An *in-silico* study of cancer cell survival and spatial distribution within a 3D microenvironment

Supplementary figures and tables.

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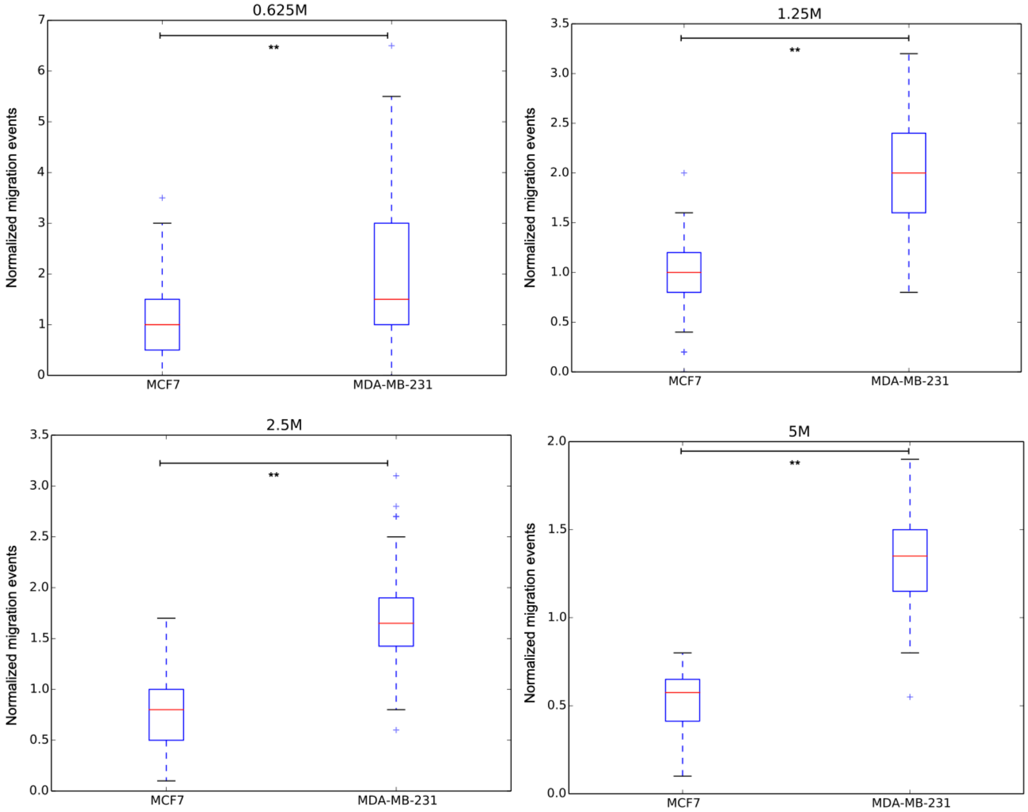

Figure 1: Distribution of the number of migratory events normalized by the initial cell density. For all cardinalities MDA-MB-231 cells migrate about twice as much when compared with MCF7 cells.

