

TOPAS-nBio v4.0 (OpenTOPAS v4.0)

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

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

University of California San Francisco

July 16, 2025

Introduction

Welcome to the TOPAS-nBio regression test results!

This document depicts the results for 13 separate regression tests, comparing TOPAS-nBio v4.0 to TOPAS-nBio v3.0.

Table of Contents I

Introduction

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

Table of Contents II

G-value of H_2O_2 : IRT

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

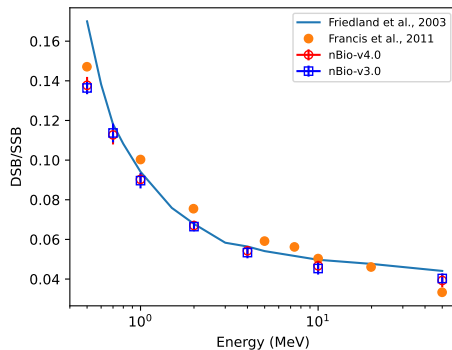
Nanodosimetry III: TsEmDNAPhysics

Nanodosimetry III: g4em-dna_opt2

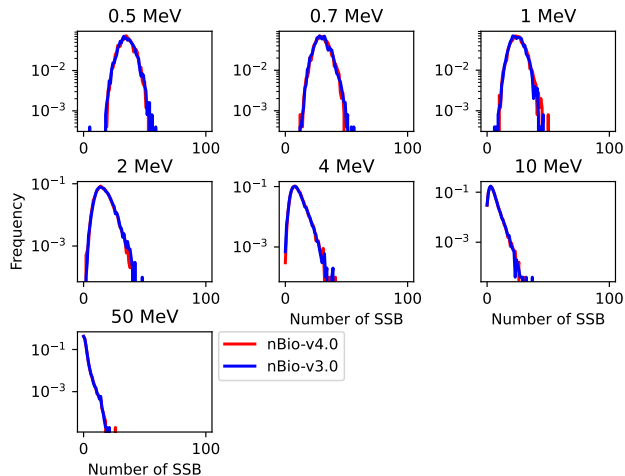
Nanodosimetry III: g4em-dna_opt4

Nanodosimetry III: g4em-dna_opt6

DBSCAN - TsEmDNAPhysics

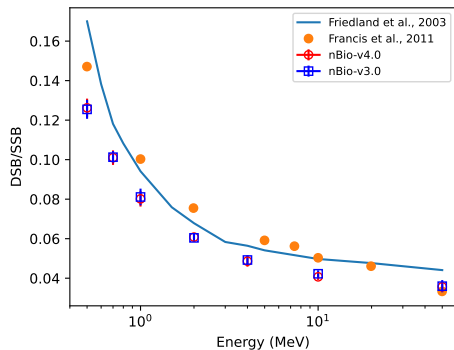


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	246.4 +/- 0.6	239.2 +/- 0.6

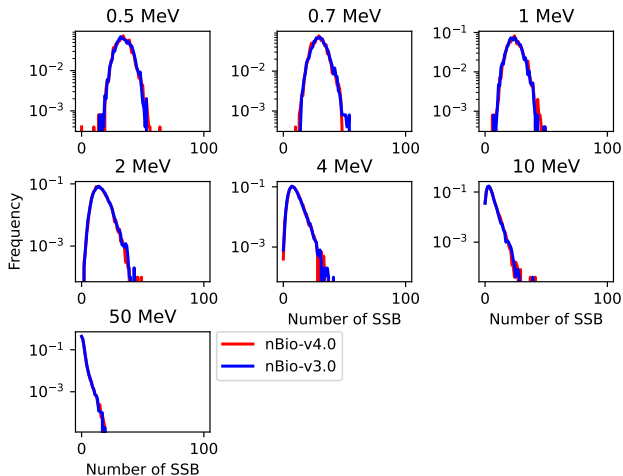


- Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed.* 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

