CONSTRUCTION OF 3D PRESYNAPTIC BOUTON MODEL

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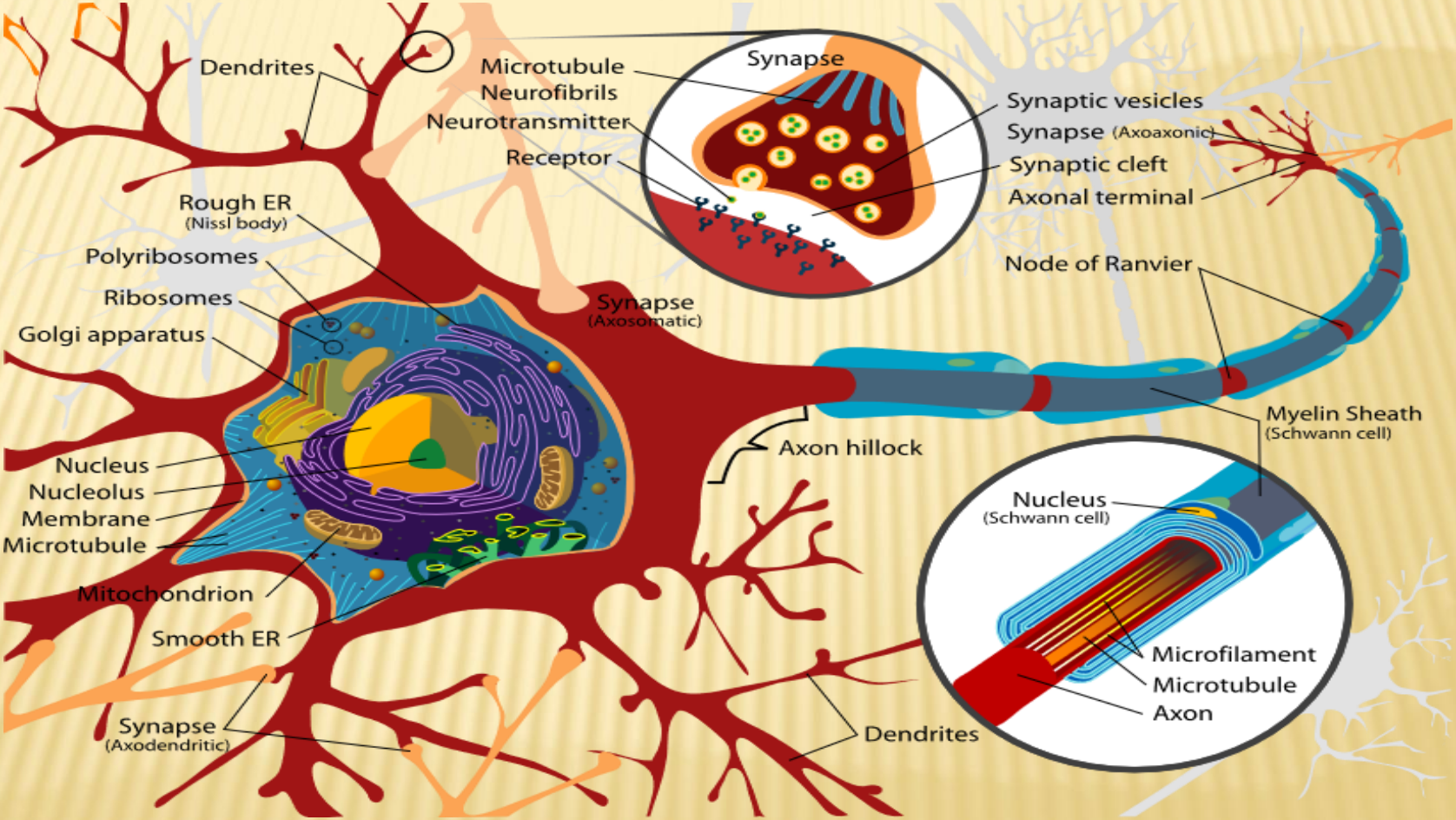
Subject of research (1)

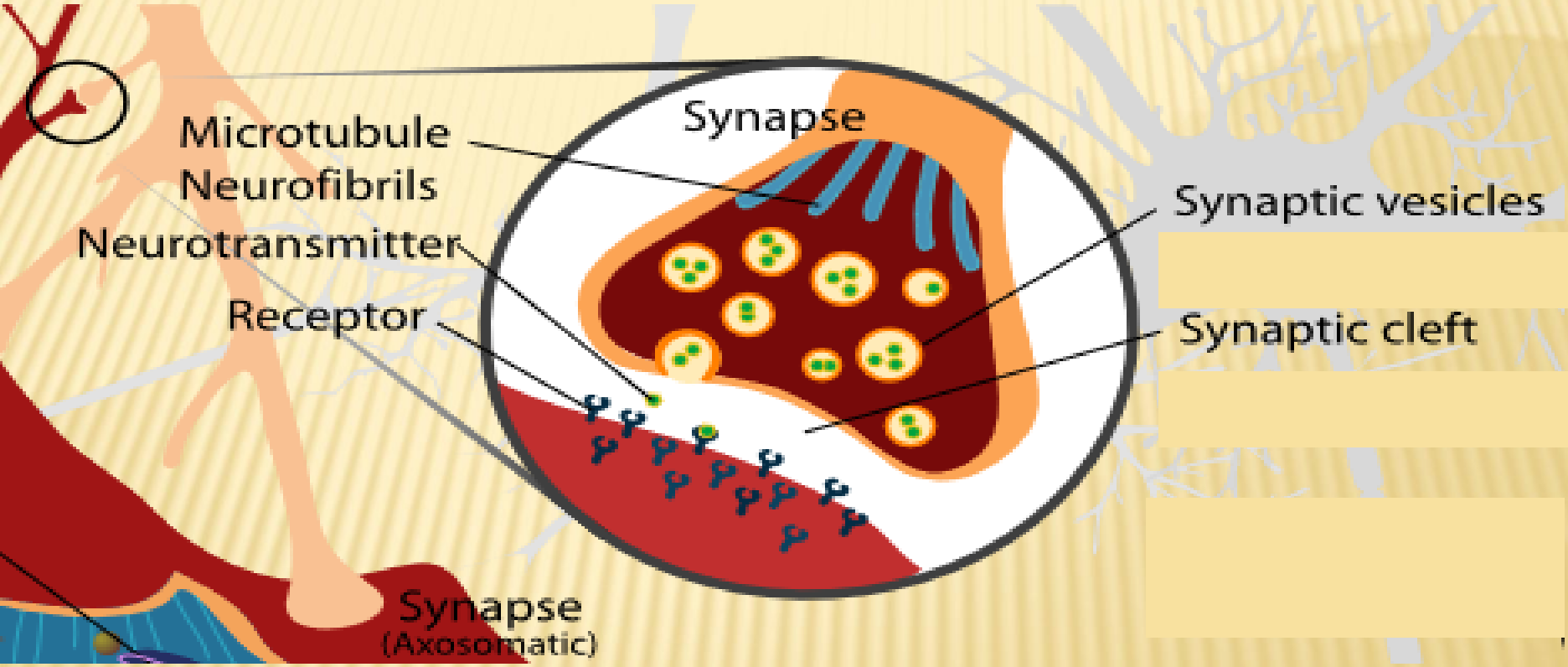
Brain → neuron → synapse → presynaptic bouton



https://en.wikipedia.org/wiki/Neuron#/media/File:Complete_neuron_cell_diagram_en.svg

Subject of research (2)

presynaptic bouton



*REMARK: The bouton may contain a **mitochondrion** as well.*

https://en.wikipedia.org/wiki/Neuron#/media/File:Complete_neuron_cell_diagram_en.svg

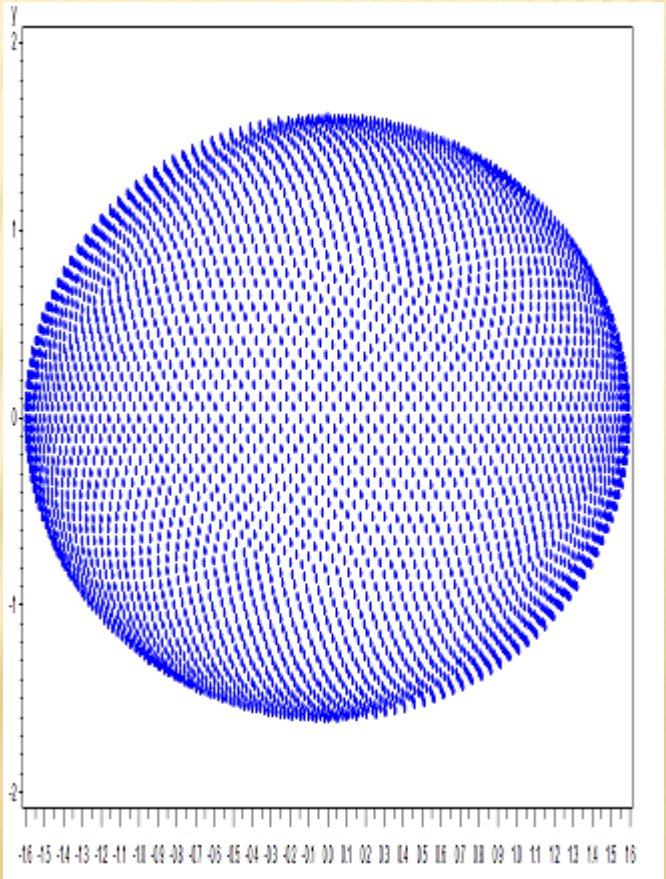
Subject of research (2)

The purpose of the work was to construct a realistic 3D model of the terminal bouton for efficient simulation of neurotransmitter (**NT**) flow

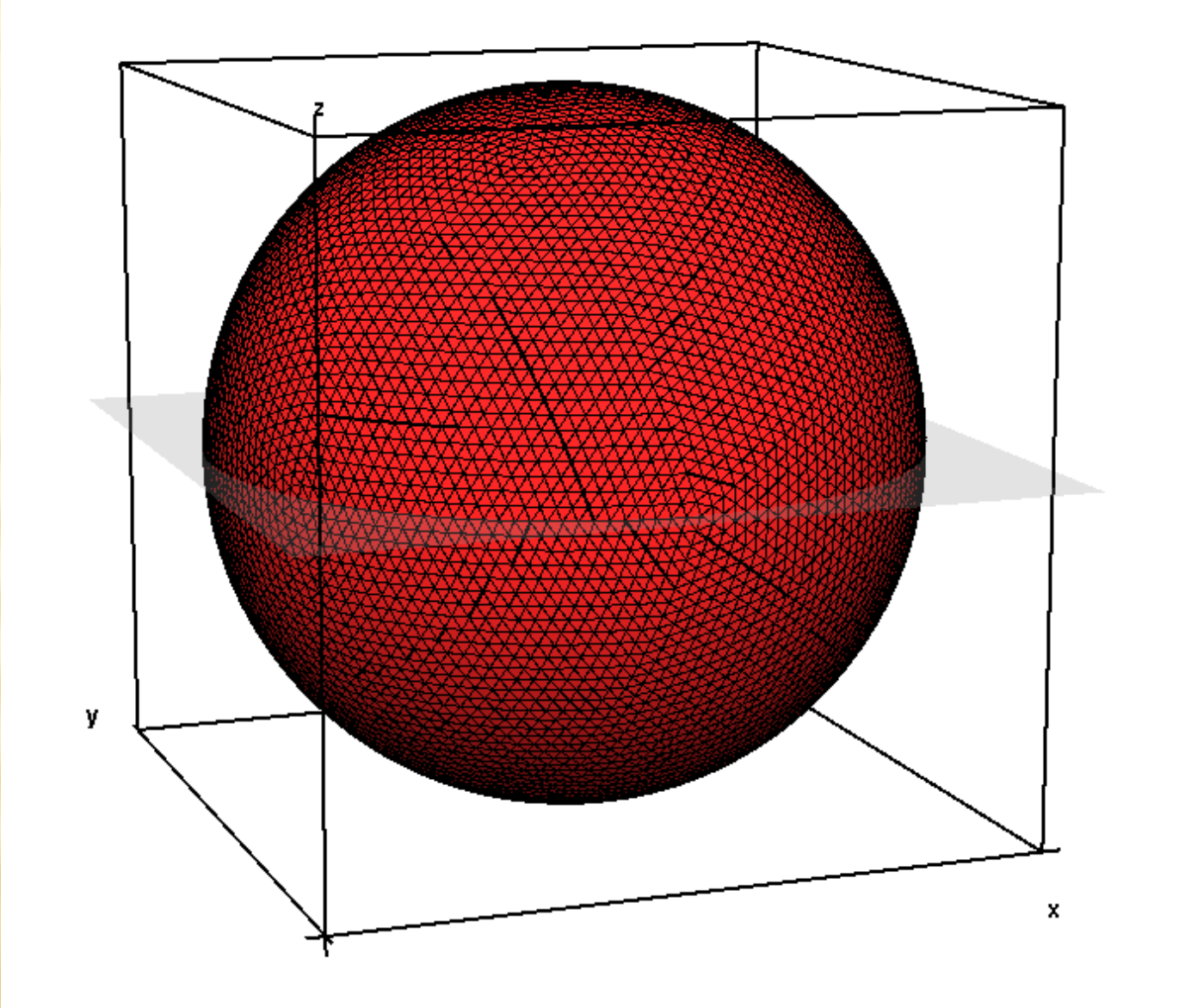
3D bouton model – geosphere - parameters

Design of the geospherical model

1. „Geosphere” wireframe model of the bouton (Ω)
    - Radius – 1.6 units (nanometers)



The simplest model – geosphere (1)



The simplest model – geosphere (2)

First model – geosphere (axes: x, y, z)

7842 vertices, 15680 faces

Center – (0,0,0) – error < 10^{-10}

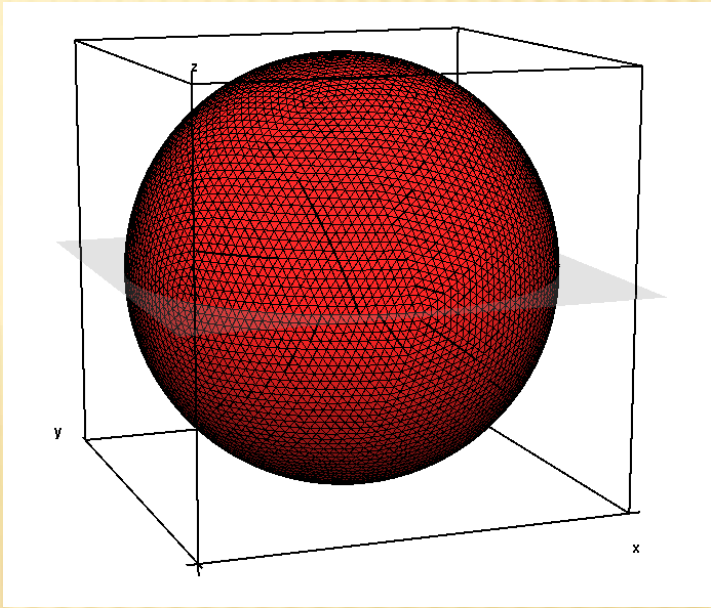
R=1.5999991µm (error < $2 \cdot 10^{-9}$)

Surface (theoretical, for R=1.6)≈32.1699

Surface (real) S≈32.1574

(S>99.96% of the theoretical value)

relative error < 0.0004 (0.04%).