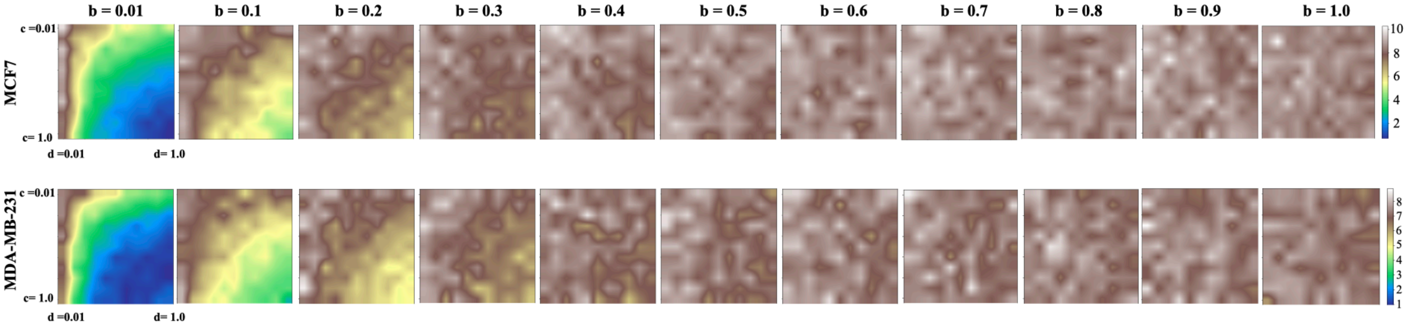

Figure 2: Errors corresponding to the wide range parameters sets. A bilinear interpolation has been applied to smooth the transitions between different values.

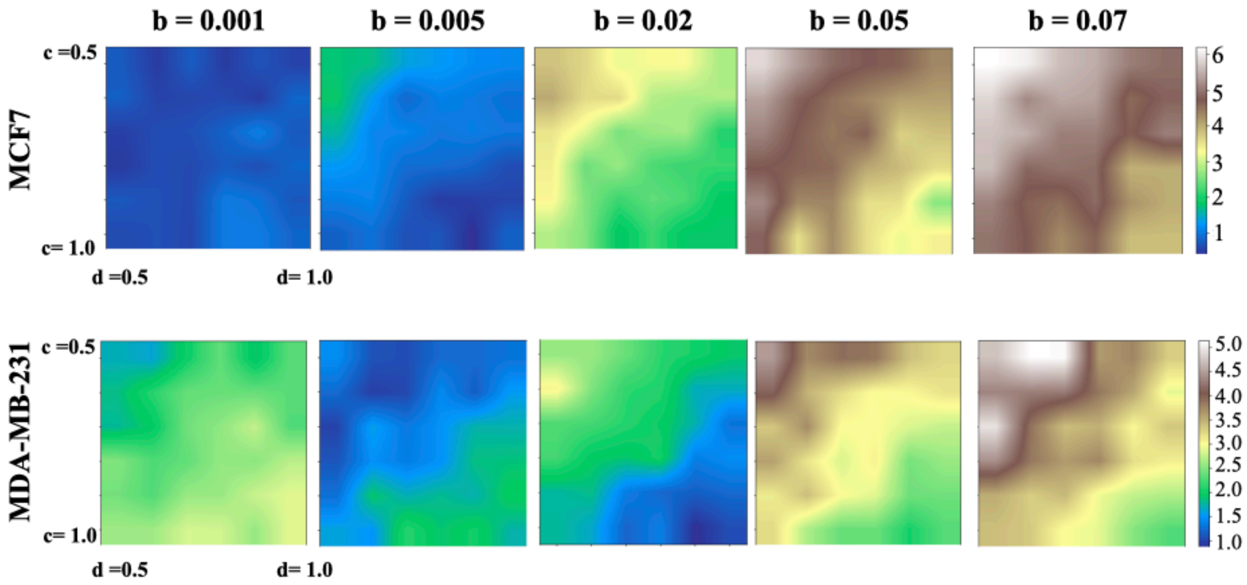

Figure 3: Errors corresponding to the narrow range parameters sets. A bilinear interpolation has been applied to smooth the transitions between different values.