DBSCAN - g4em-dna_opt2

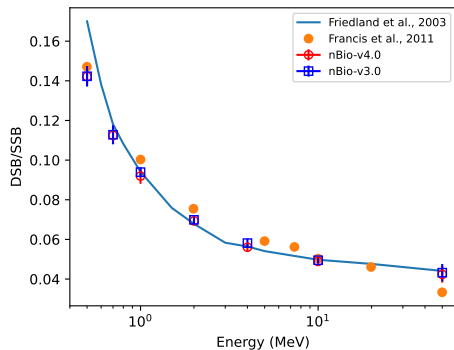


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	235.8 +/- 1.4	235.7 +/- 1.2

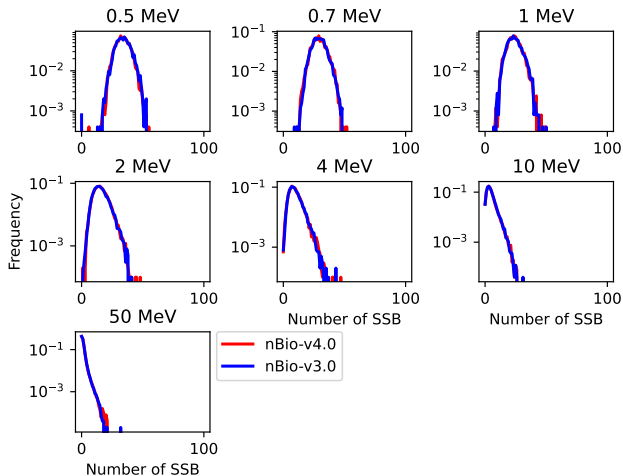


- Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed.* 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

DBSCAN - g4em-dna_opt4

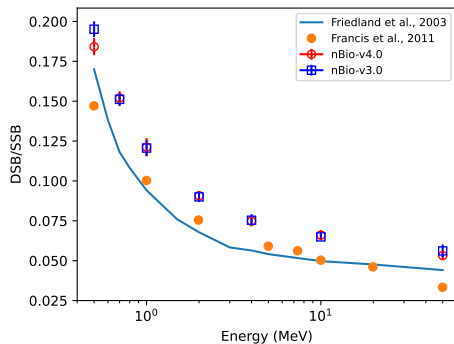


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	613.7 +/- 1.1	938.1 +/- 2.2

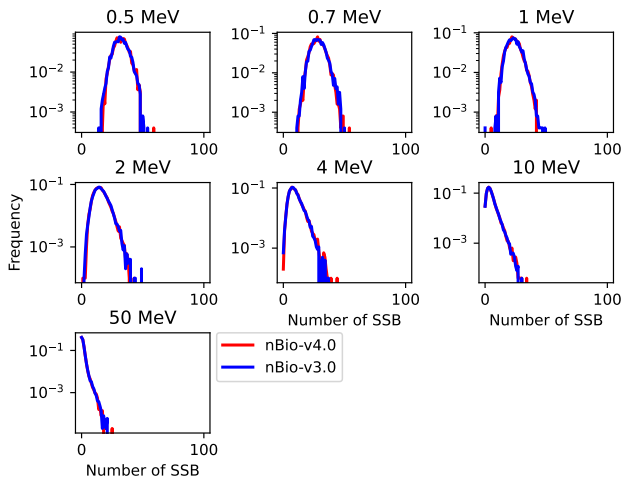


- Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed.* 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

DBSCAN - g4em-dna_opt6

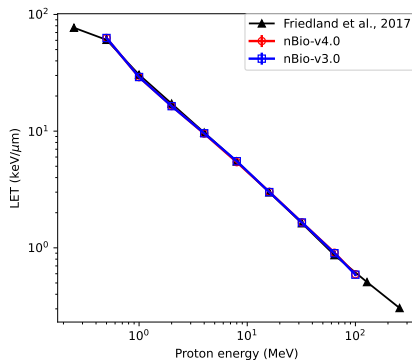


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	177.5 +/- 1.4	202.5 +/- 2.2