TetView®

a) The file in .OBJ format => 2 input files for SAS(R) package (Python program was used for transformation)

First file – surface points; Second file – faces (triangles)

b) The file in .OBJ format => input file for SAS(R) package

The simplest model – geosphere (3)

Characteristics of 2D surface mesh (reference for next models)

Quality measures of the input mesh triangles:

a) perimeter / square root of the surface (**P_TO_S2**)

b) the longest edge / the radius of the inscribed circle (**E_TO_R**)

c) the aspect ratio = the longest edge / the shortest altitude (**E_TO_A**)

used for example in TetGen(R) program by Hang Si (2013)

The ideal values of these parameters (equilateral triangle):

P_TO_S2=2x($27^{1/4}$)≈4.559014; E_TO_R=2*($3^{1/2}$)≈3.4641; E_TO_A=2/($3^{1/2}$)≈1.1547

For the real mesh:

The minimum value: P_TO_S2≈4.559034; E_TO_R≈3.4683; E_TO_A≈1.1575

The mean values: P_TO_S2≈4.5769; E_TO_R≈3.6886; E_TO_A≈1.2999

The maximal values:P_TO_S2≈**4.6104**; E_TO_R≈**3.9245**; E_TO_A ≈**1.4527**

[24] Si H., 2013. TetGen, towards a quality tetrahedral mesh generator. WIAS Preprint No. 1762, 2013. submitted to ACM TOMS

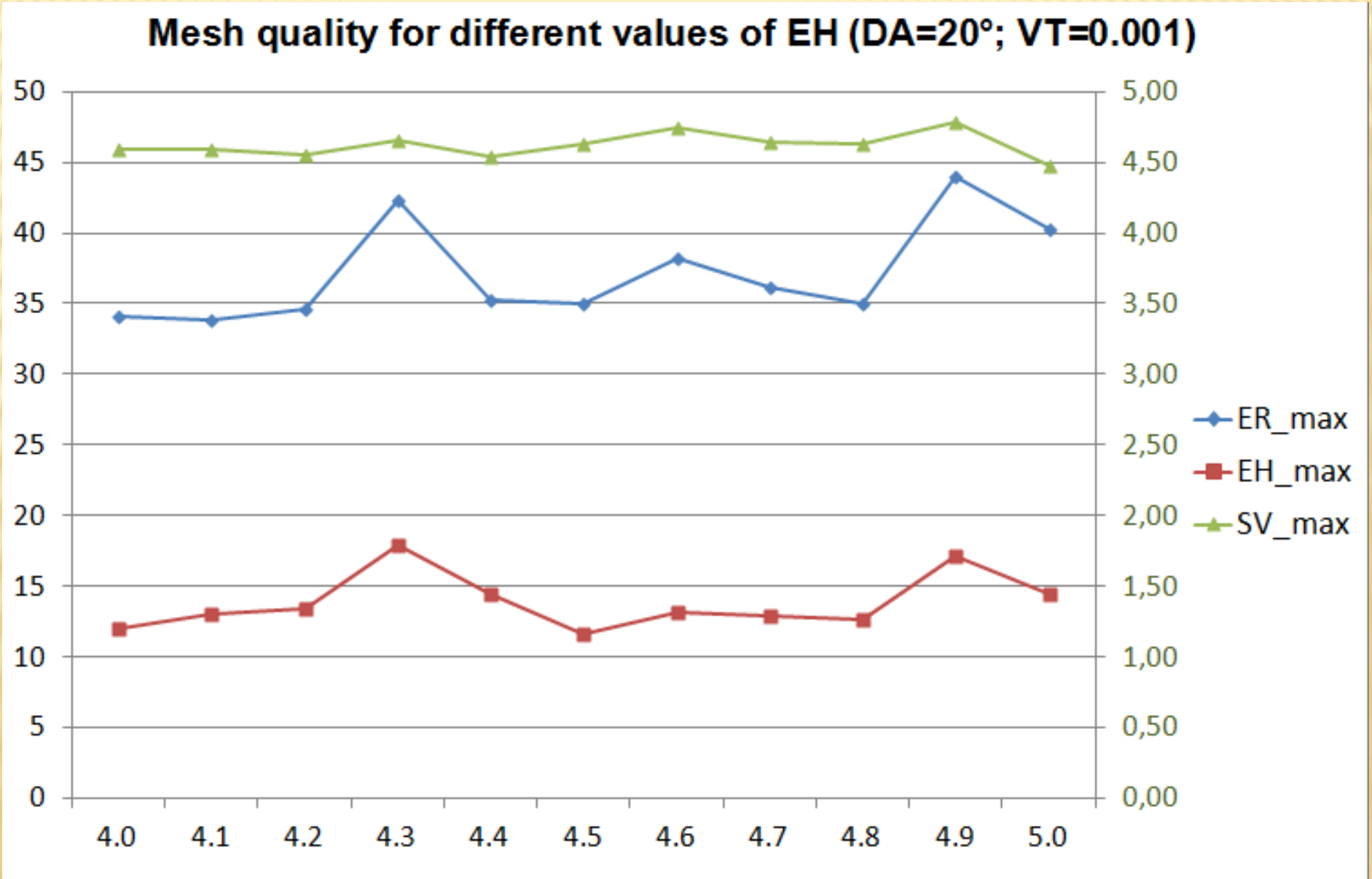
3D bouton model – geosphere – mesh quality

Mesh quality measures of the **tetrahedron**:

E/R, ER, E_TO_R – ratio of the longest edge to the radius of the inscribed circle, range: from less than 5 to over 40
E/H, EH, E_TO_H,– ratio of the longest edge to the shortest altitude, range: from less than 1.23 to over 17.95
S/V, SV, S_TO_V – ratio of square root of the surface to the cubic root of the volume, range: from less than 2,685 to over 4,785
ER – defined by Ciarlet (1978)
EH – used by Si (2015)
SV – experimental (introduced here)
Mesh size (mesh density):
NO_VER – number of vertices
NO_TET – number of tetrahedra
Ideal values: ER=$2x6^{0,5}\approx4.899$; EH=$0.5x6^{0,5}\approx1.224745$; SV=$3^{1/4}x72^{1/6}\approx2.684$

Ciarlet P.G., The Finite Element Method for Elliptic Problems. North Holland, 1978.
Si H., 2015. TetGen, a Delaunay-based quality tetrahedral mesh generator. ACM Transactions on Mathematical Software, 41.

3D bouton model – geosphere – mesh quality



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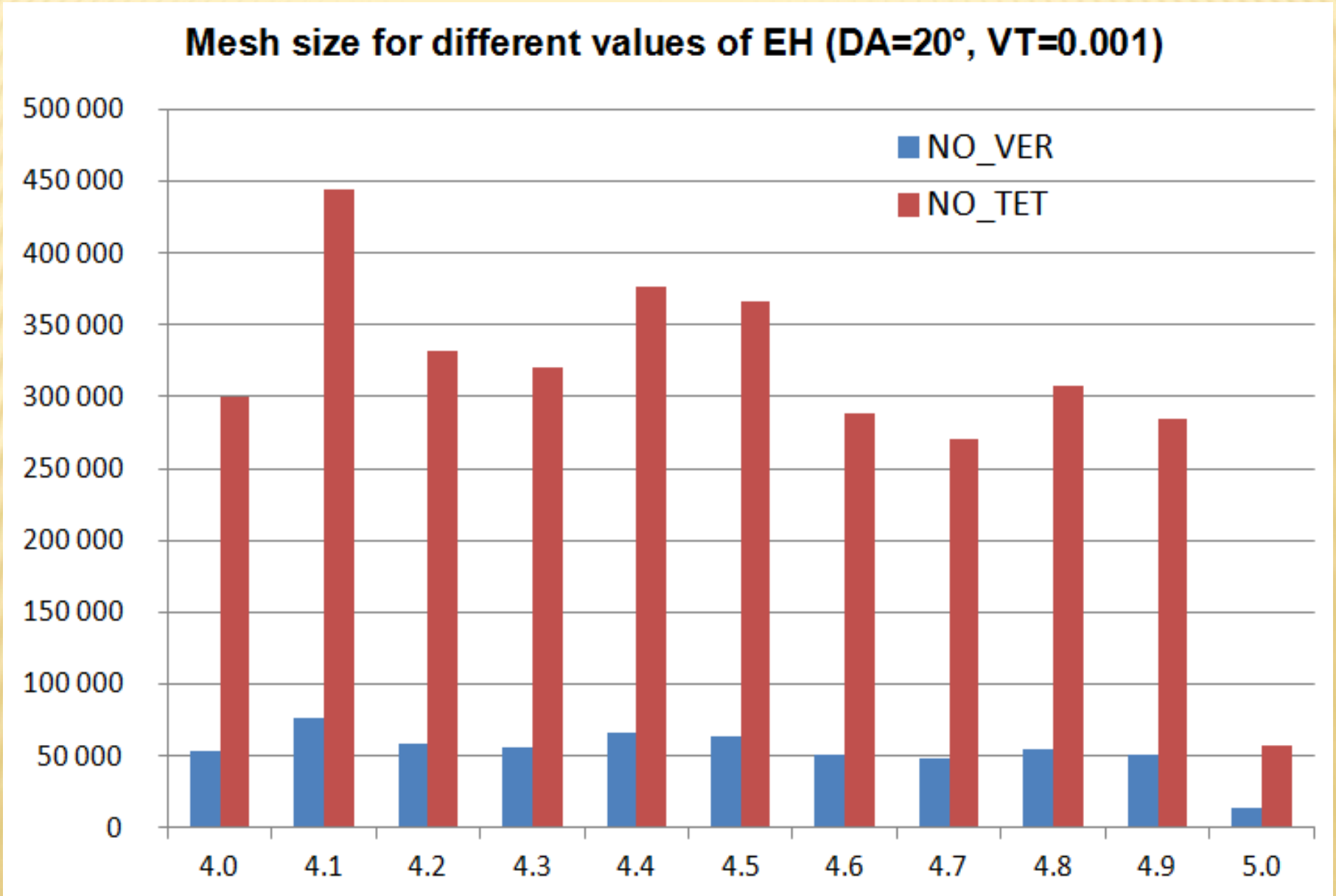

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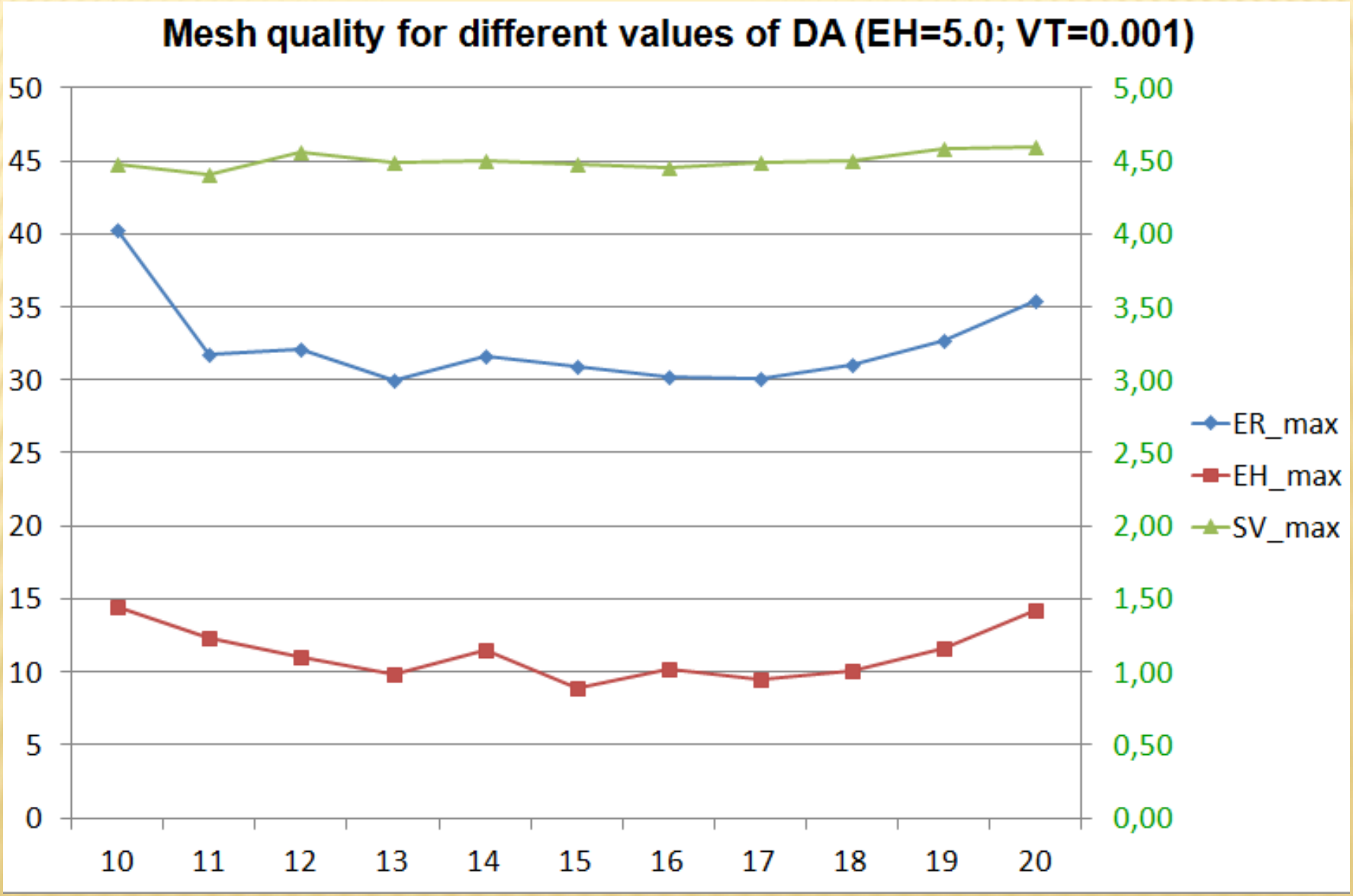

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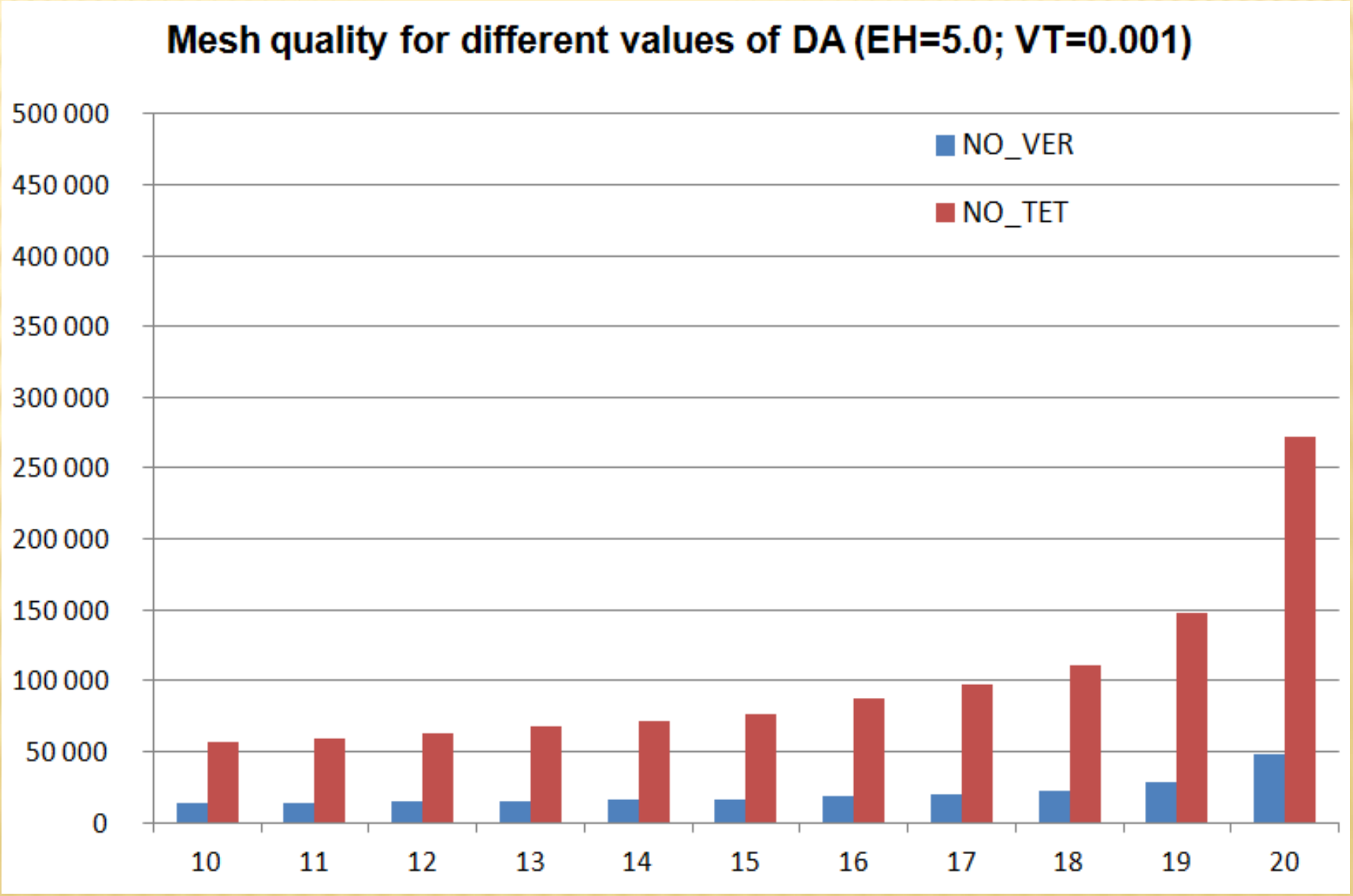
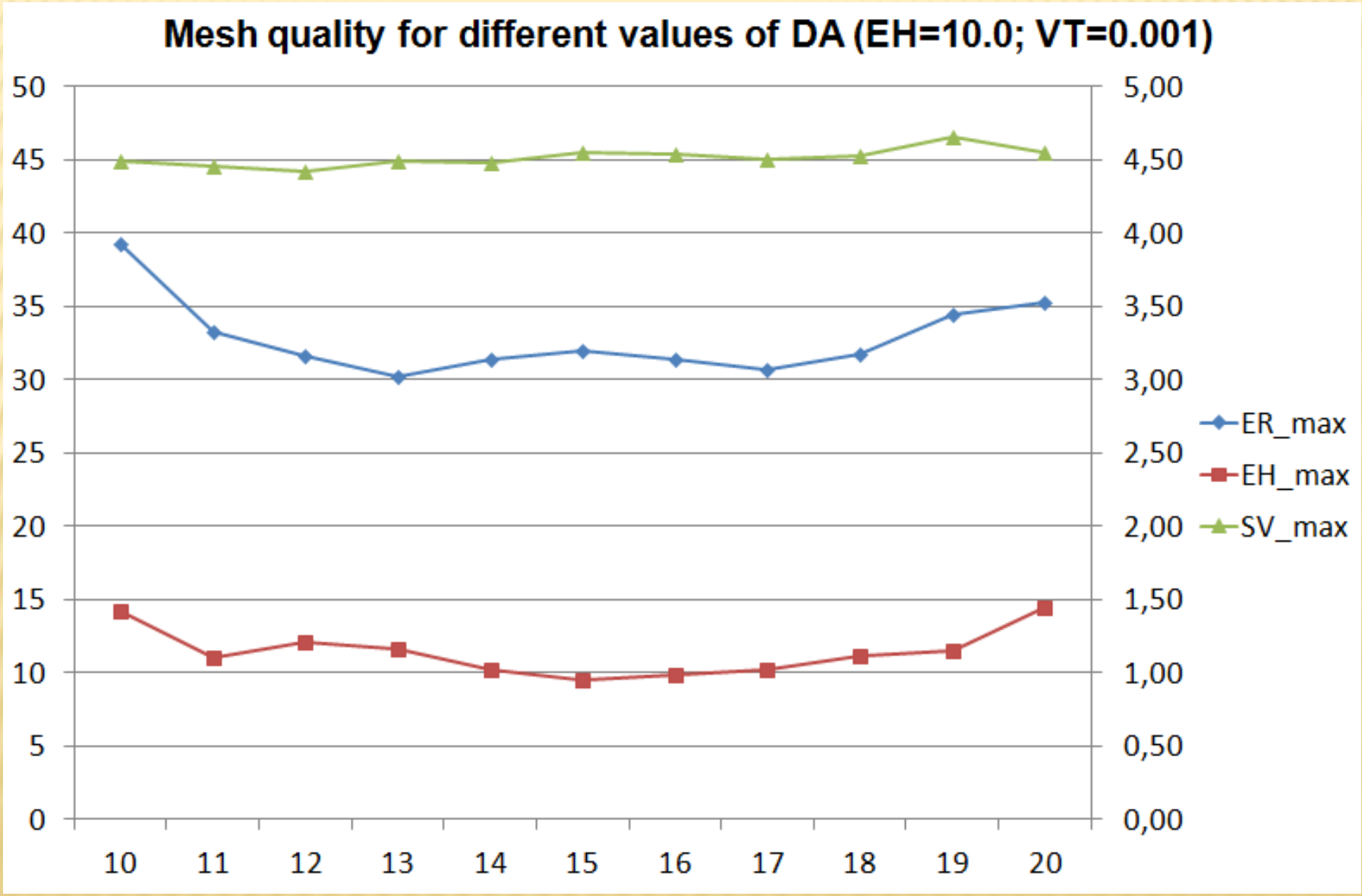