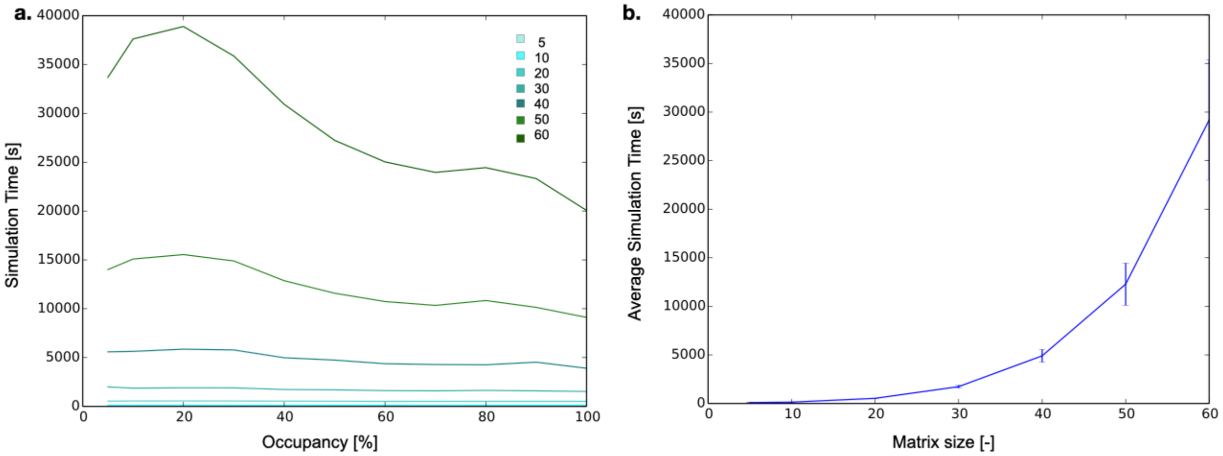

Figure 4: Computational time. In a. the simulation time associated with each combination of scaffold size and occupancy is reported, while in b. the average simulation time for each matrix size is shown (data reported as mean and standard deviation).