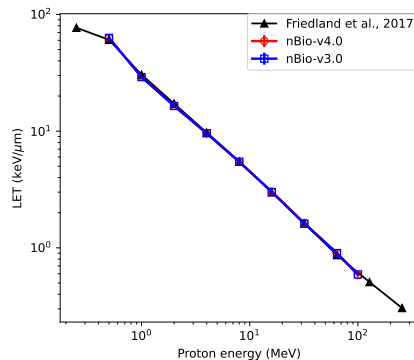


- Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed.* 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

LET I



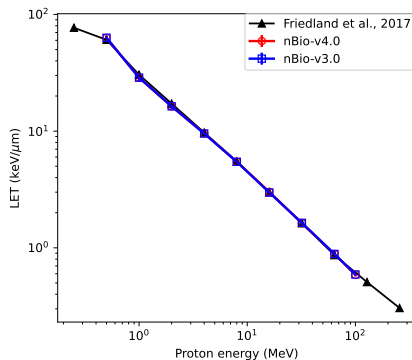
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	266.8 +/- 1.7	304.9 +/- 1.2



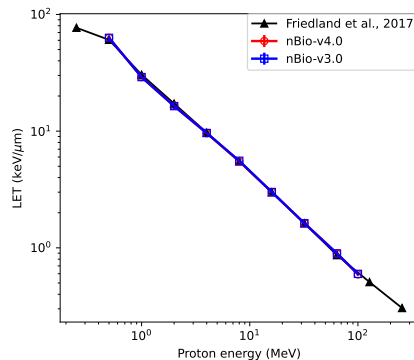
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	275.0 +/- 1.4	344.5 +/- 10.0

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

LET II



	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	688.0 +/- 1.7	1017.4 +/- 10.0

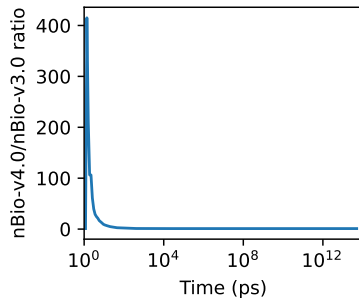
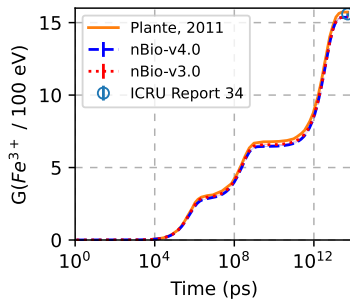


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	301.4 +/- 2.3	330.2 +/- 12.5

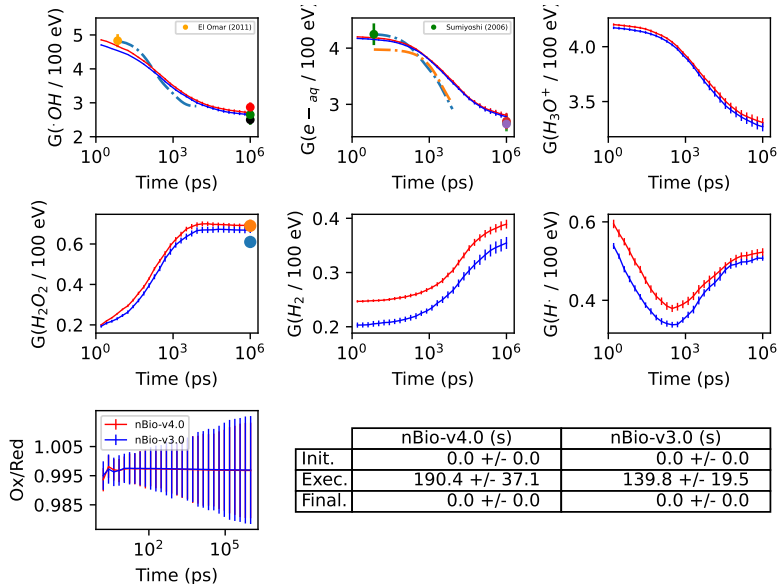
▶ LET as a function of proton energy for g4em-dna_opt4 (left) and g4em-dna_opt6 (right).