3D bouton model – geosphere – mesh quality



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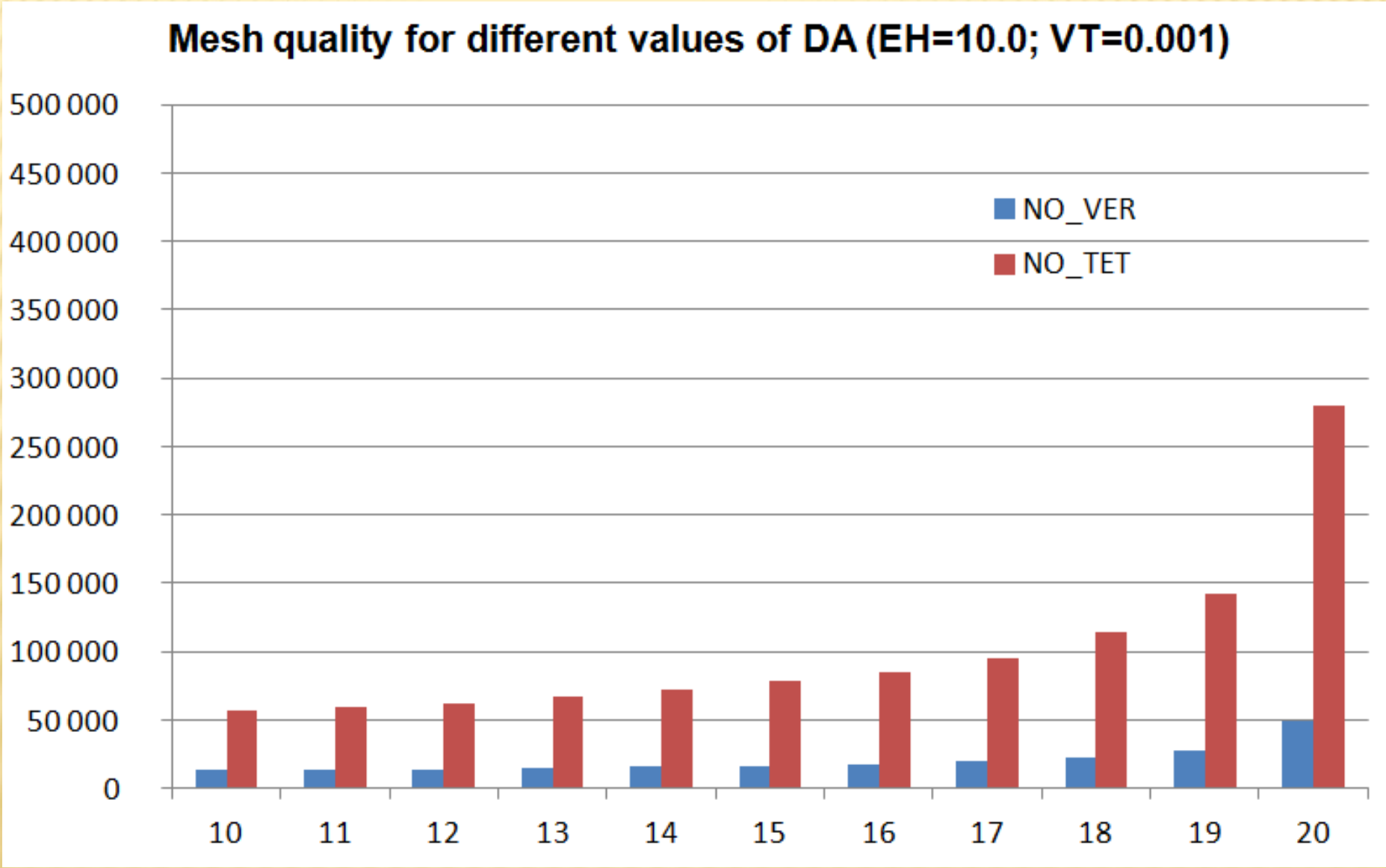
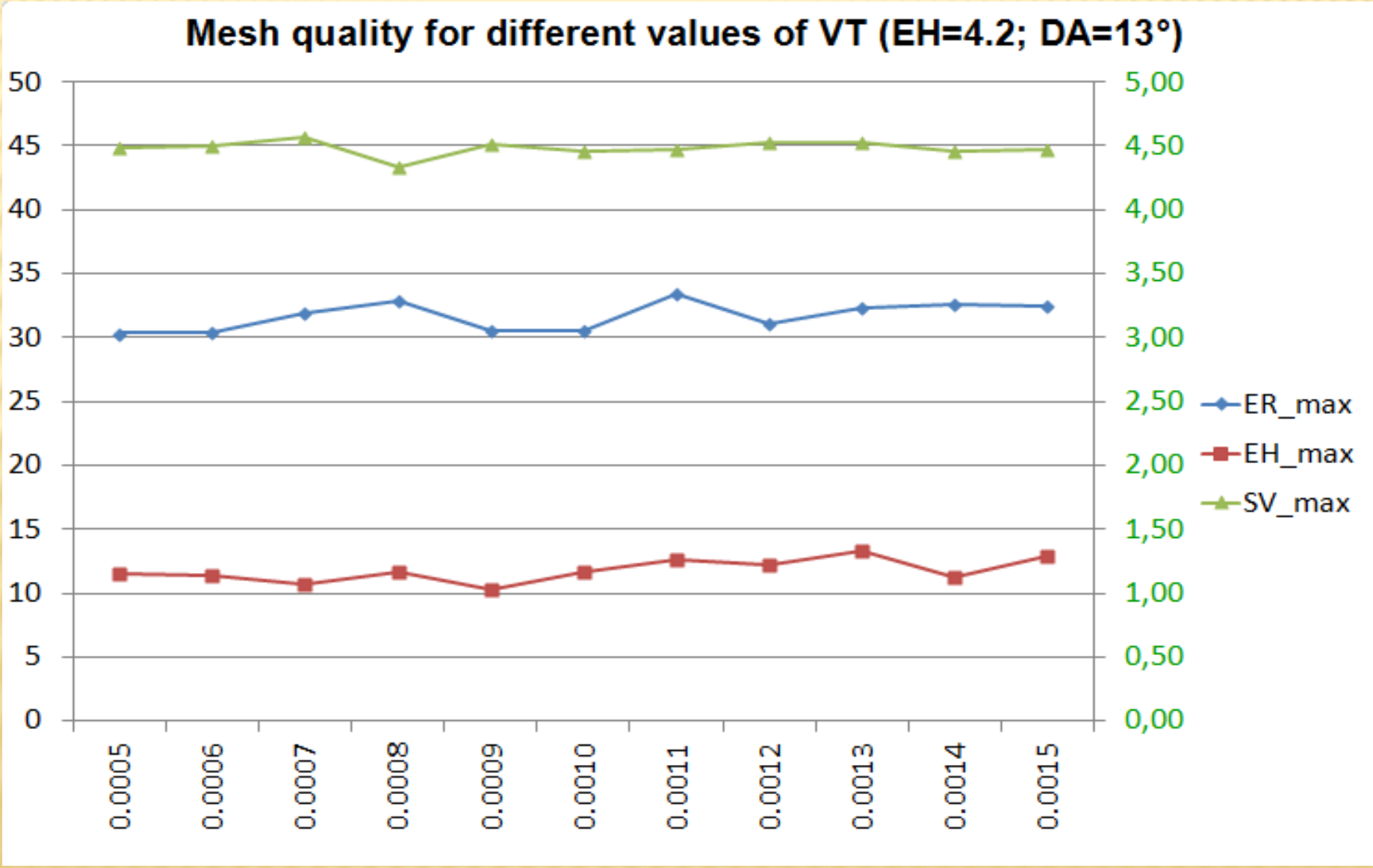
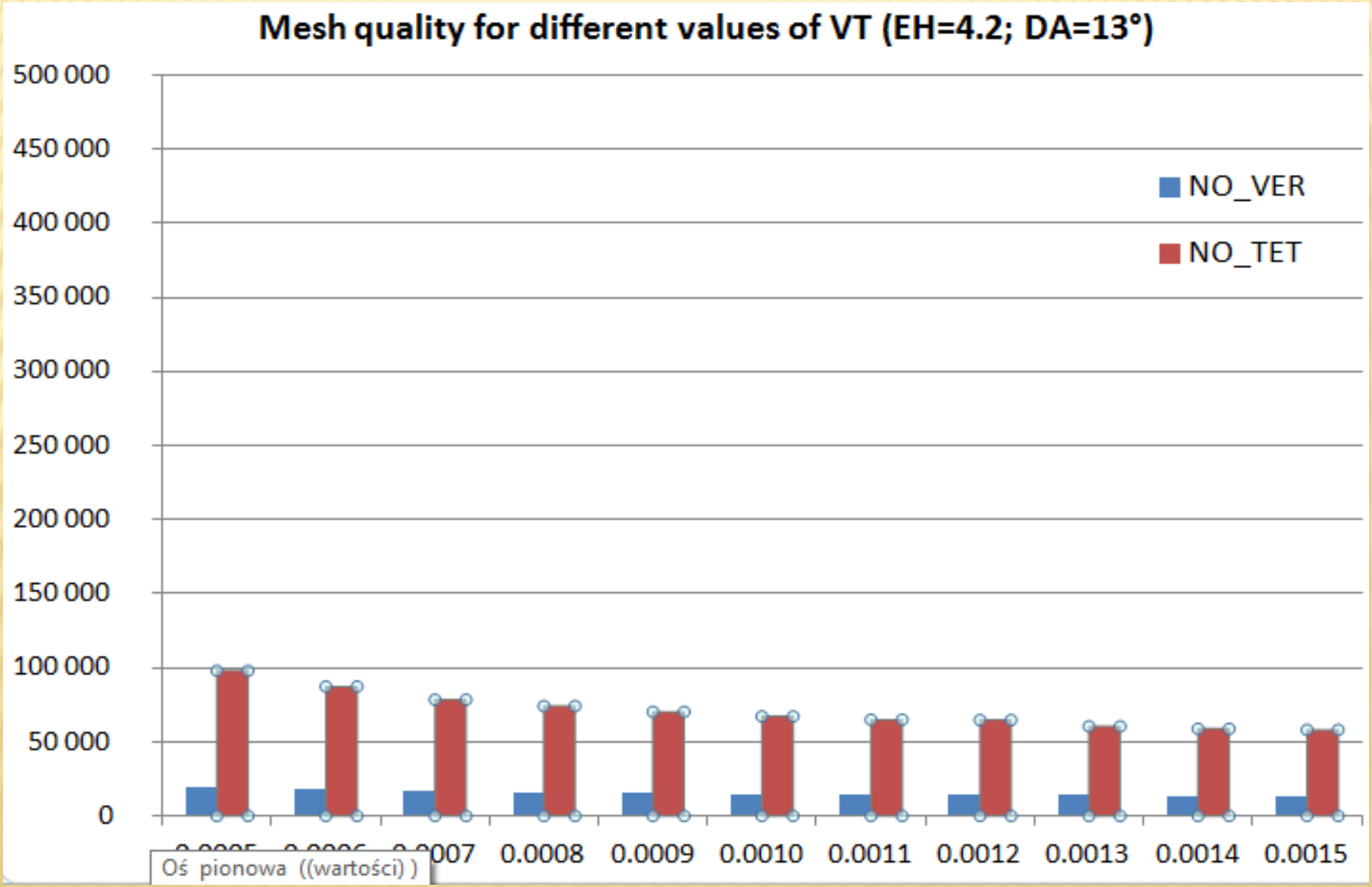


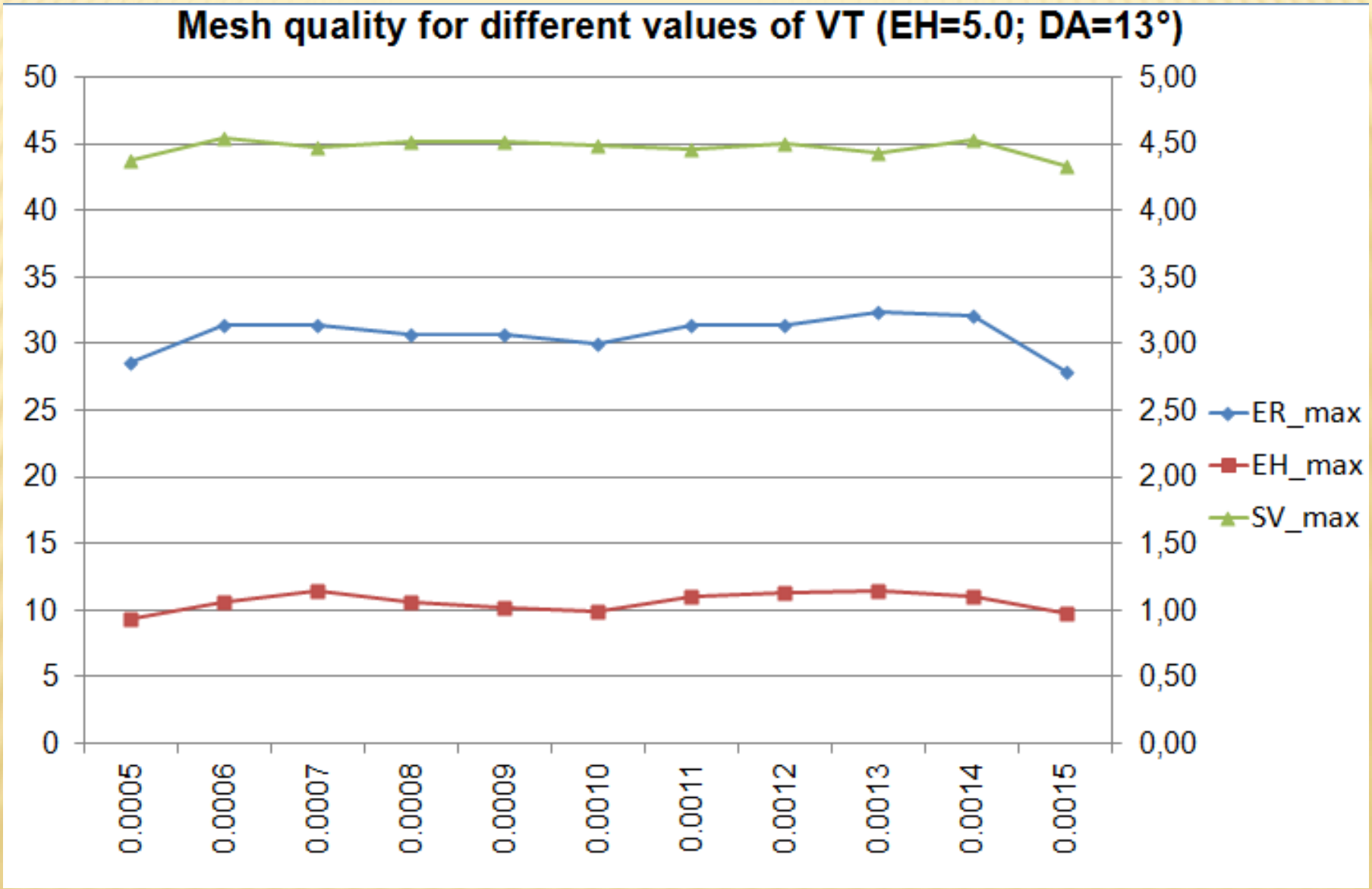
3D bouton model – geosphere – mesh quality