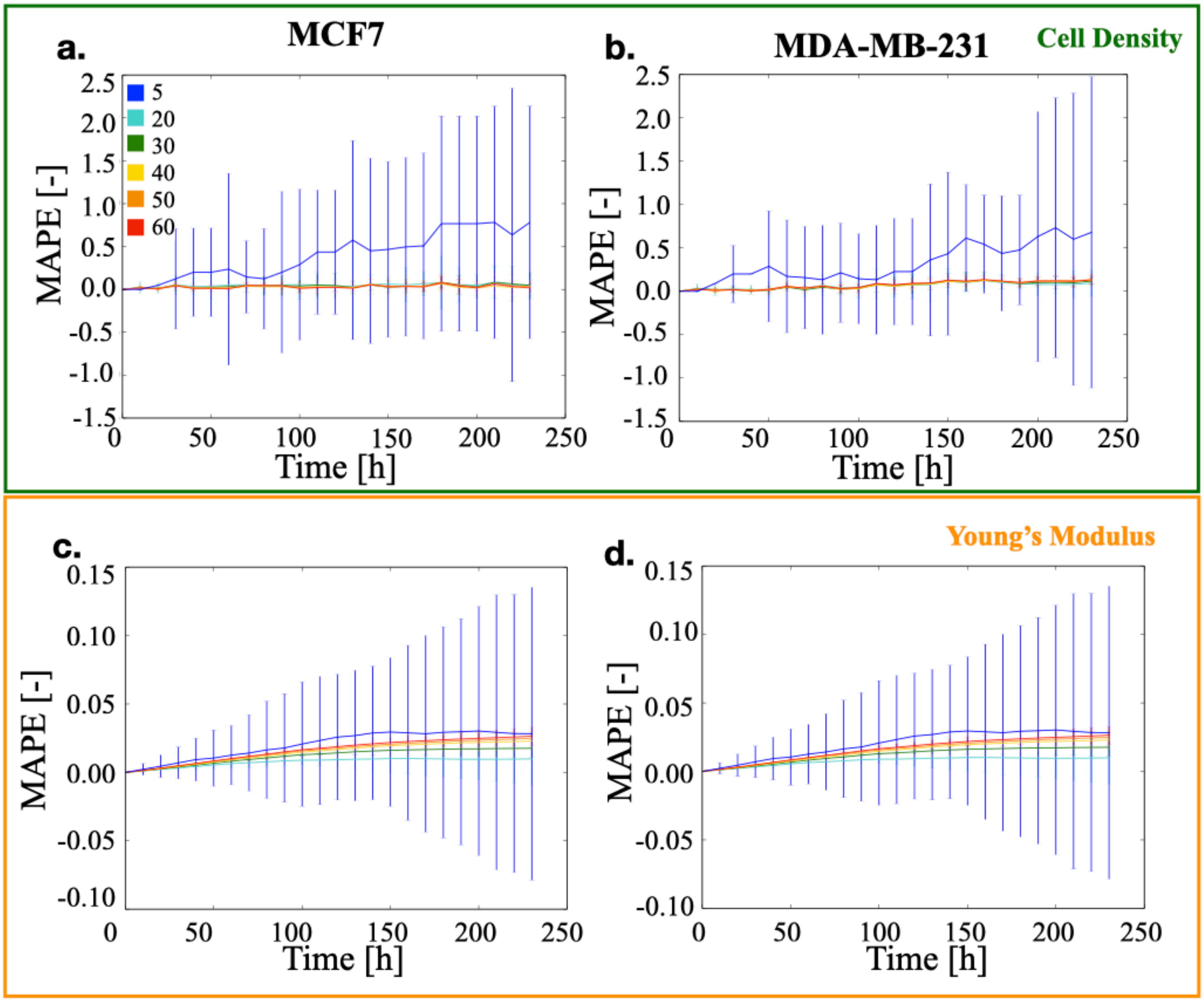

Figure 5: Analysis of the influence of the lattice size on the simulation's outputs. For graphical clarity only one in ten points is reported.