Fricke: IRT

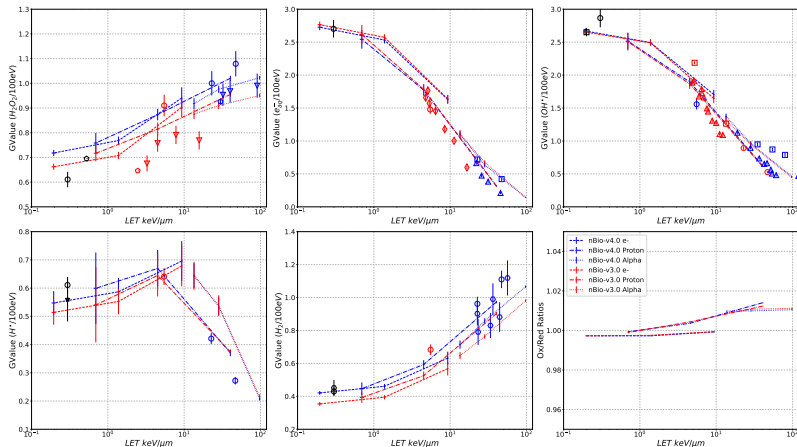
	nBio-v4.0	nBio-v3.0
Exec. (s)	52.123 +/- 1.720	58.806 +/- 2.009
Value (/100eV)	15.370 +/- 0.008	15.373 +/- 0.007



G-value: step-by-step

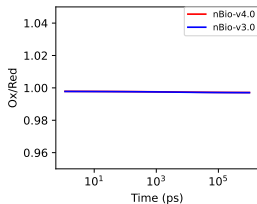
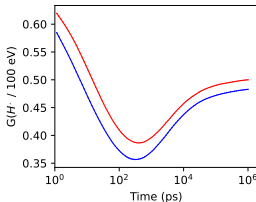
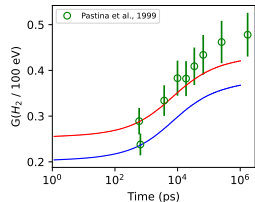
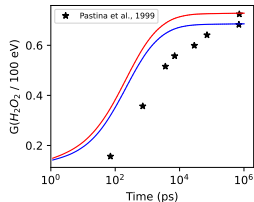
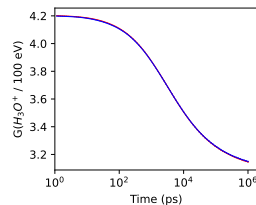
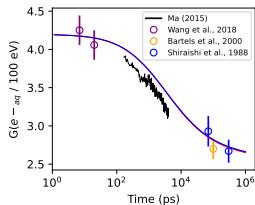
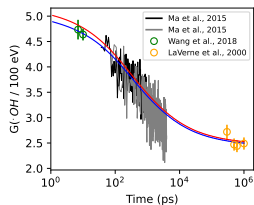


G-value vs. LET: step-by-step



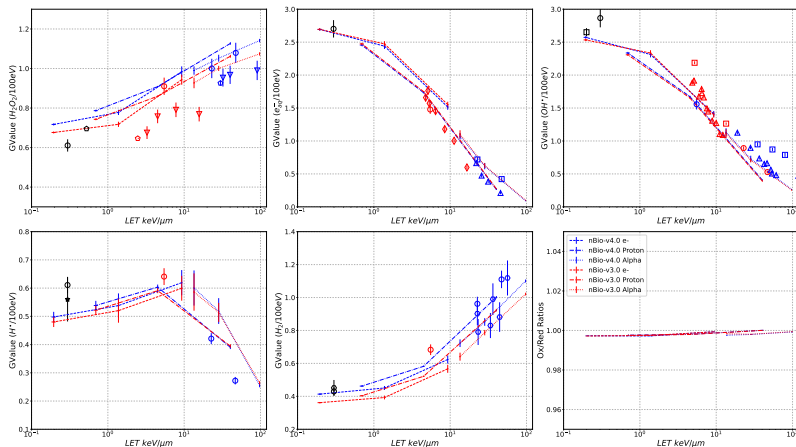
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	1769.253 +/- 36.755	1548.273 +/- 35.277