3D bouton model – geosphere – mesh quality



3D bouton model – geosphere – mesh quality



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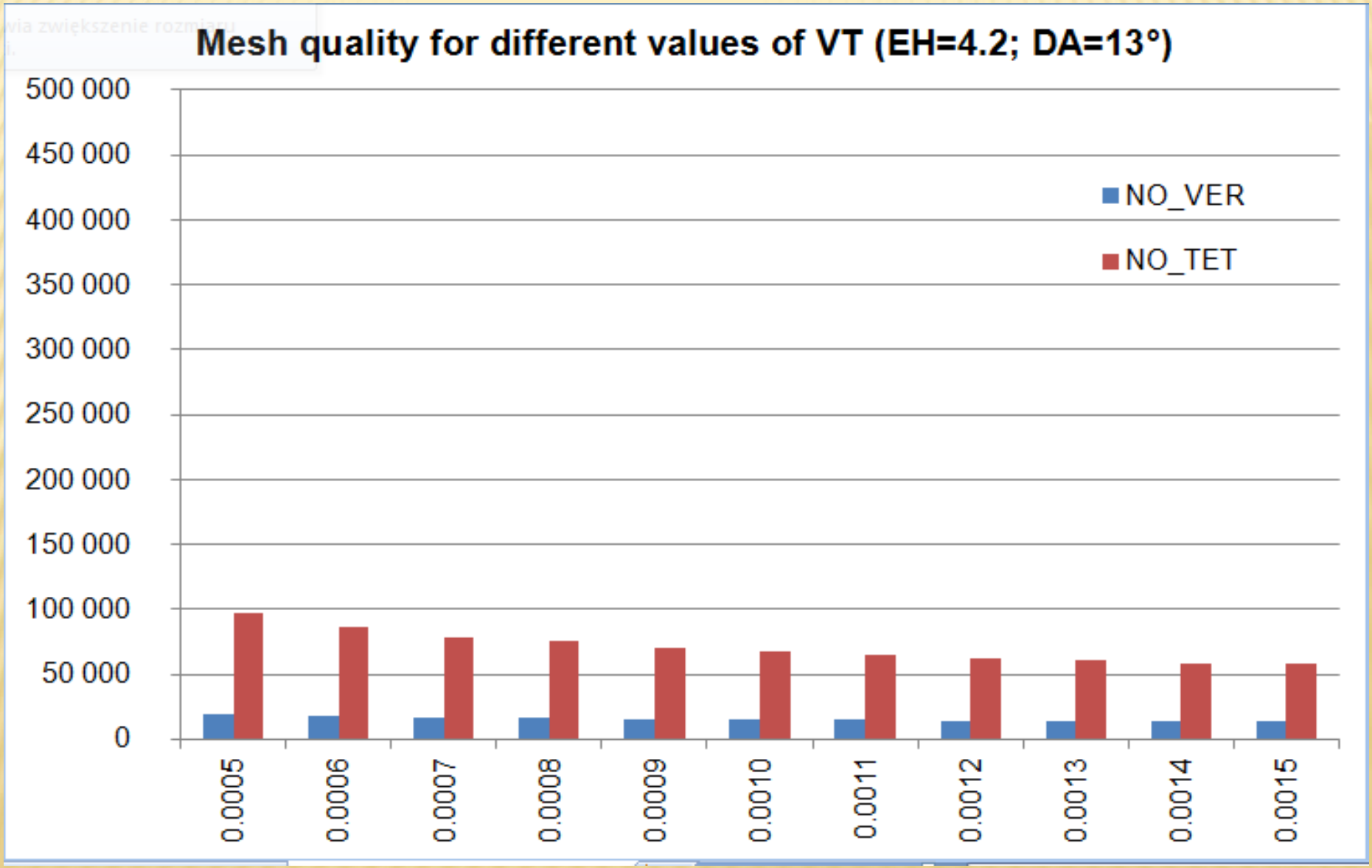
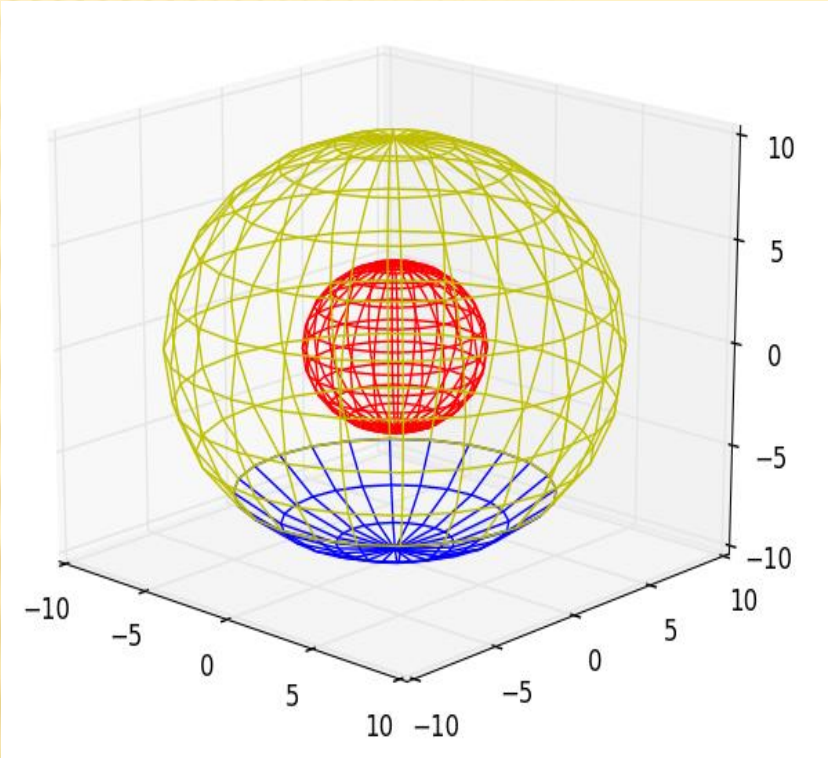
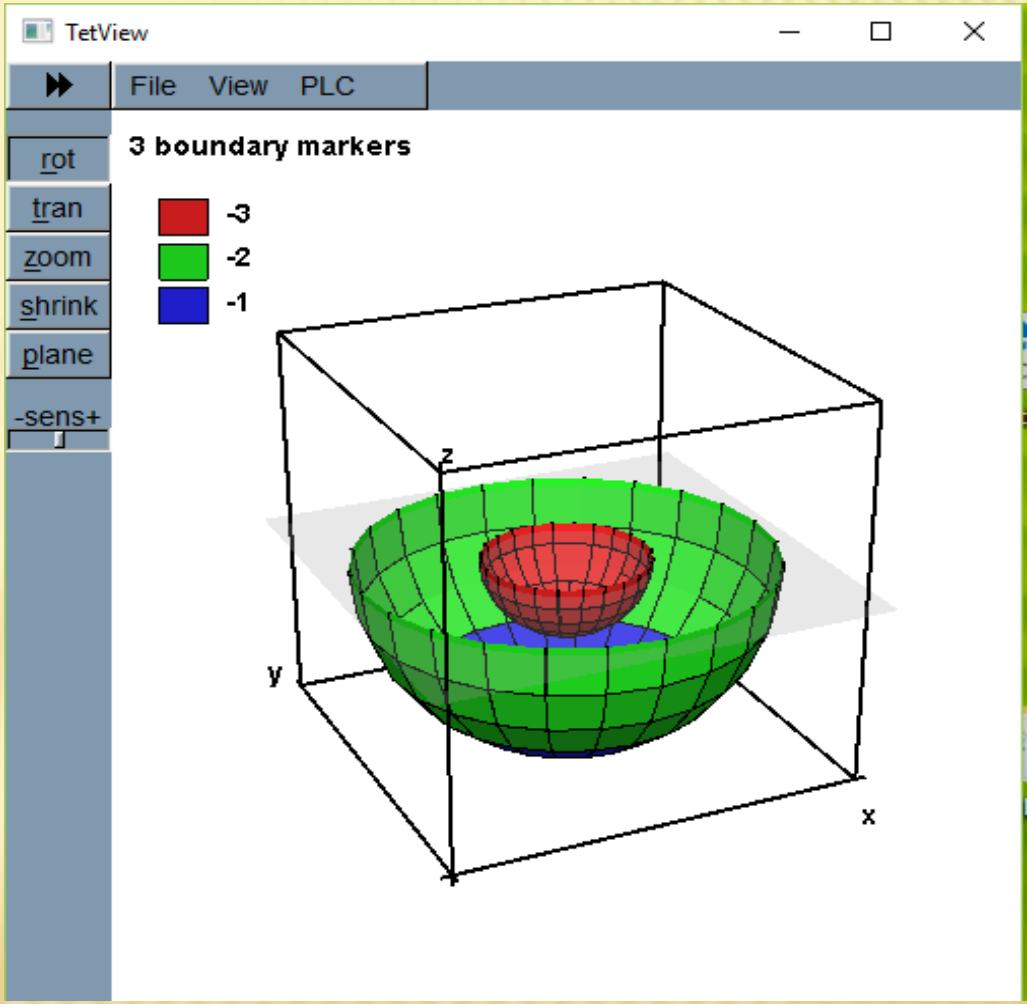


GLOBE = 2 CONCENTRIC SPHERES





1. bouton (Ω) (yellow)
   - Radius – 10 units
2. NT synthesis domain (Ω_3) (red)
   - Radius – 2,5 units
3. NT docking site ($\partial\Omega_d$) (blue)
   - 90°S to 45°S

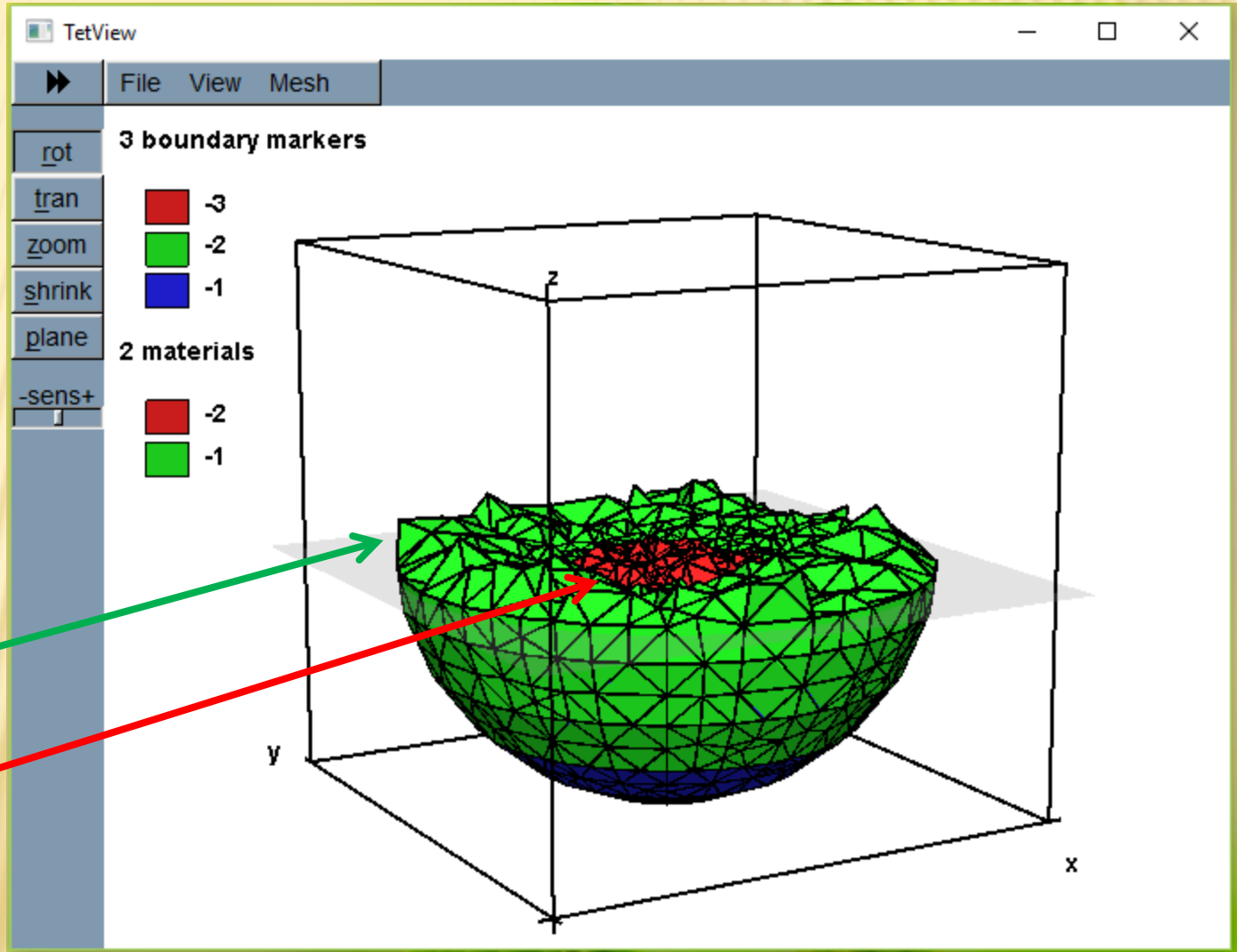
One of generated meshes before applying FEM

The view of the generated mesh ***(TetView®)***

1. Synthesis
2. Docking
3. Other

Rescaled Bouton: (unit=0,16μm)

R = 0,16x10μm
= 1,6 μm
r = 0,16x4μm
= 0,64 μm



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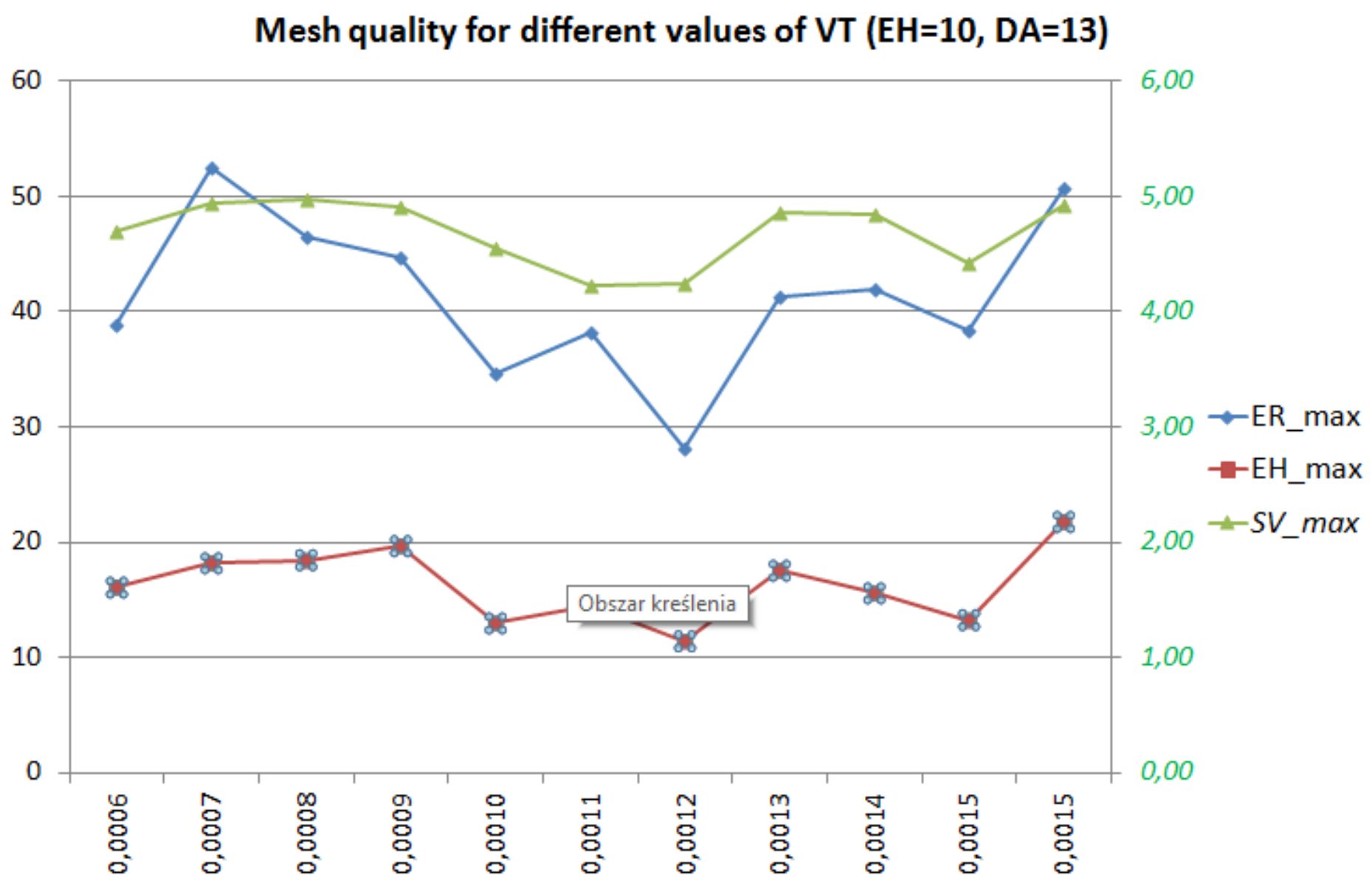