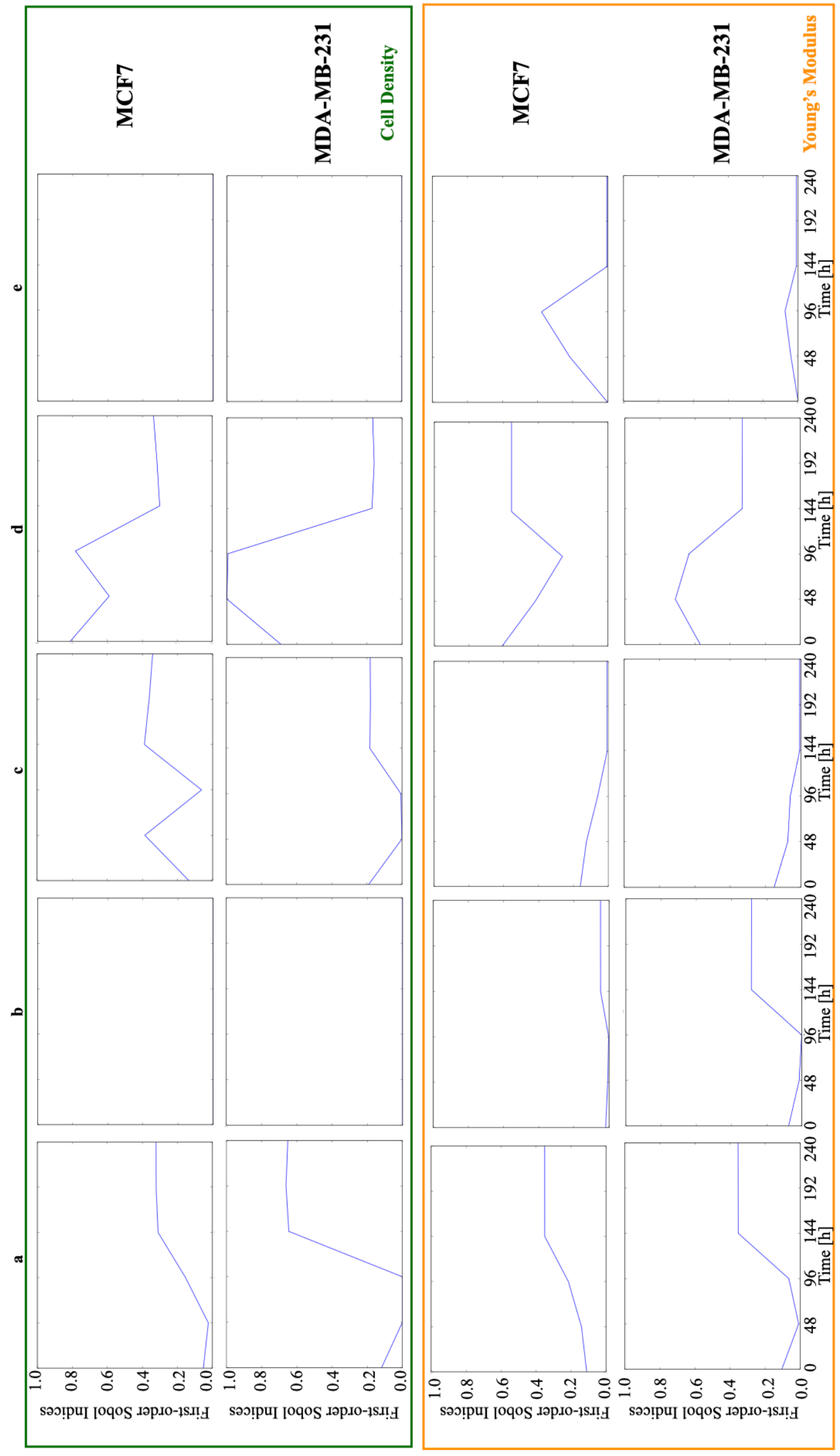

Figure 6: First order Sobol indices computed for each behavioural parameter and output. Both the x and the y axis are shared among all panels.