G-value: IRT



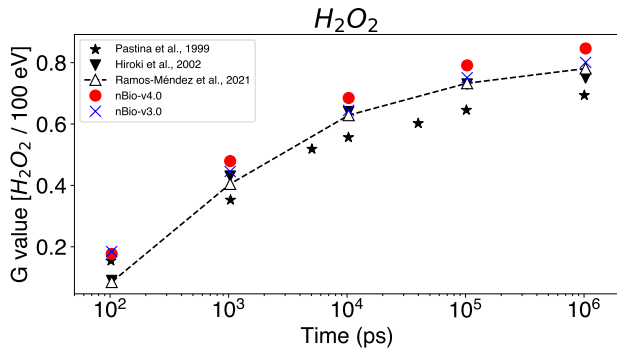
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	49.502 +/- 1.436	99.338 +/- 3.006

G-value vs. LET: IRT



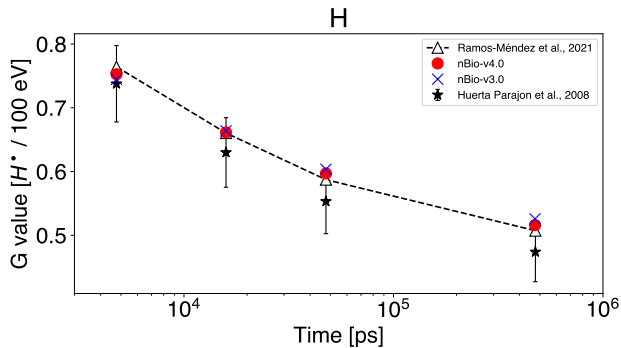
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	59.315 +/- 1.344	78.096 +/- 1.074

G-value of H_2O_2 : IRT



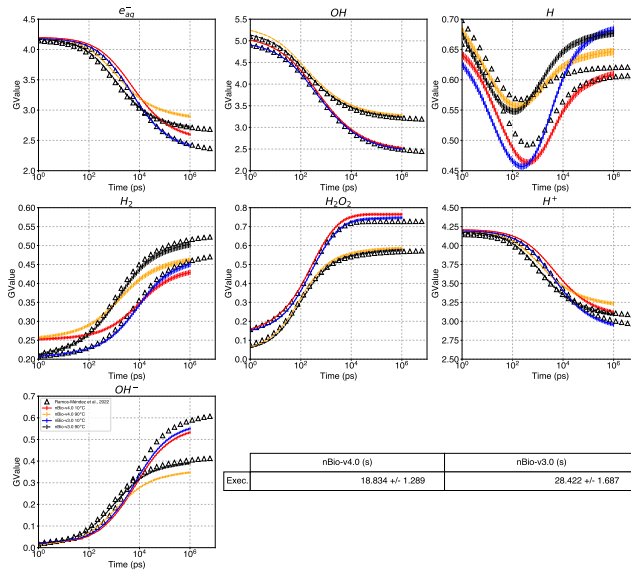
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	43.487 +/- 0.086	115.608 +/- 0.399