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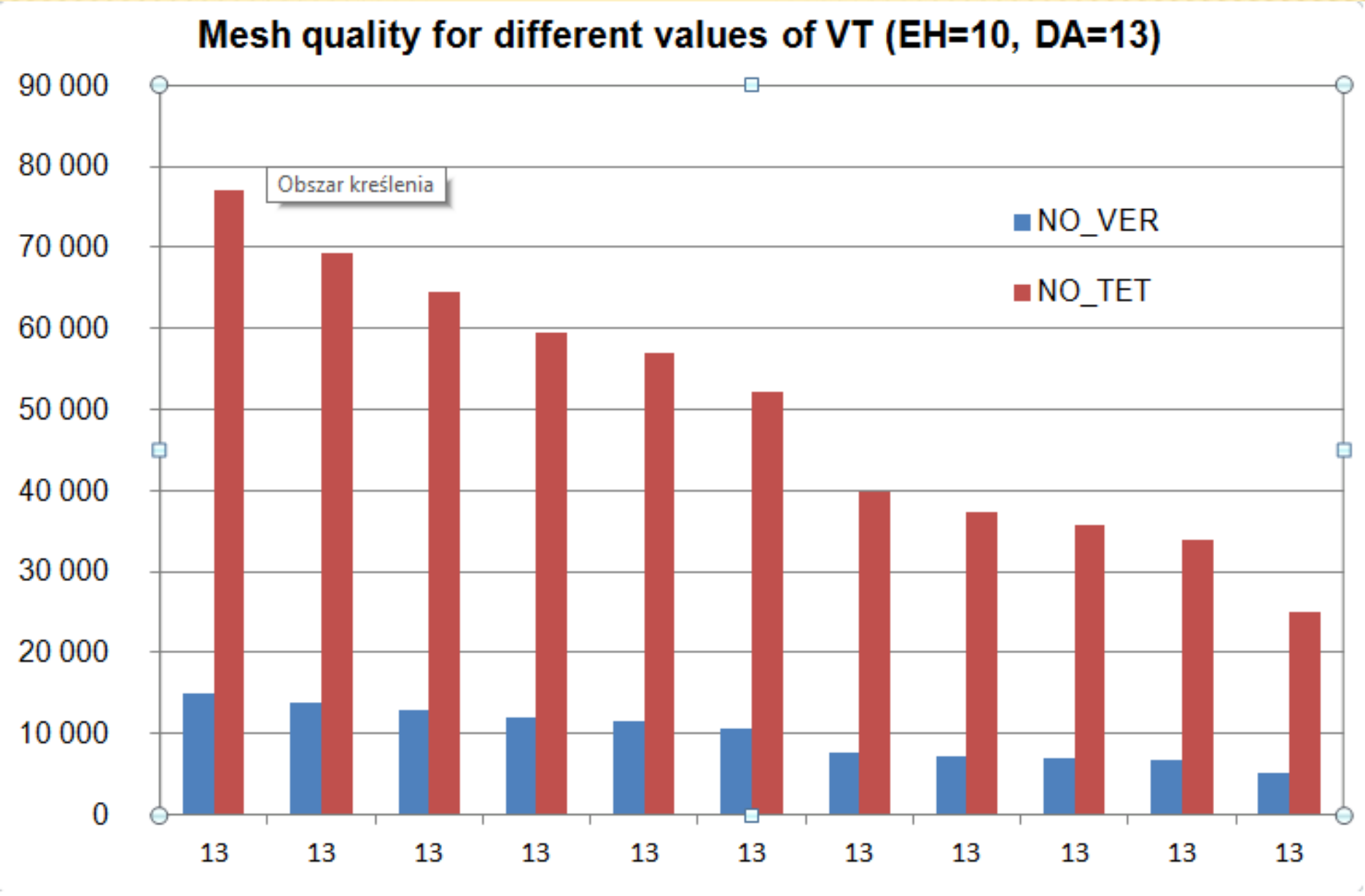

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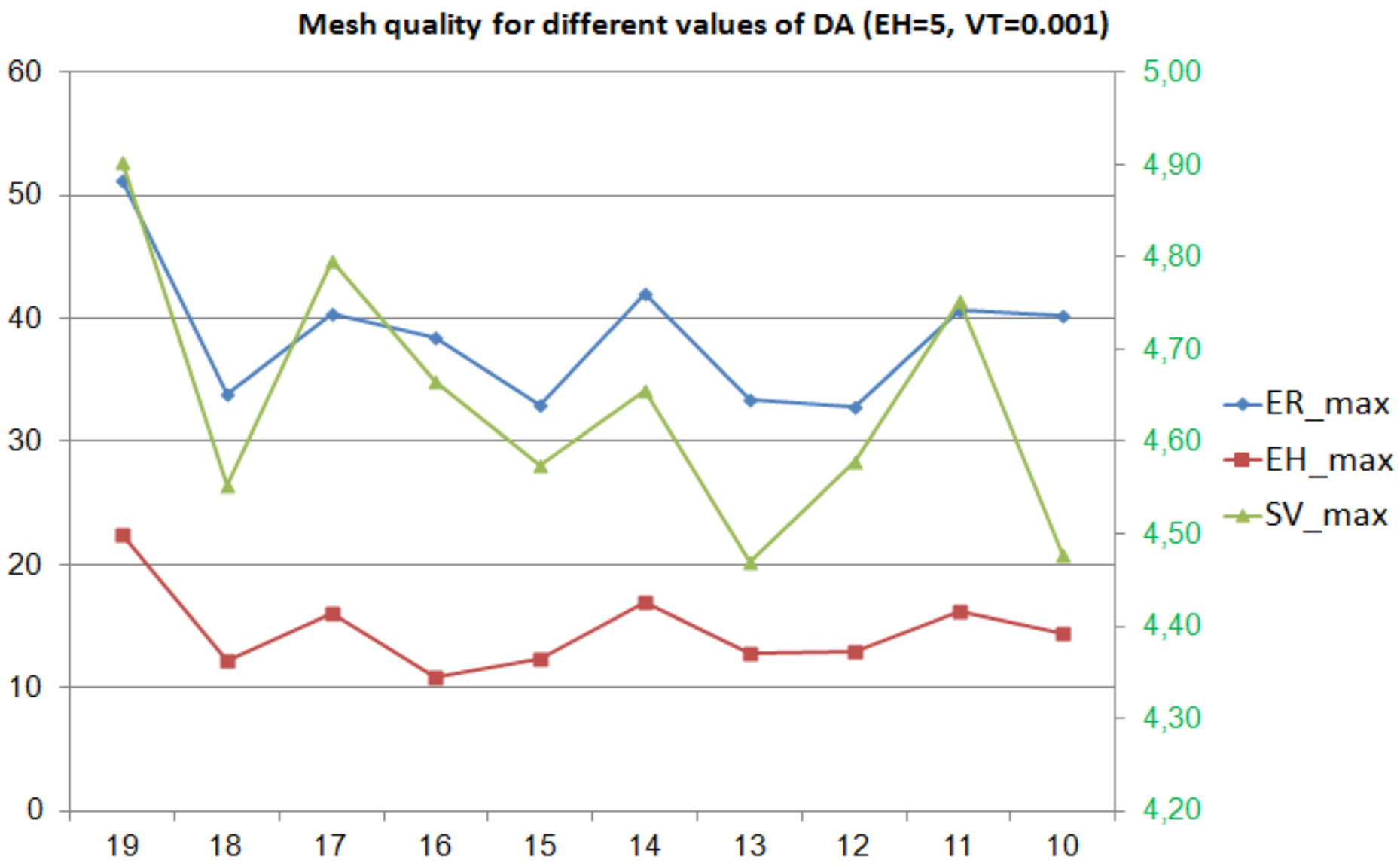

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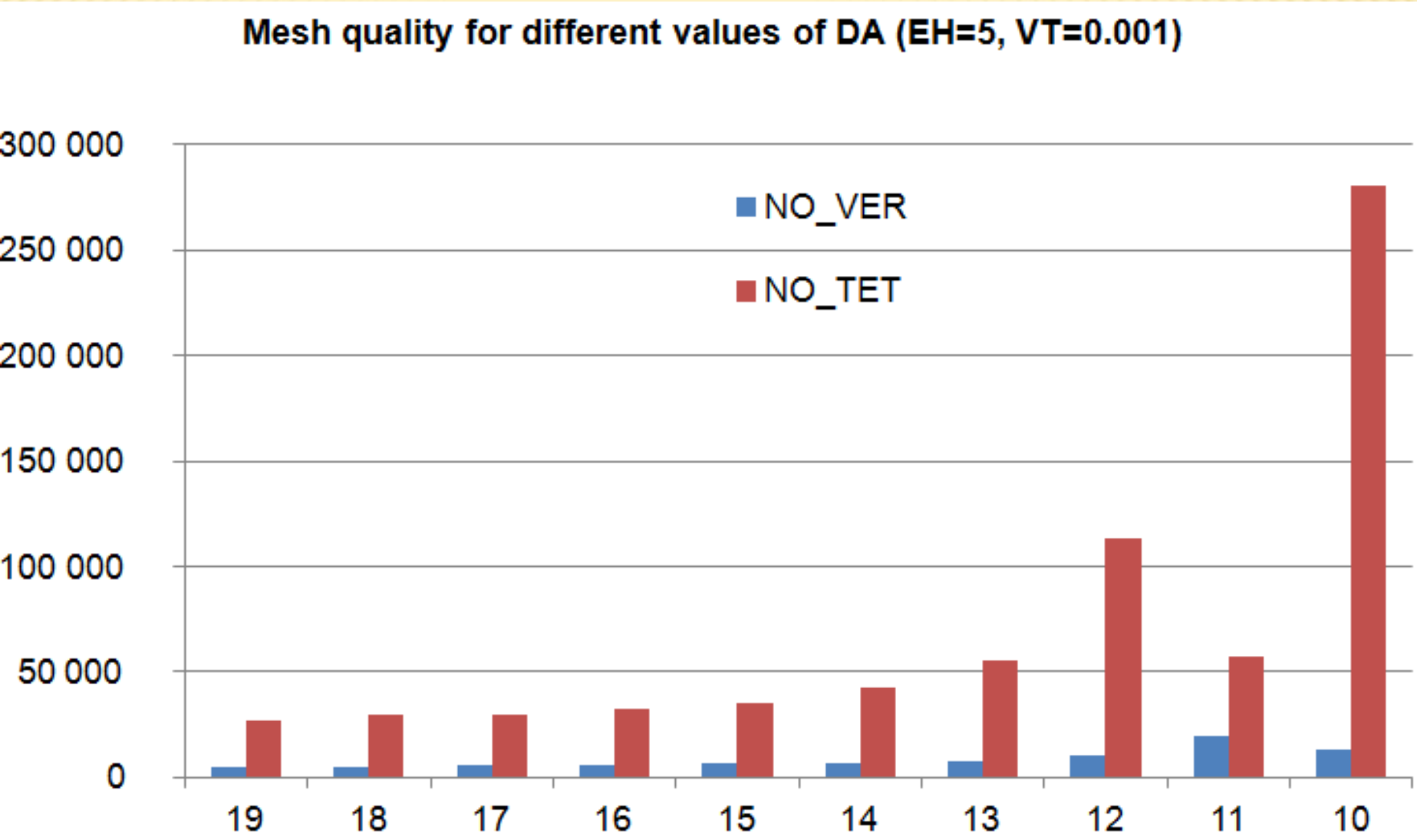
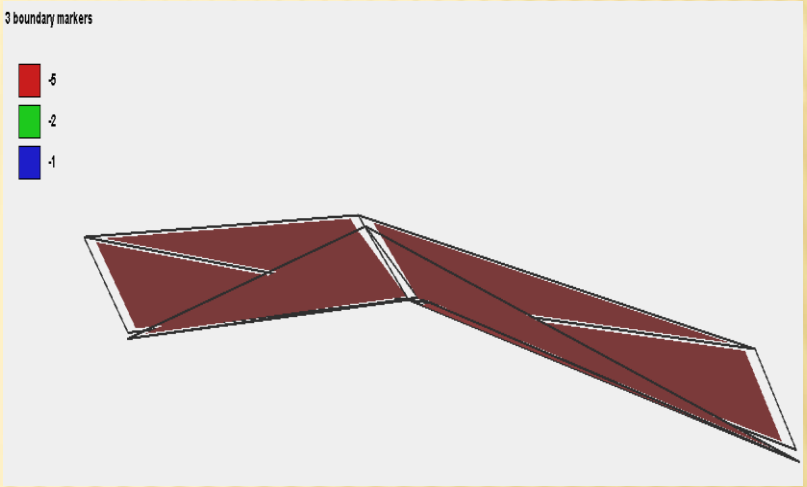
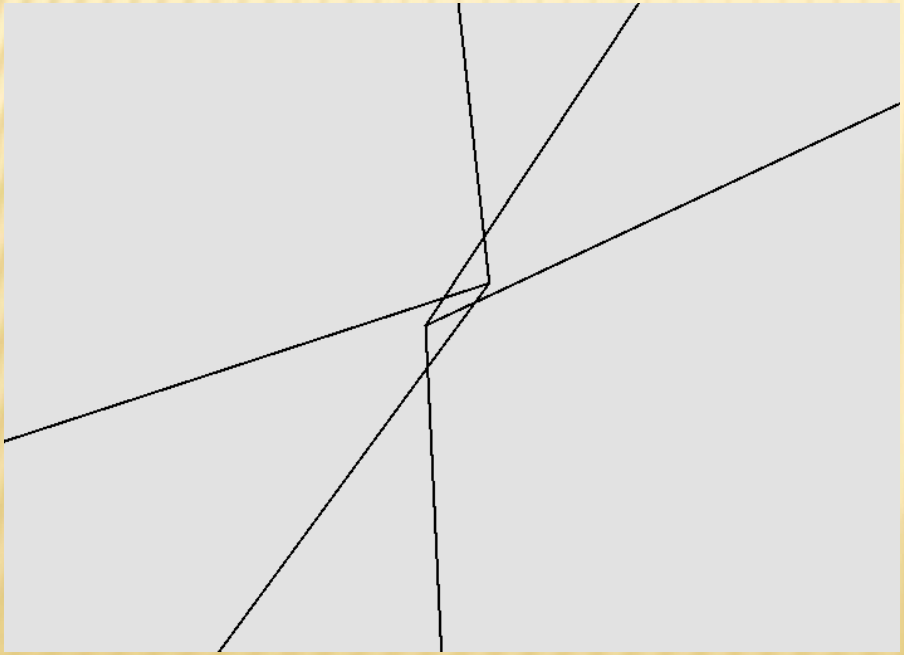
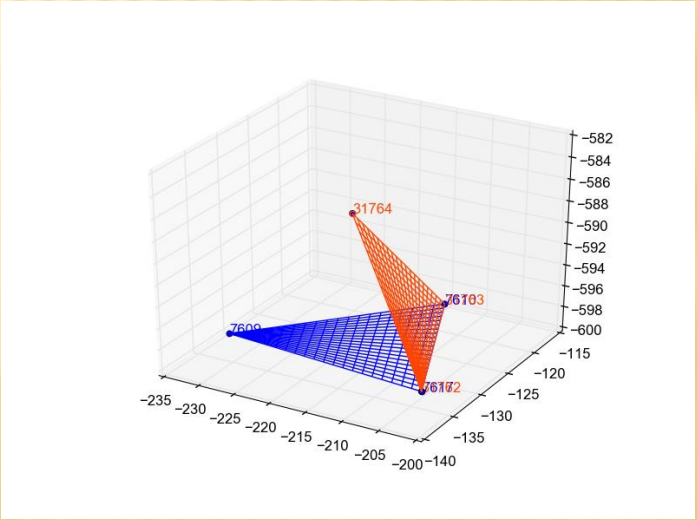