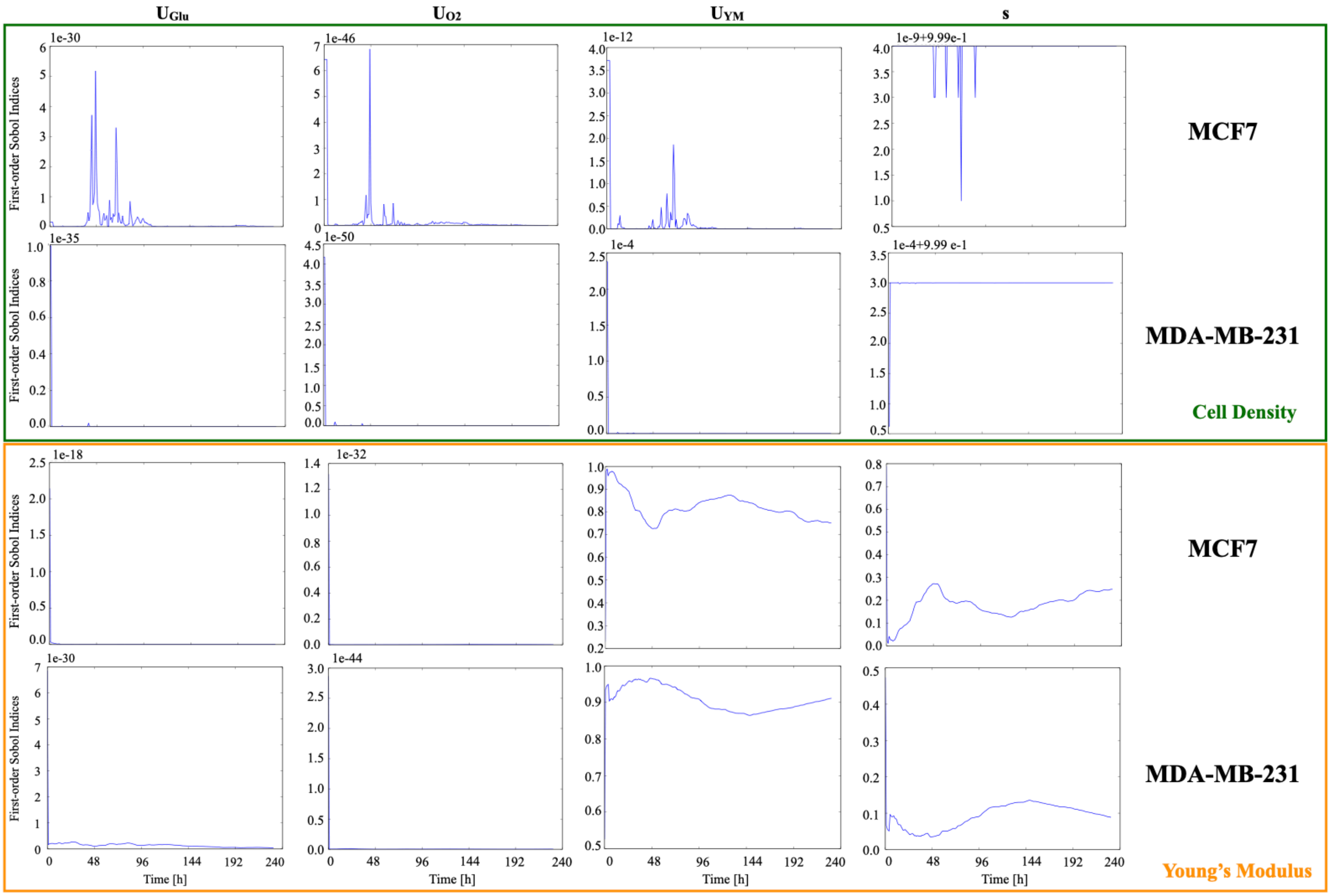

Figure 7: First order Sobol indices computed for each environmental parameter and output. The x axis is shared among all panels.