G-value of H: IRT



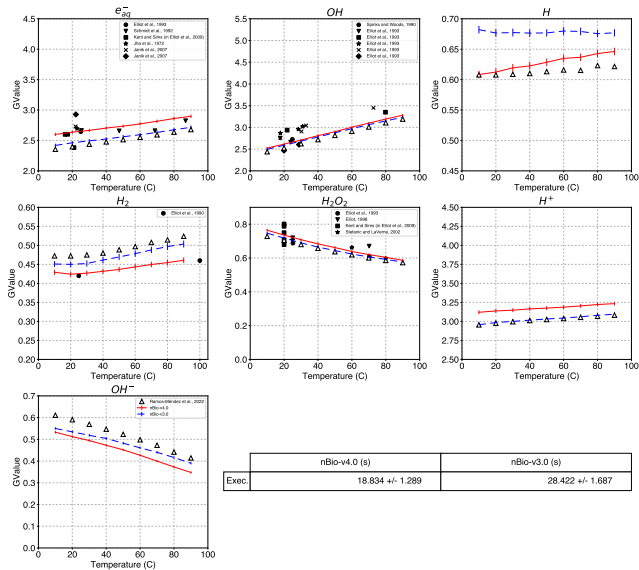
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	131.561 +/- 1.218	397.215 +/- 25.305

G-value and Temperature I: IRT

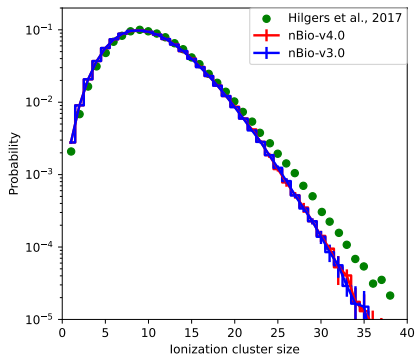


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	18.834 +/- 1.289	28.422 +/- 1.687

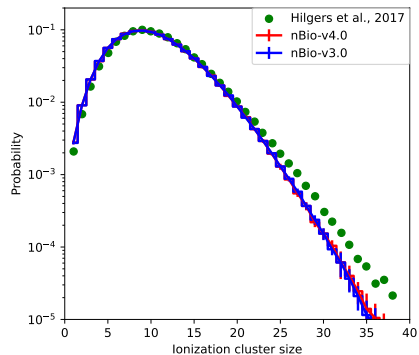
G-value and Temperature II: IRT



Nanodosimetry I: TsEmDNAPhysics and g4em-dna_opt2

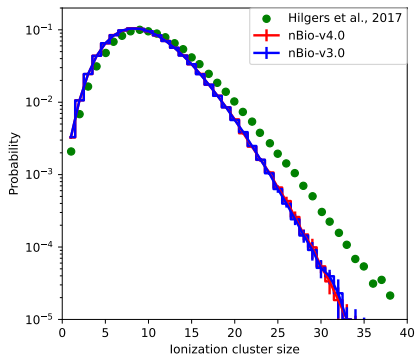


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	11579.9 +/- 15.1	14398.1 +/- 46.0

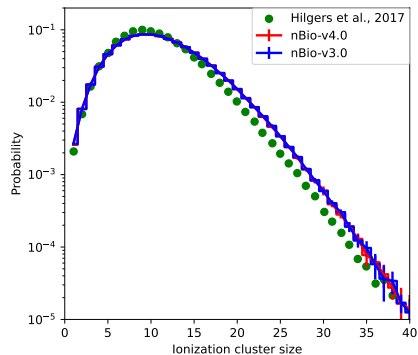


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	11425.1 +/- 52.8	9463.3 +/- 51.6

Nanodosimetry I: g4em-dna_opt4 and g4em-dna_opt6

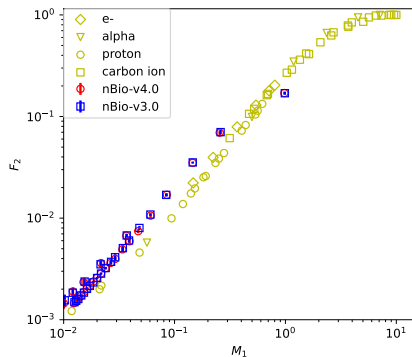


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	9512.8 +/- 20.7	7557.2 +/- 15.9