PROBLEMS WITH REAL BOUTON

- Intersections
- Leakage



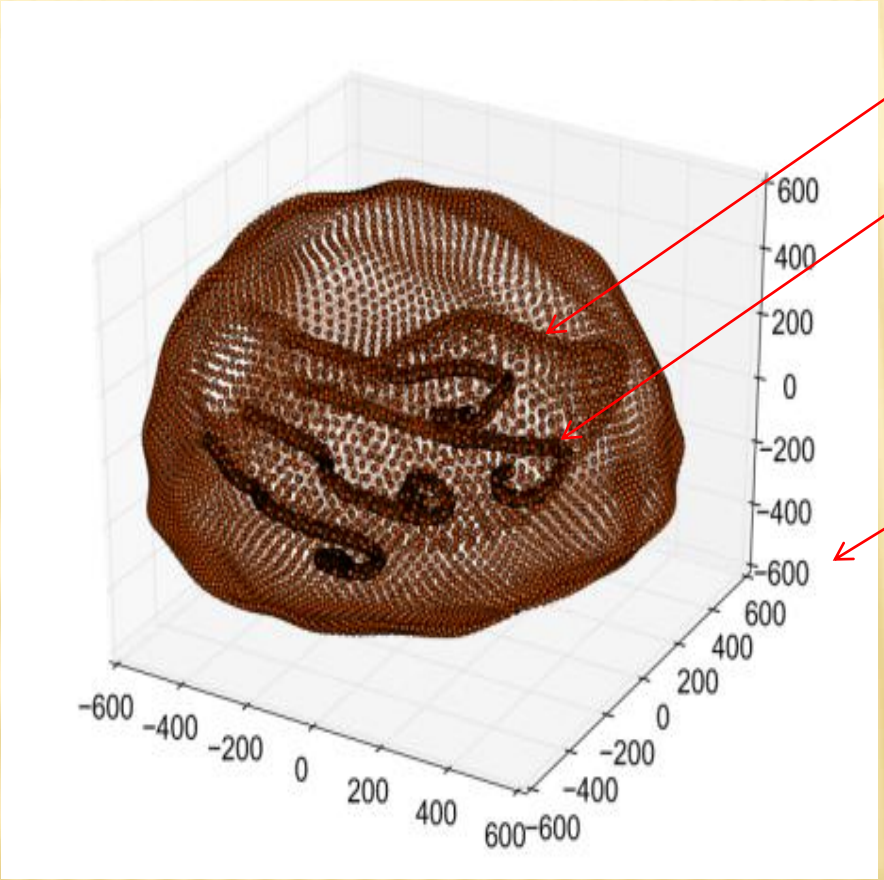




Real presynaptic bouton – cross-section

Zhang et al. 1998, *Neuron*

3D model of a presynaptic bouton



mitochondrion

microtubule

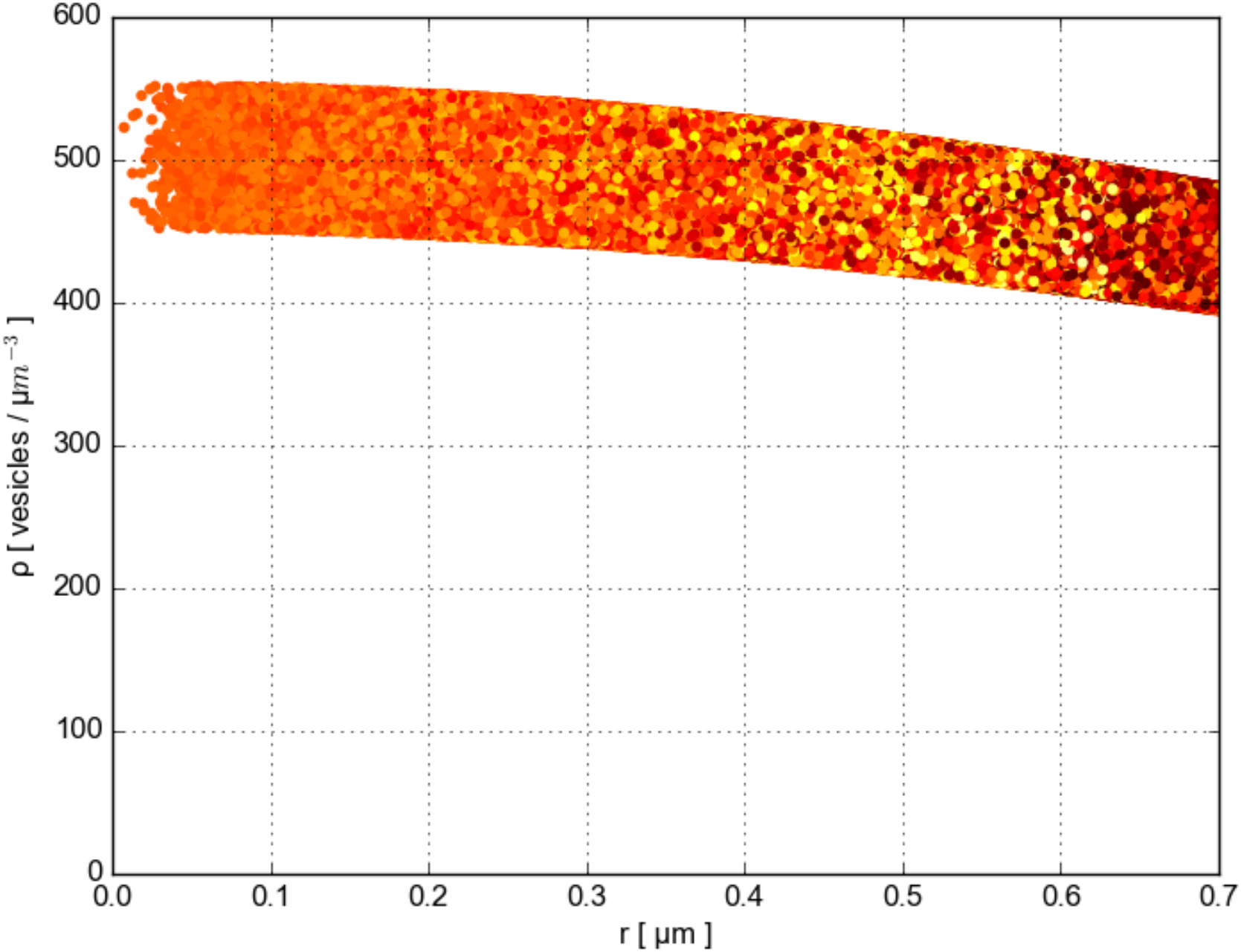
coordinates in nanometers

REAL BOUTON MODEL - OPTIMIZATION

eh	da	vol	v	t	f	e	ehmin	ehmax	vmax	damin
80	10	1000	577806	2828839	5906813	3655779	1,227 4	276,68	1129,6	0,31035
79	10	1000	578942	2835972	5921210	3664179	1,231 9	389,24	1090,1	0,26259
78	10	1000	578942	2835972	5921210	3664179	1,231 9	389,24	1090,1	0,26259
77	10	1000	578774	2833491	5916361	3661643	1,228 9	277,31	1058,4	0,27932
76	10	1000	578774	2833491	5916361	3661643	1,228 9	277,31	1058,4	0,27932
75	10	1000	577769	2828521	5906298	3655545	1,226 8	215,45	999,99	0,33202
74	10	1000	578713	2833402	5916189	3661499	1,232	240	1094,3	0,5764
73	10	1000	578255	2831259	5911890	3658885	1,232 4	356,44	1025,5	0,23726