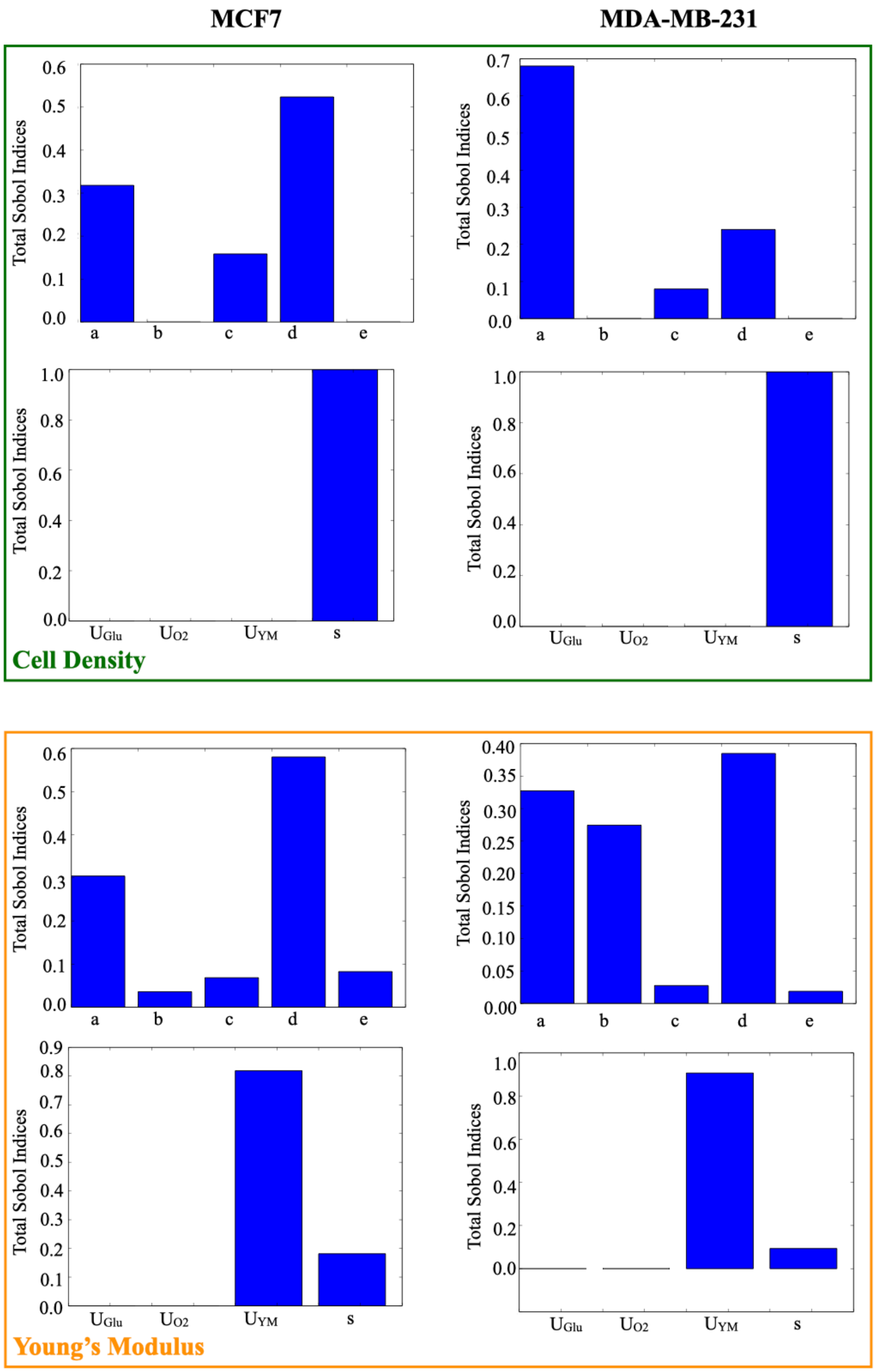

Figure 8: Total average Sobol indices computed for each environmental parameter and output.