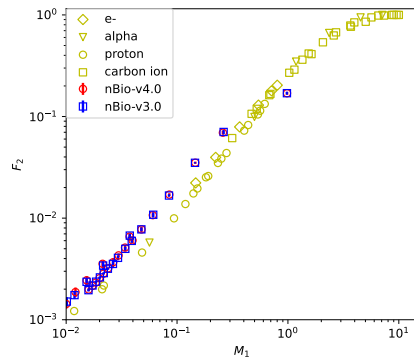


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	8176.1 +/- 29.0	6869.1 +/- 38.5

Nanodosimetry II: TsEmDNAPhysics and g4em-dna_opt2



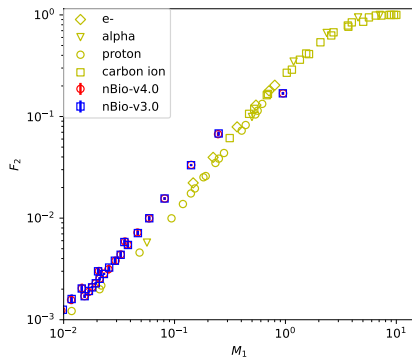
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	114.8 +/- 0.4	114.7 +/- 0.5



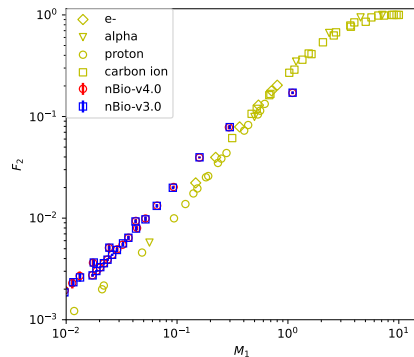
	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	90.8 +/- 0.5	90.7 +/- 0.4

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



	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	1617.2 +/- 1.9	1701.2 +/- 3.5