CONCLUSIONS

1. The constructed mesh is suitable for performing numerical calculations.
2. However, some improvements can still be made.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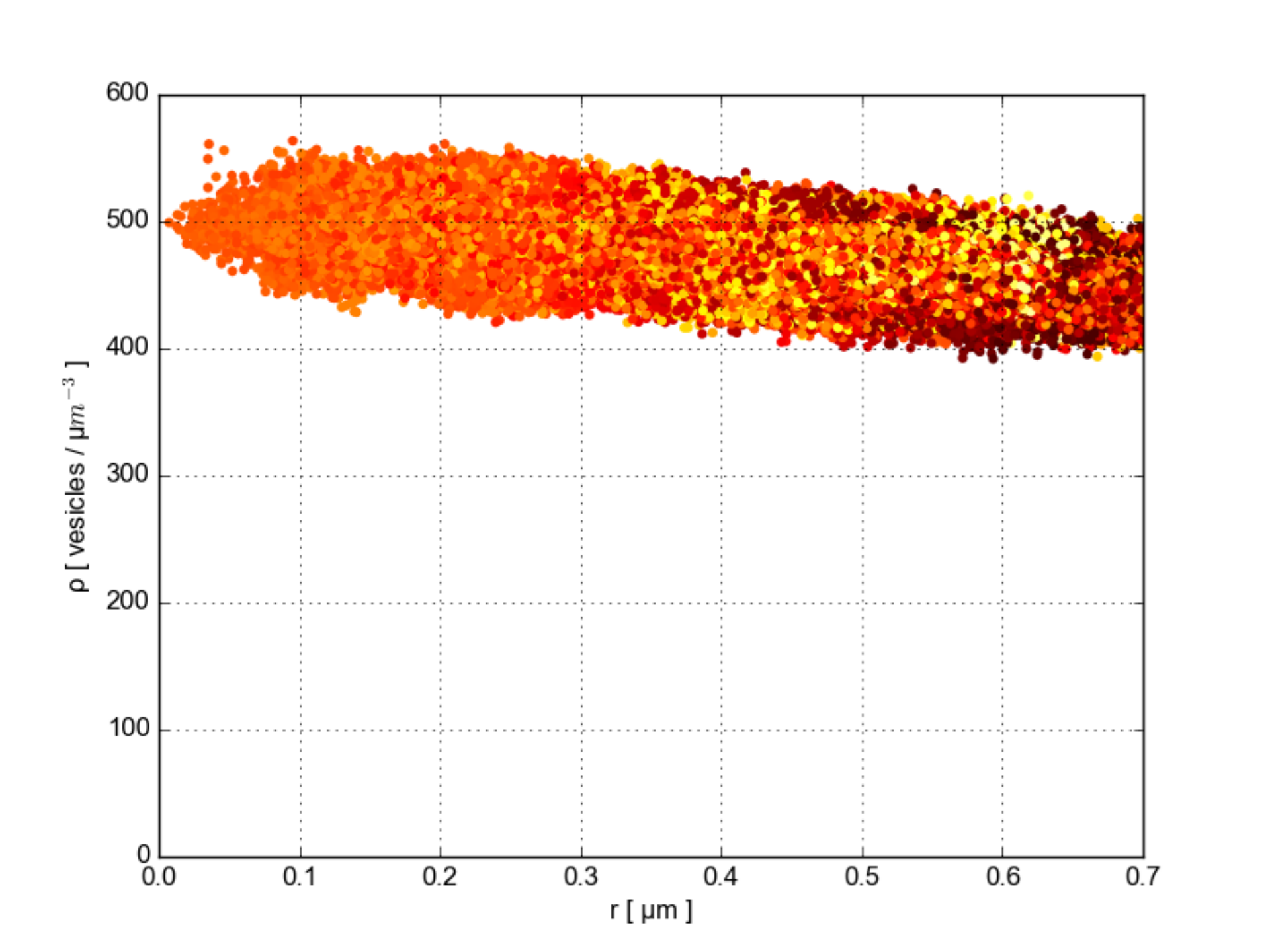
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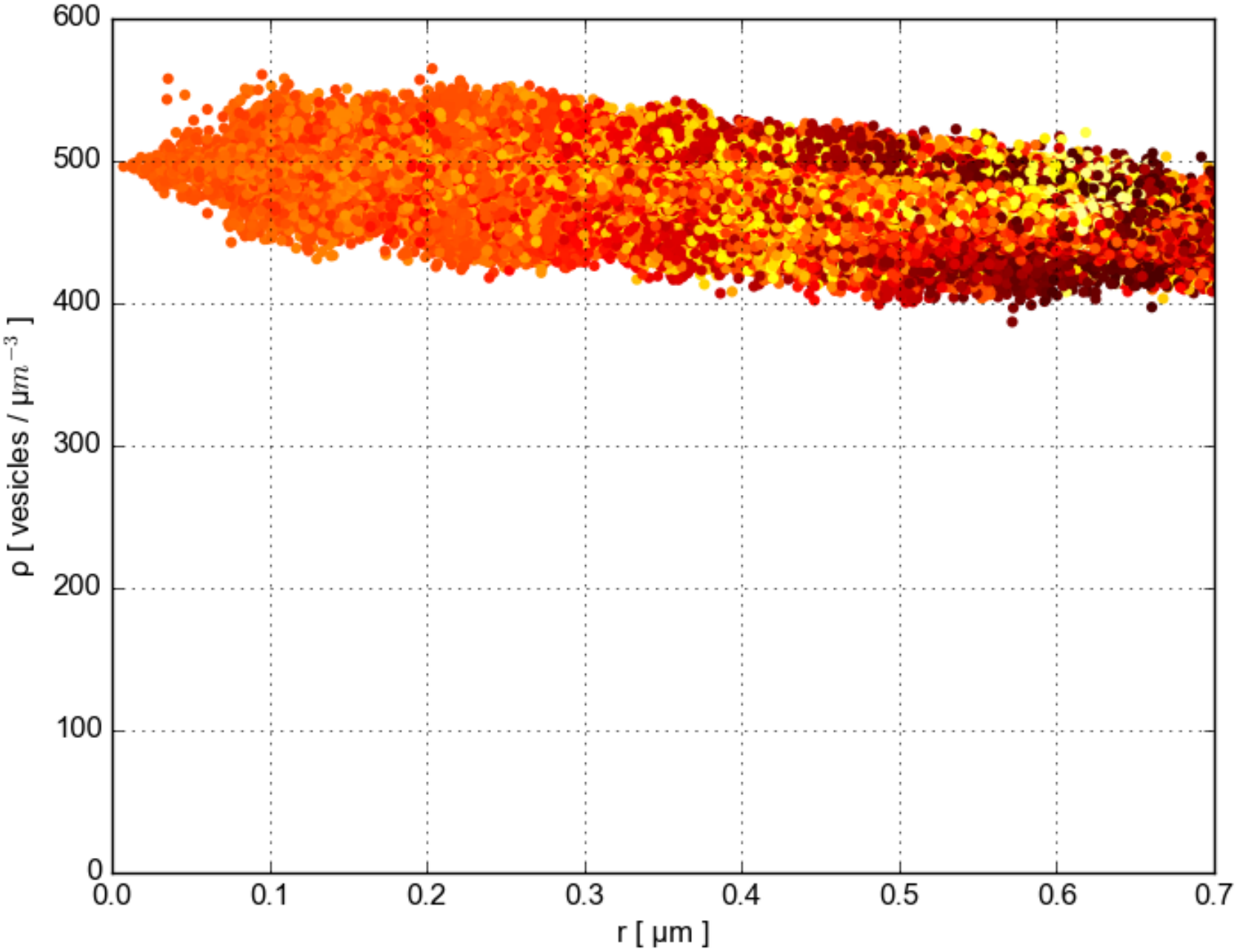
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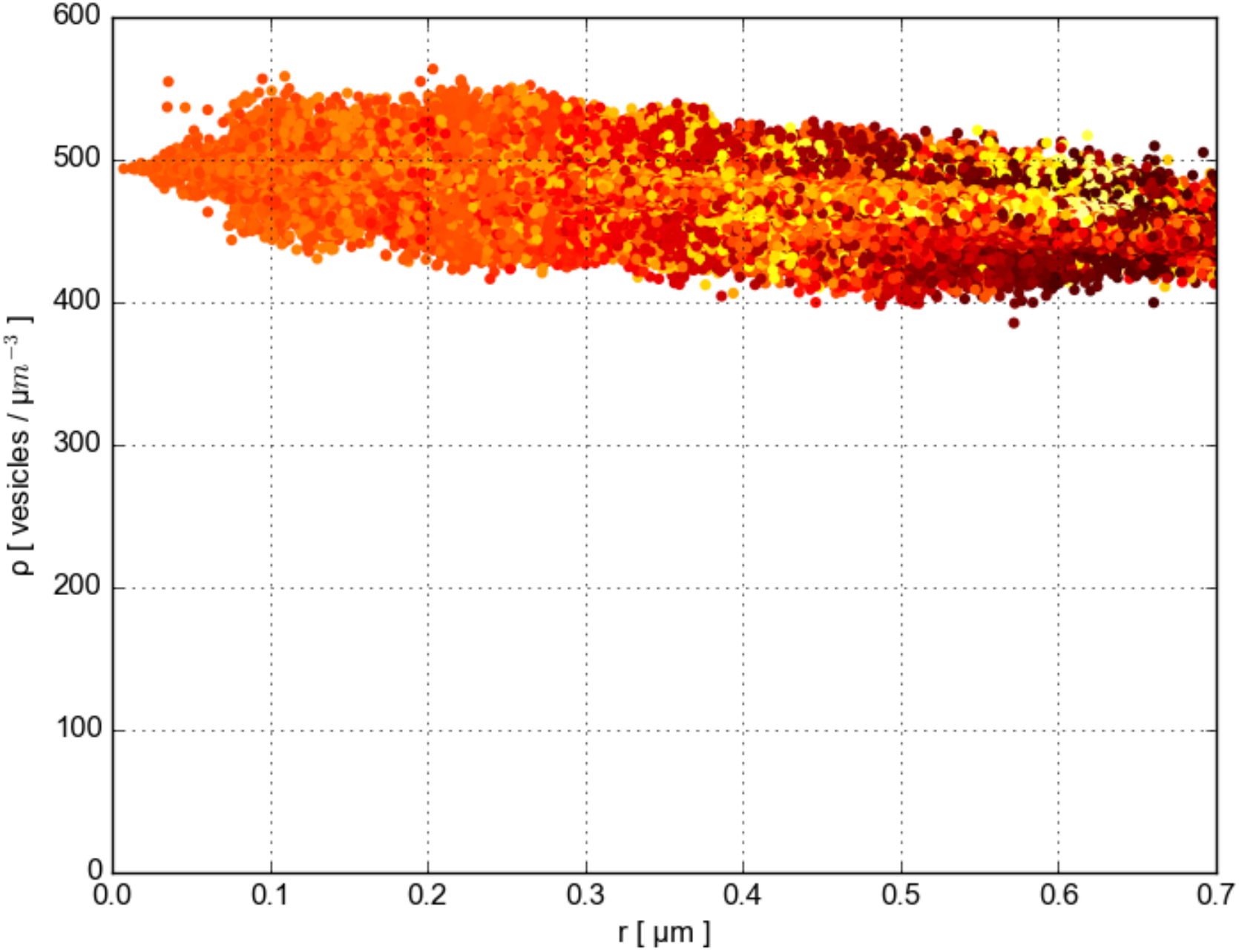
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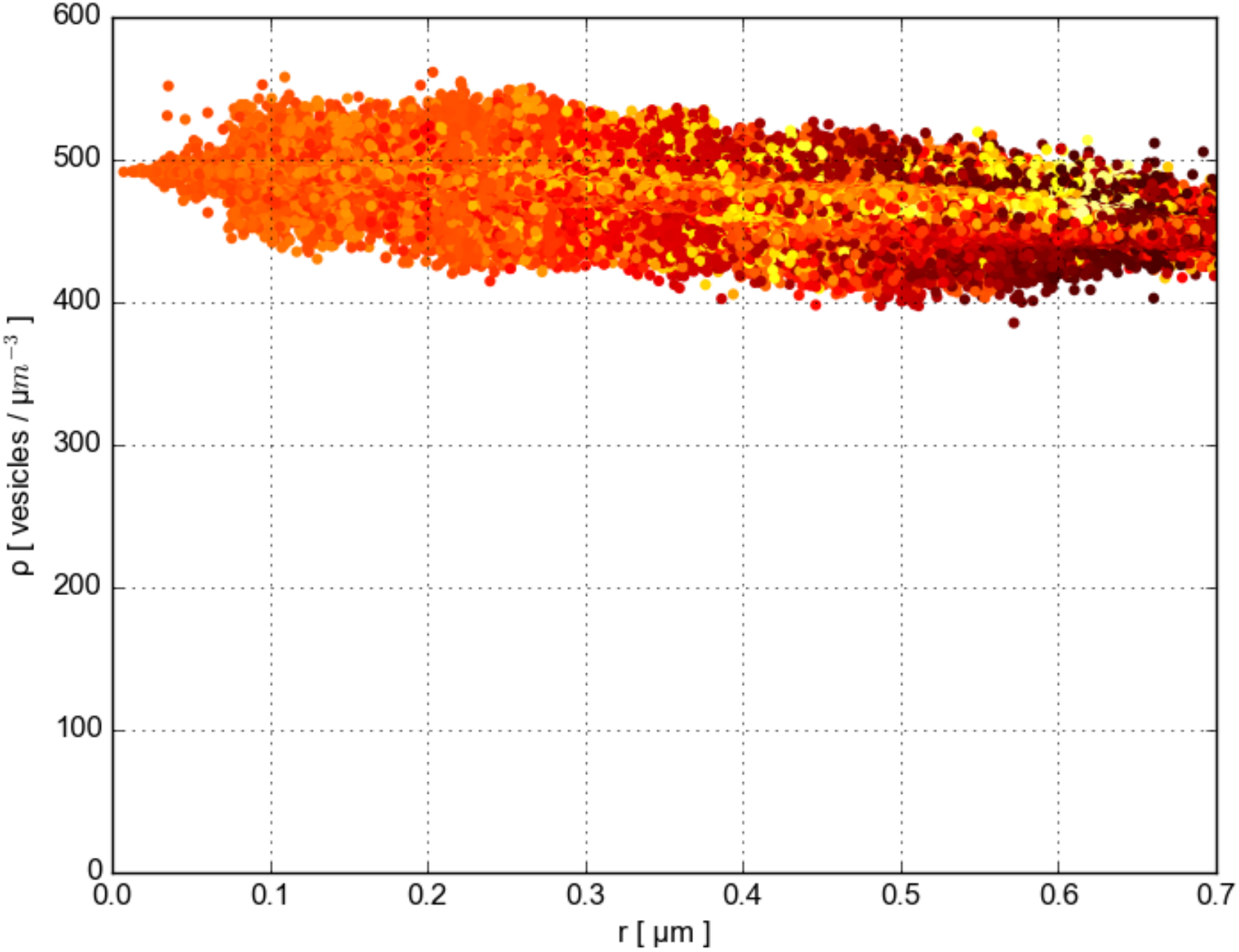
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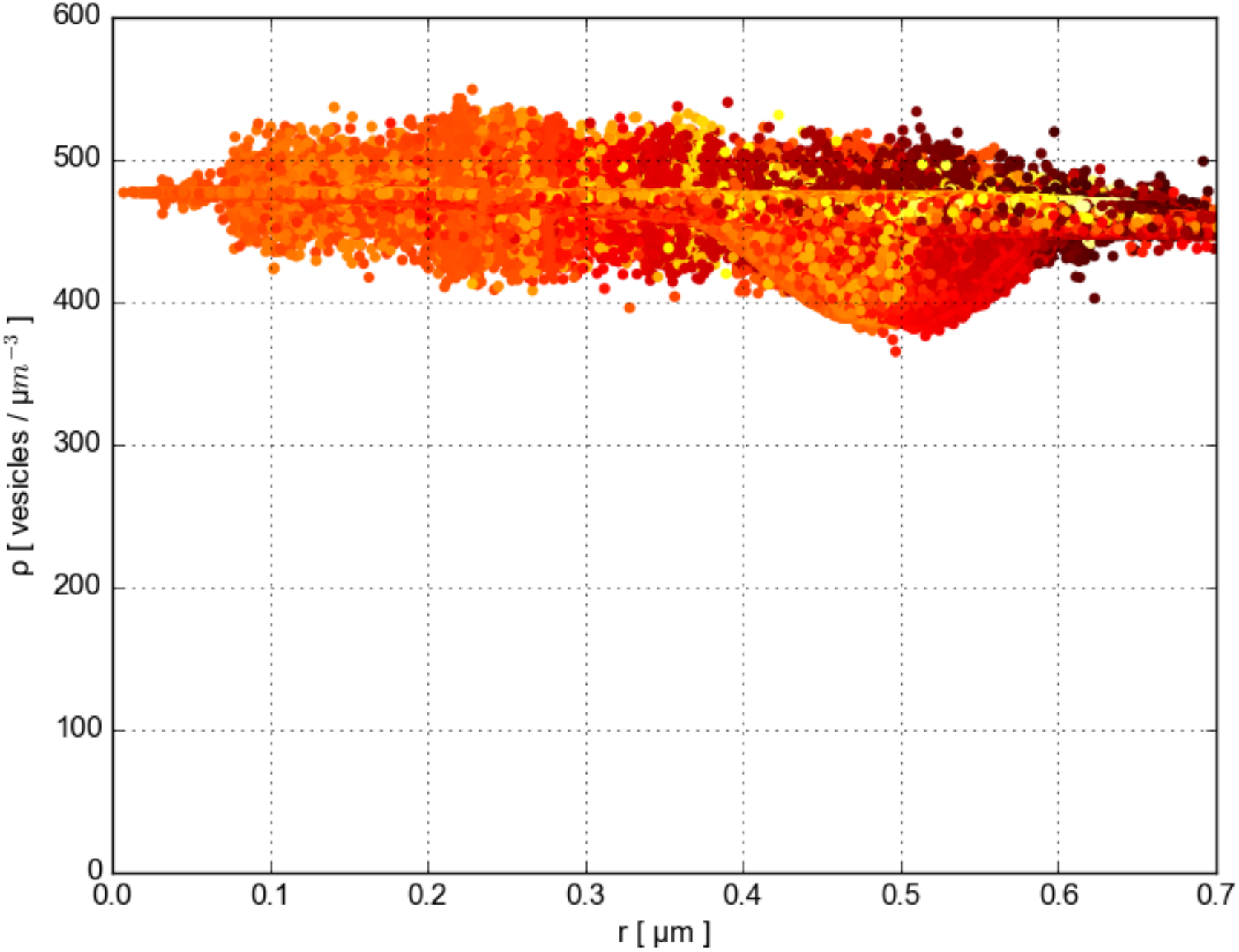
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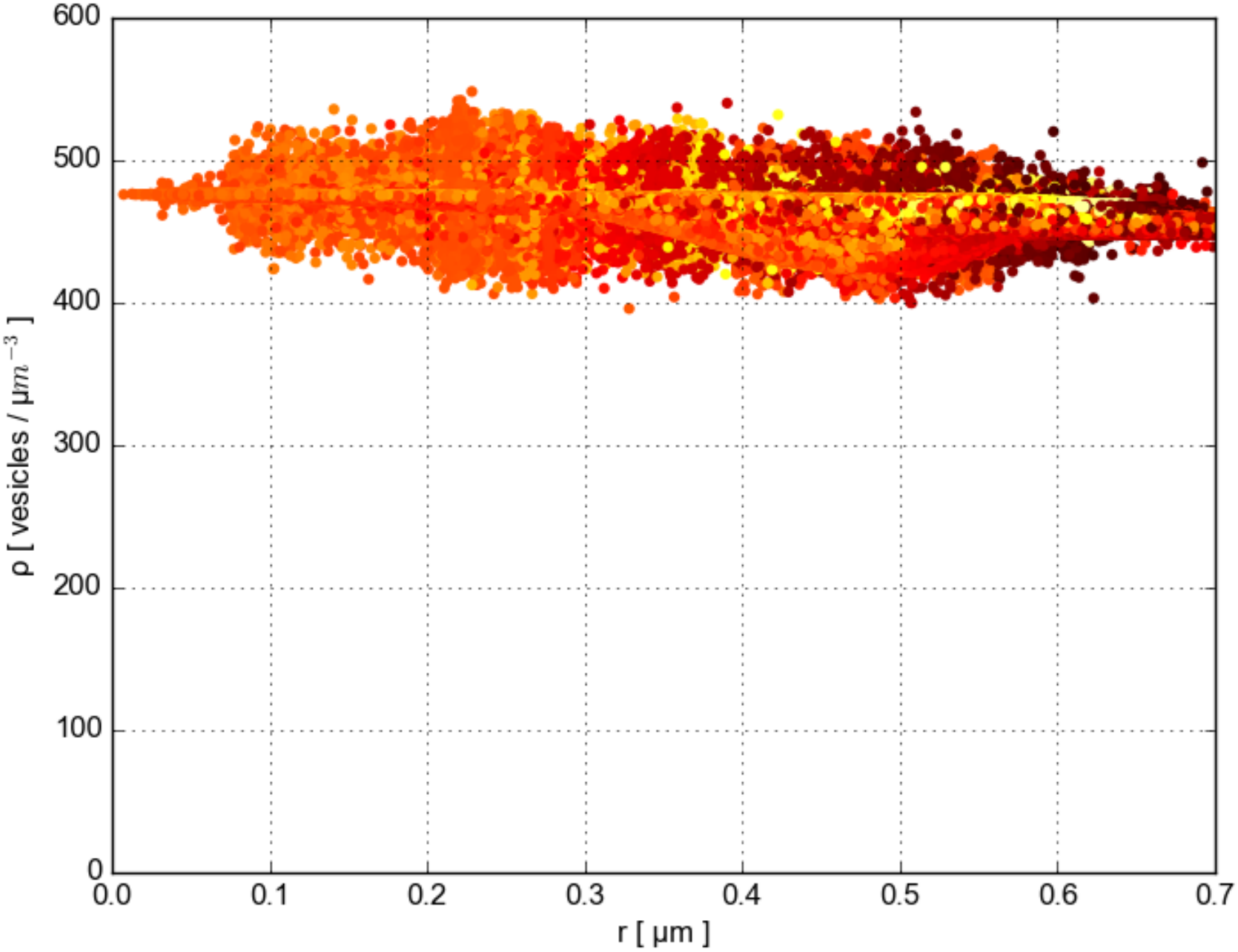
