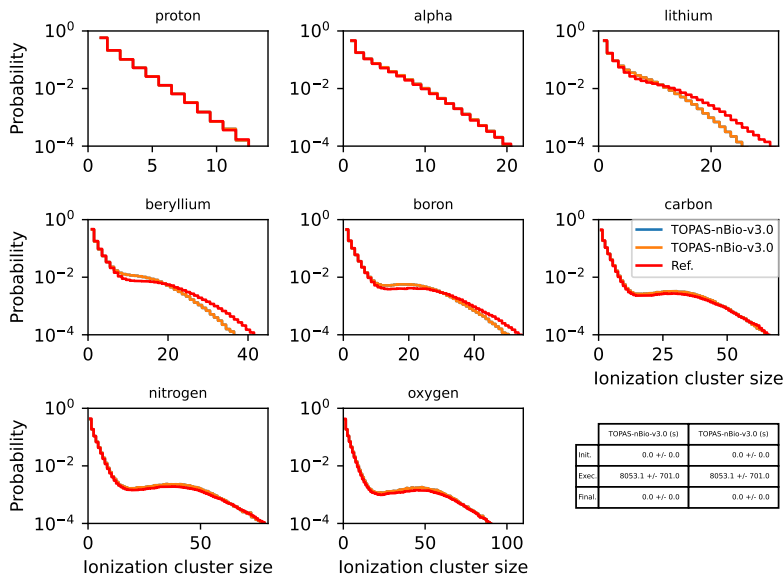
Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol*. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee

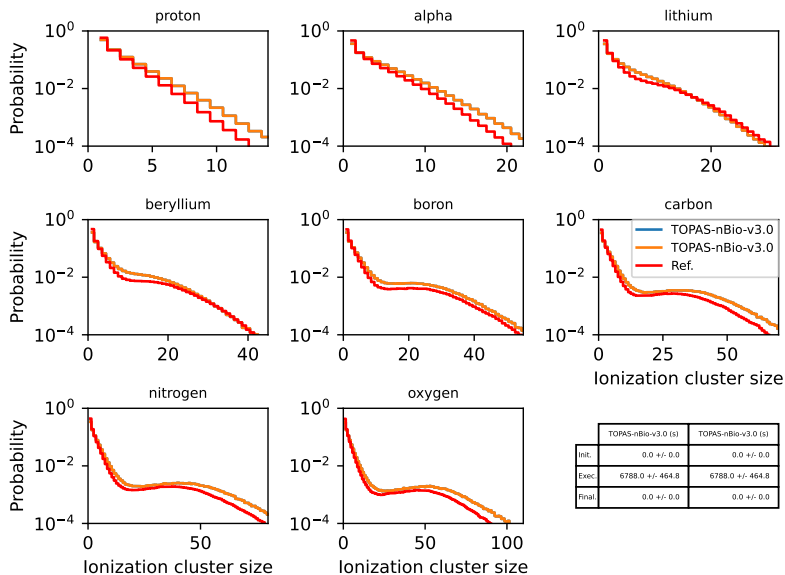# Nanodosimetry III: g4em-dna_opt4

▶ 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