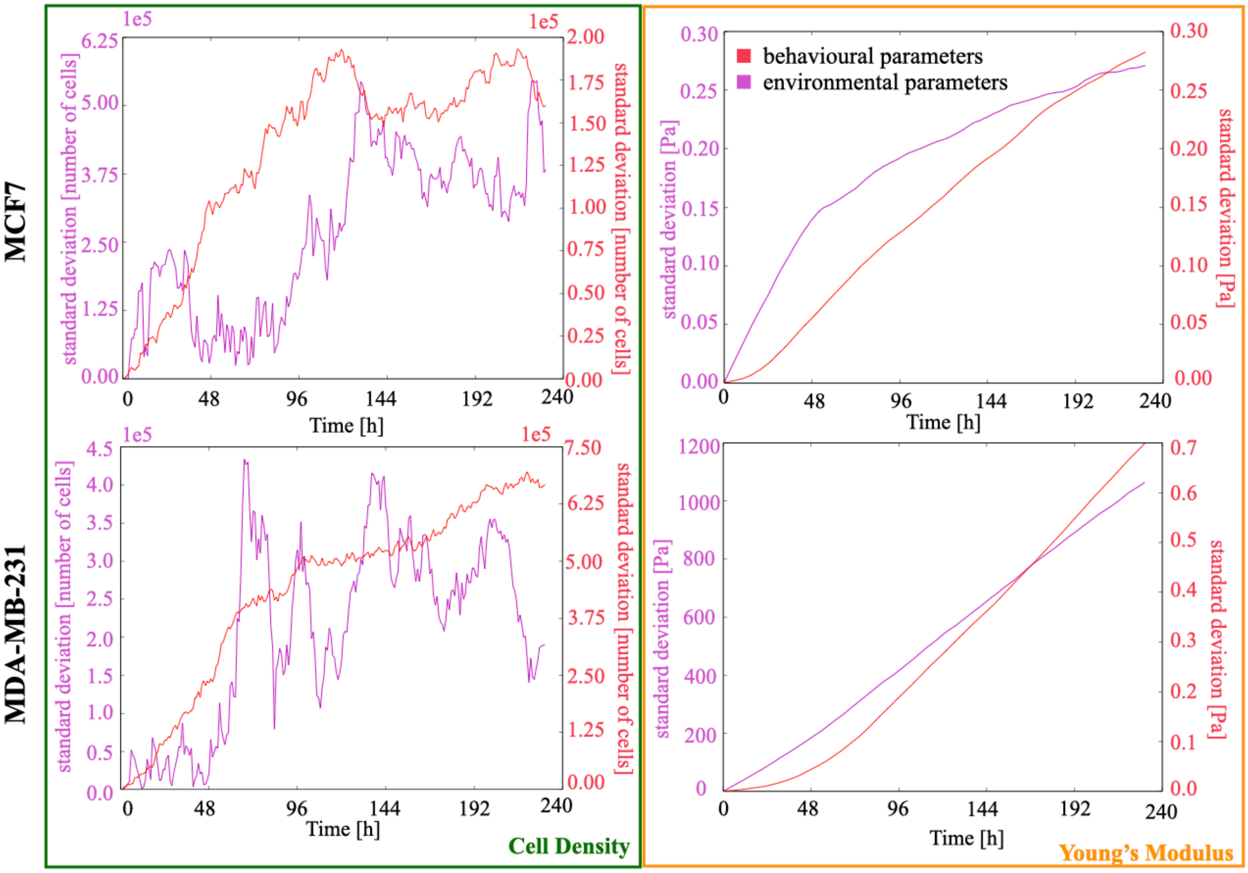

Figure 9: Standard deviation due to the variation of the parameters involved in the sensitivity analysis.

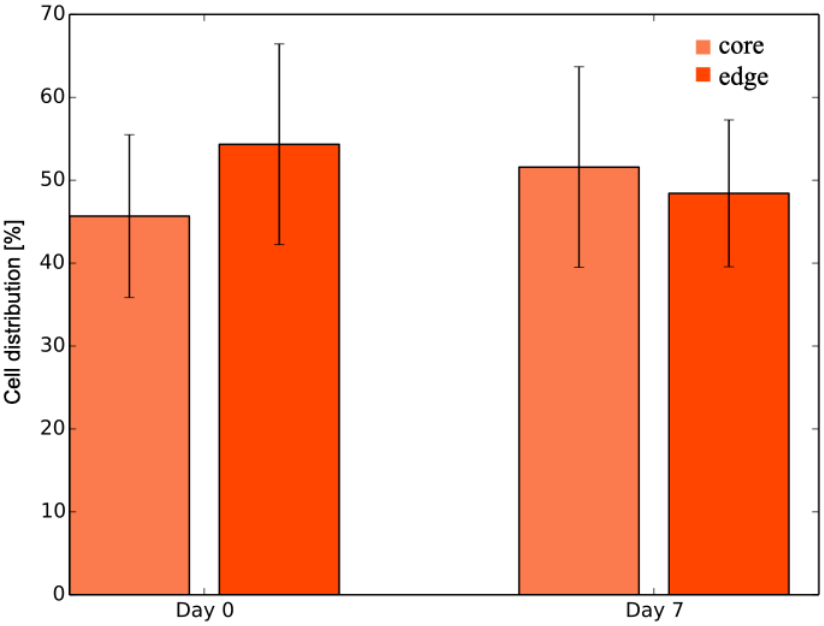

Figure 10: Experimental cell distribution within the scaffold. A starting population of 1M cells reduced importantly the difference in cell density between core and edge regions measured in [8]. Indeed at the end of the experiment the cell population is approximately uniformly distributed within the whole structure.

Coefficient	MCF 7	MDA-MB-231
a	0.38	0.44
b	0.005	0.02
c	1	1
d	0.9	0.9
e	0.008	0.01
f	0.000003	0.003

Table 1: Values of the coefficients used for the simulation of MCF7 and MDA-MB-231 cells

Parameter	value
CPU	32 Intel(R) Xeon(R) CPU E5-2640 v2 @ 2.00GHz
RAM	65GB

Table 2: Specifications of the workstation used for the SALSA simulations

Parameter	Value
Side	1 cm
Layers	10
Initial population composition	all proliferant cells
Initial population cardinality	625 K, 1.25 M, 2.5 M, 5M
Iteration	240
Media replace frequency	1 day

Table 3: Parameters of the virtual scaffold. The complete configuration files are available, together with SALSA source code, at http://www.mcbeng.it/en/category/software.html