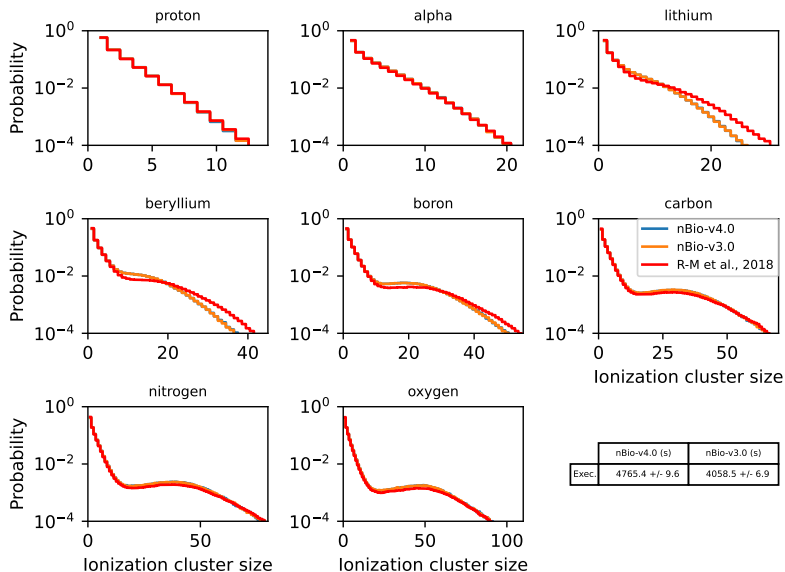


	nBio-v4.0 (s)	nBio-v3.0 (s)
Exec.	1175.0 +/- 2.1	1930.9 +/- 4.9



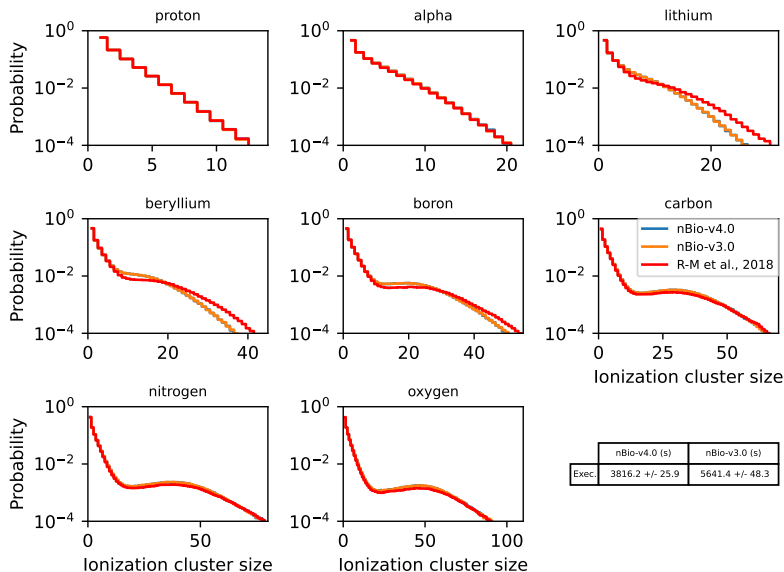
Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry III: TsEmDNAPhysics



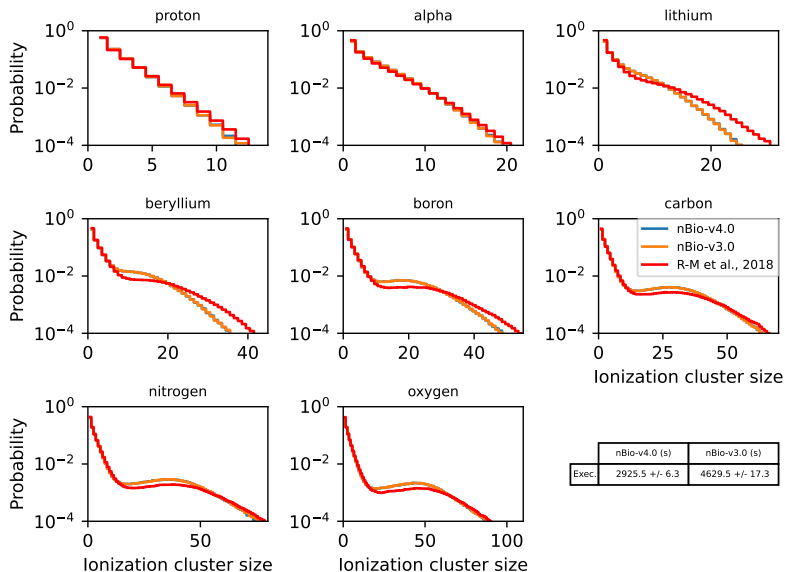
Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol.* 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee

Nanodosimetry III: g4em-dna_opt2



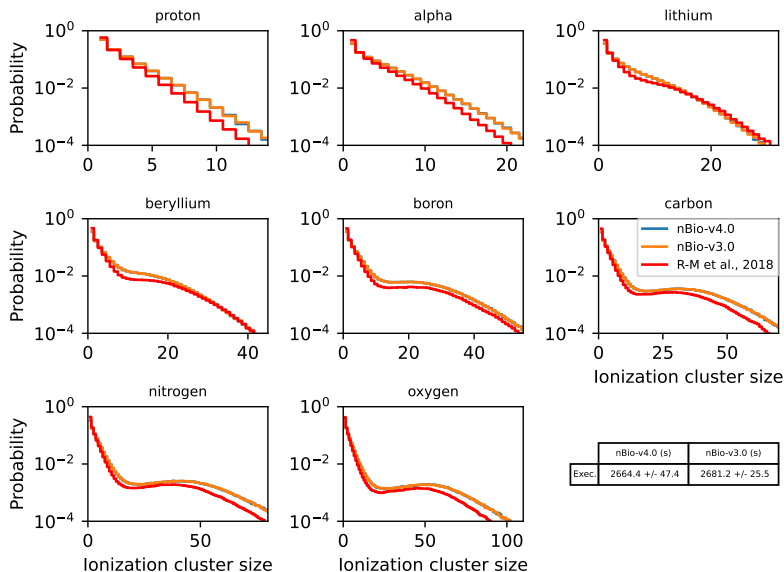
Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol.* 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee

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