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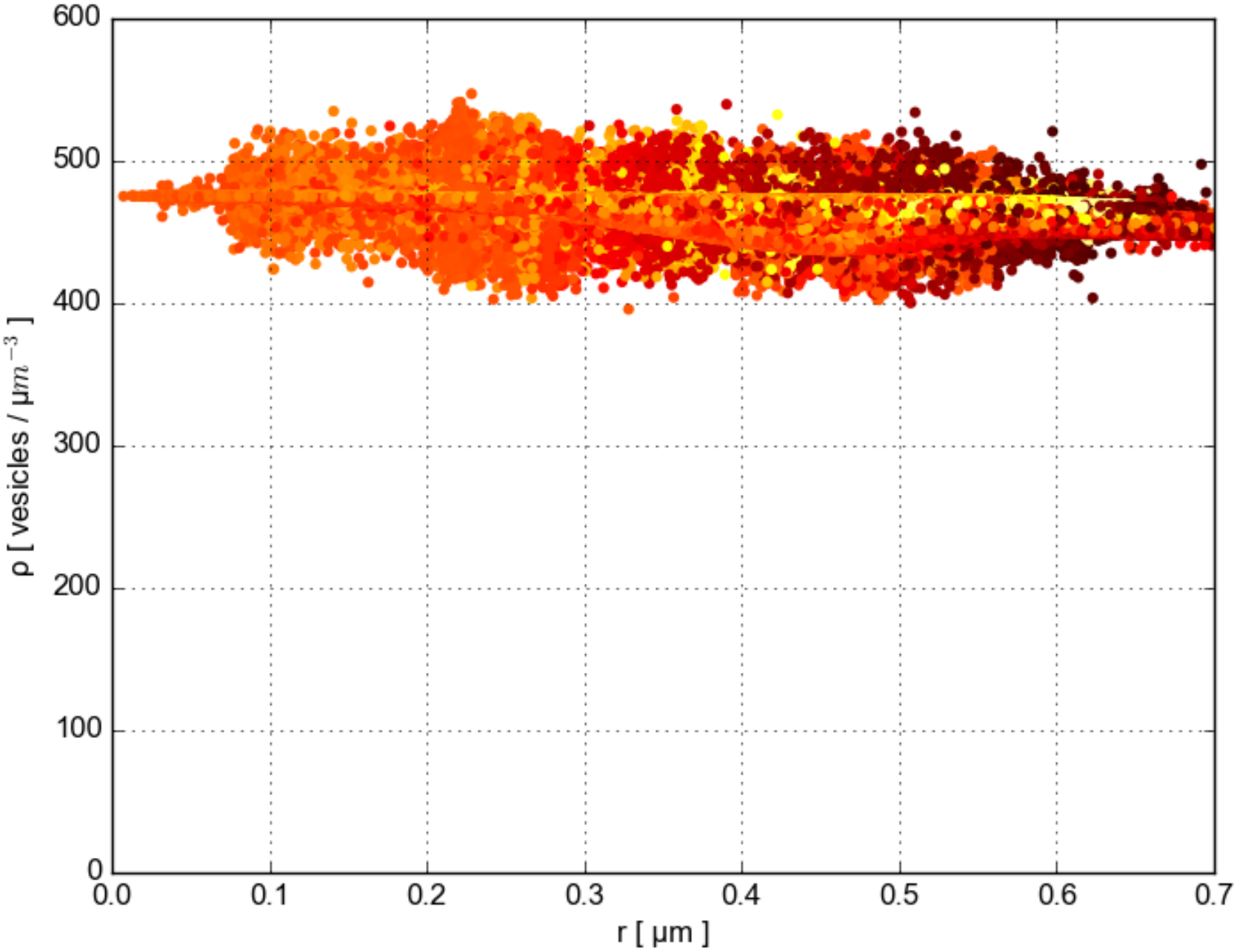
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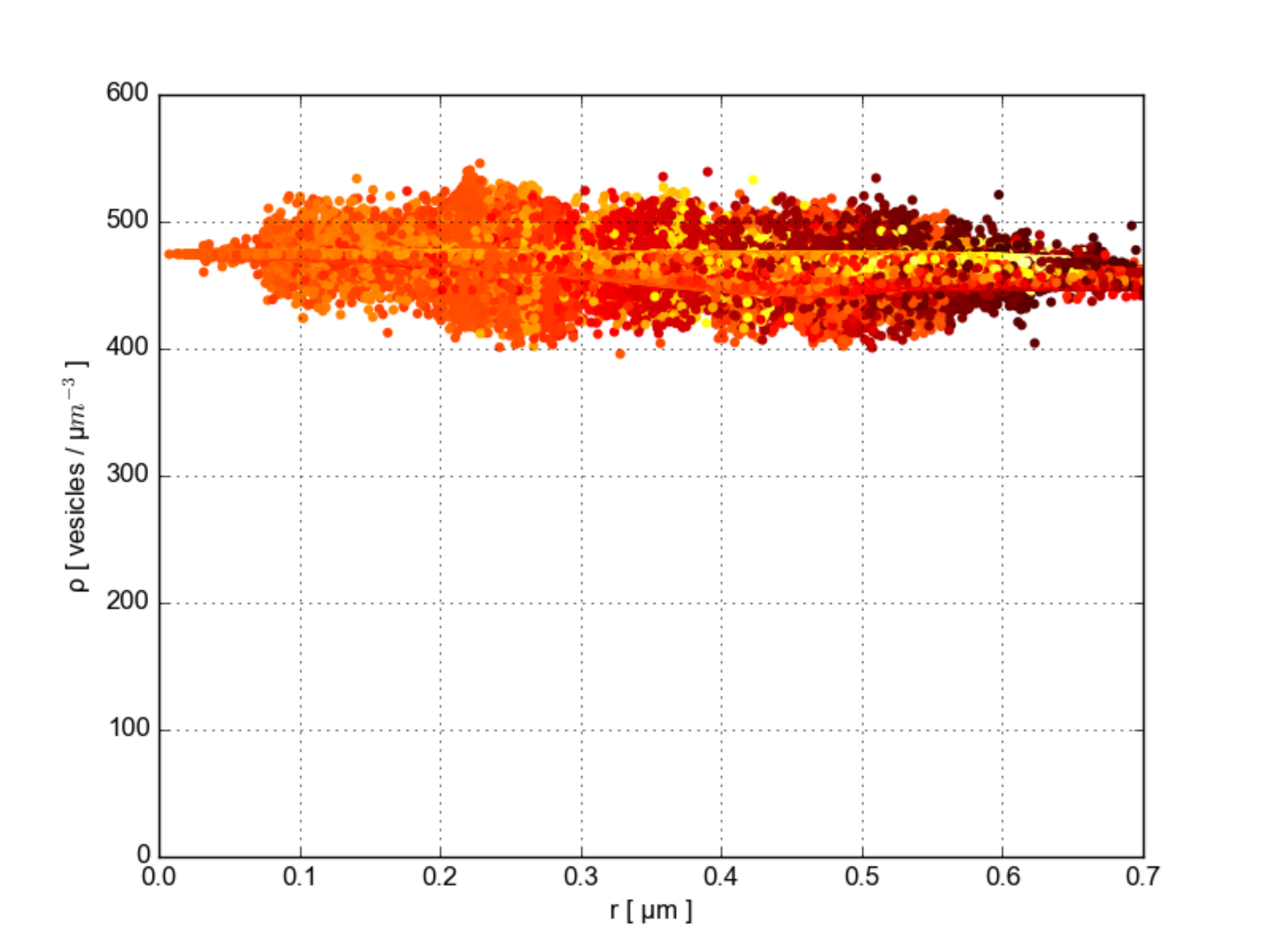
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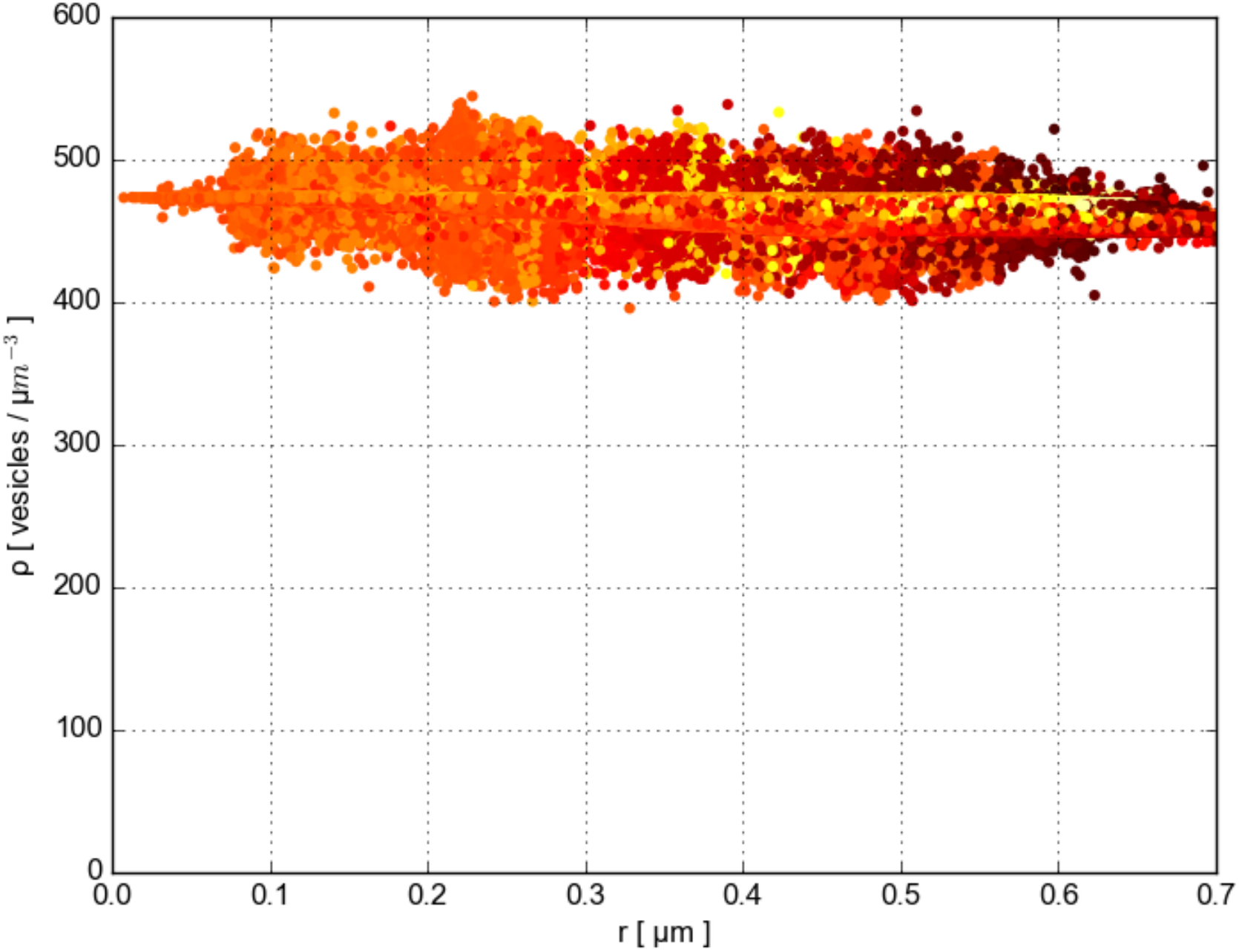
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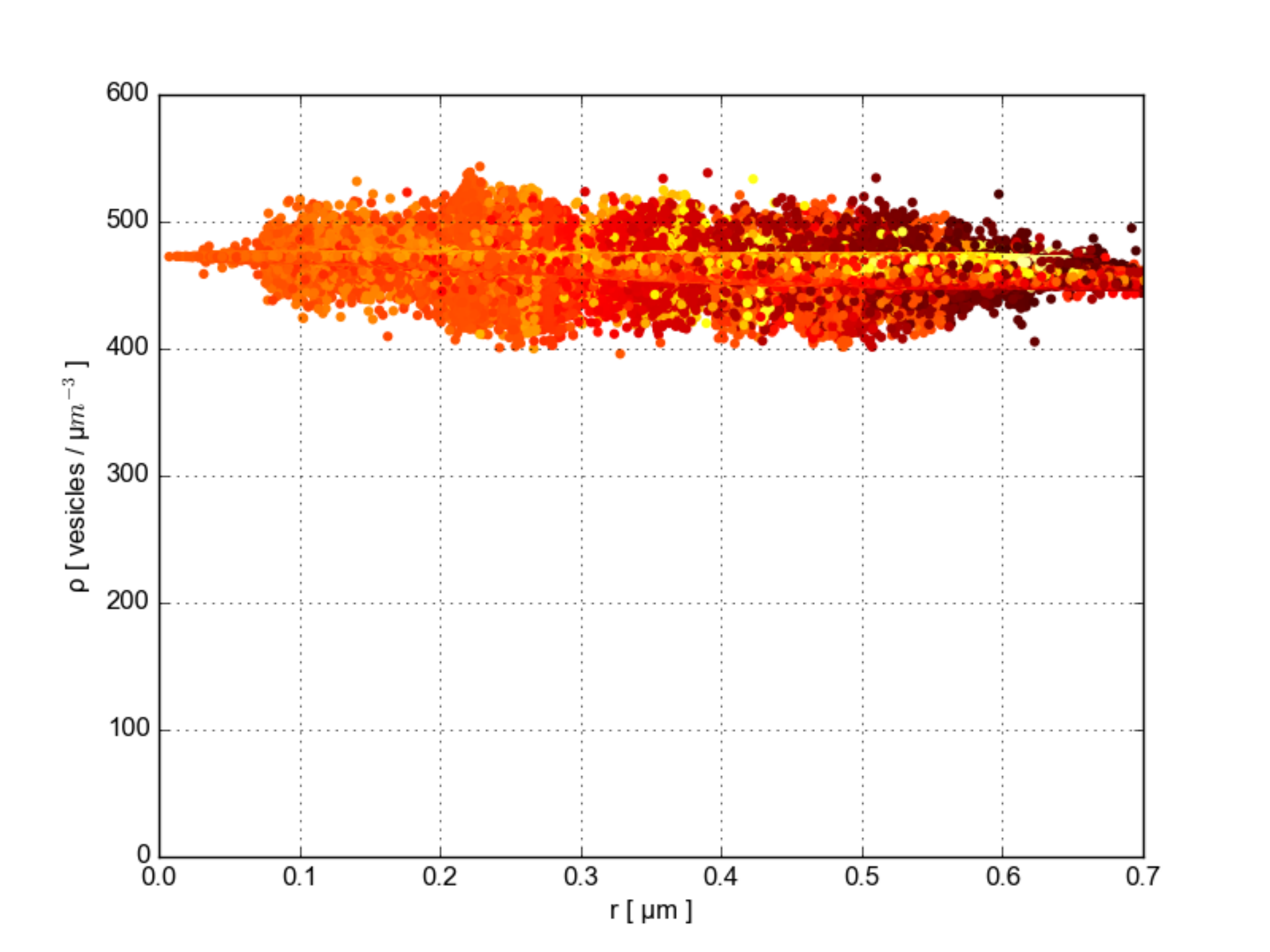
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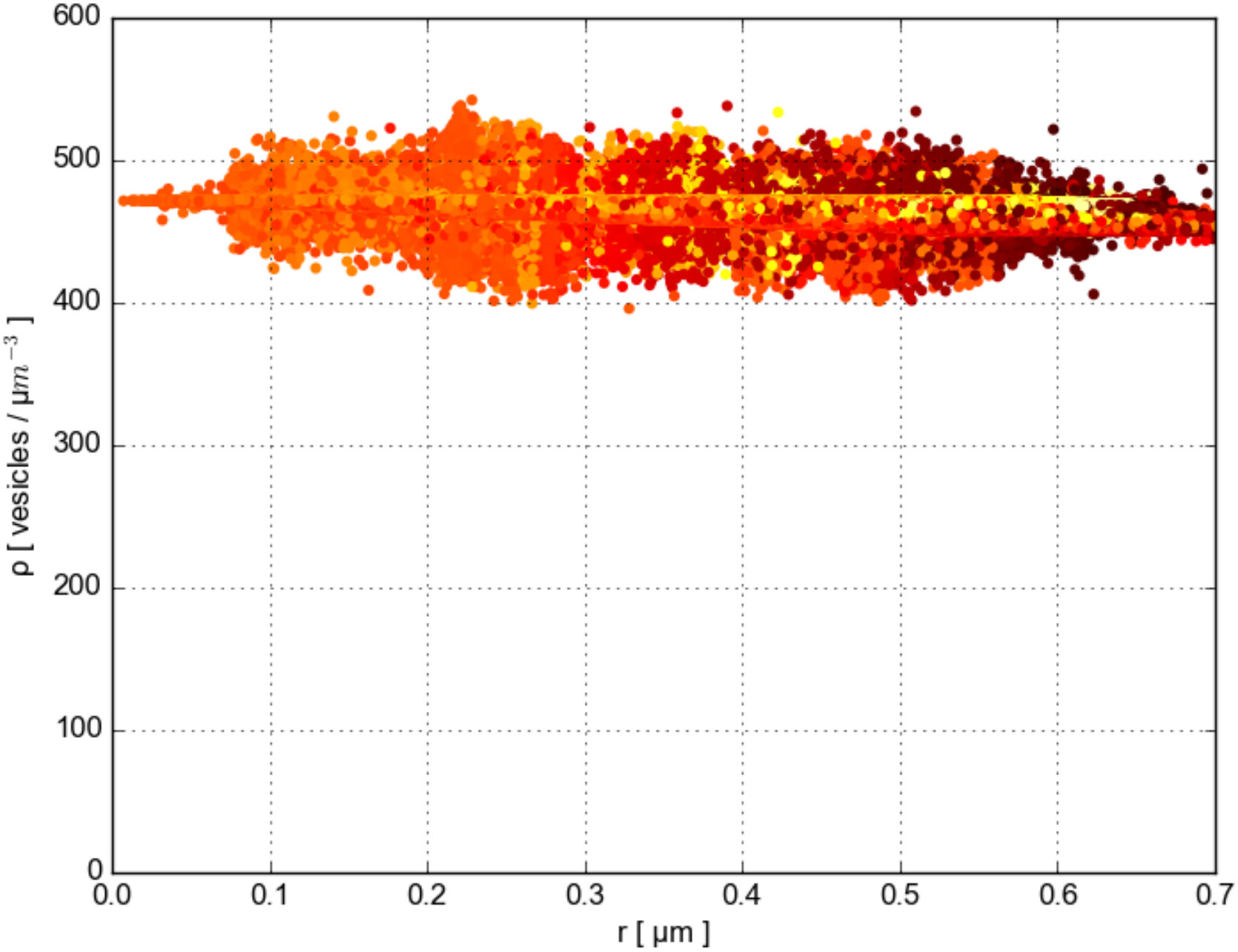
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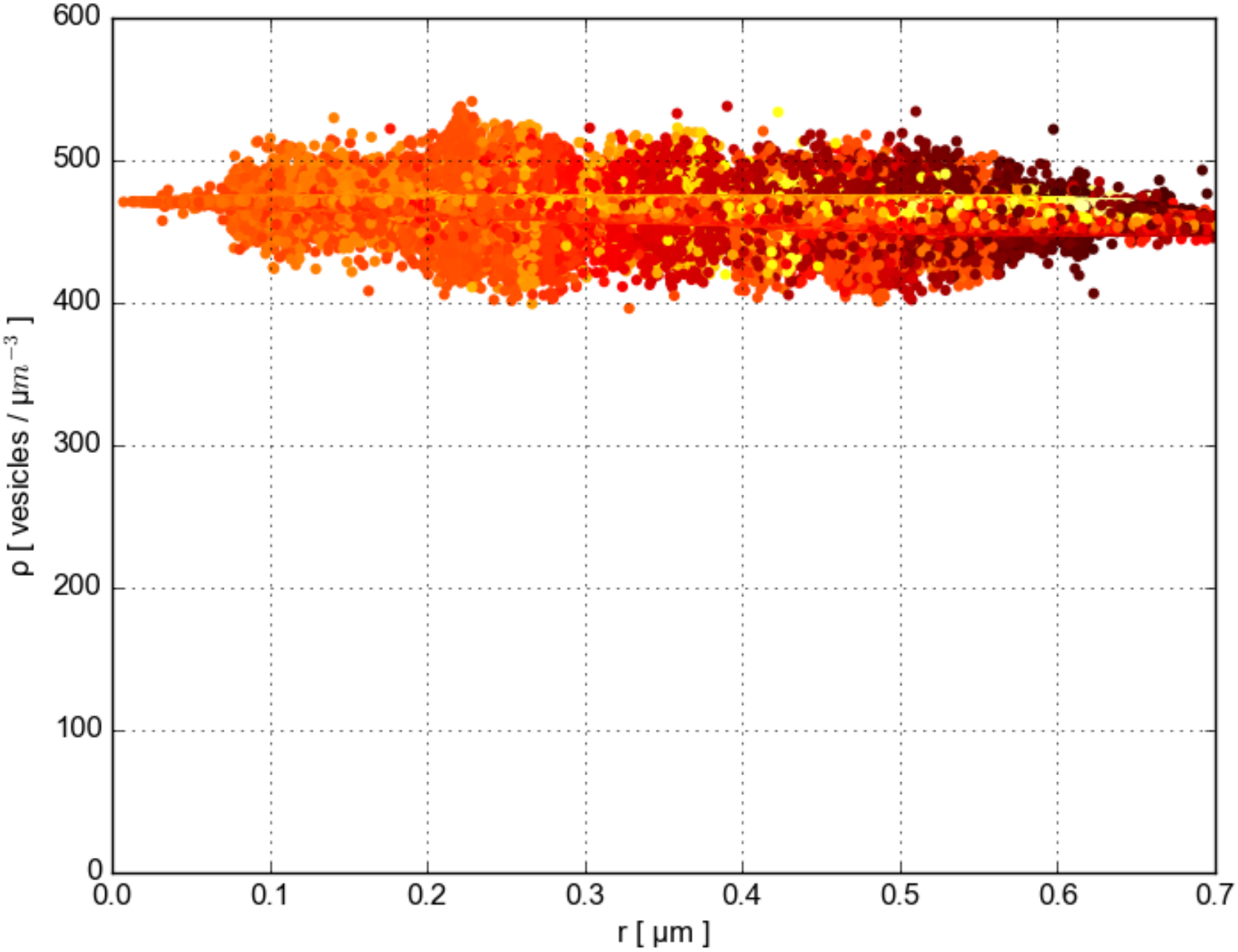
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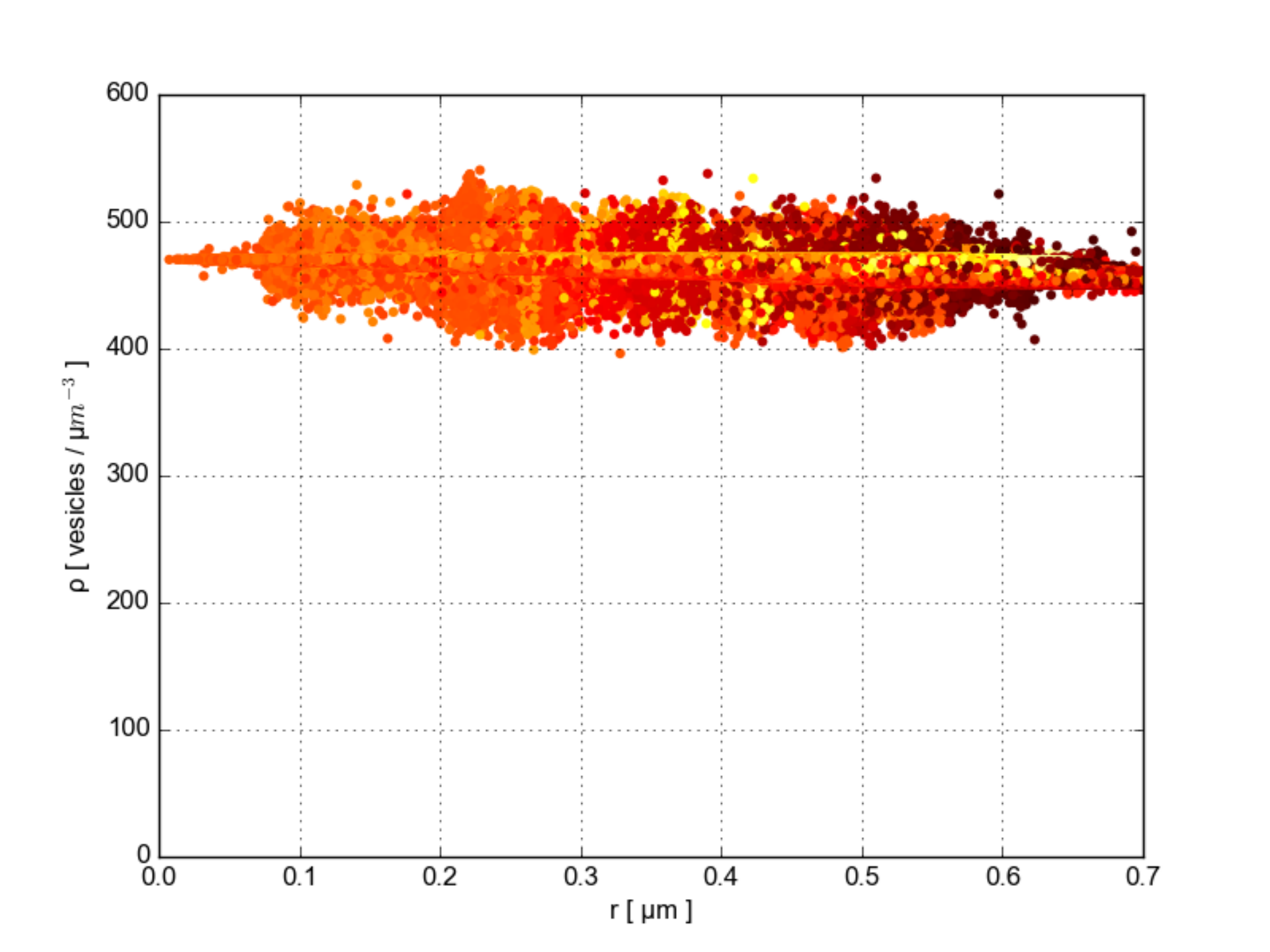
ρ [vesicles / μm^{-3}]
r [μm]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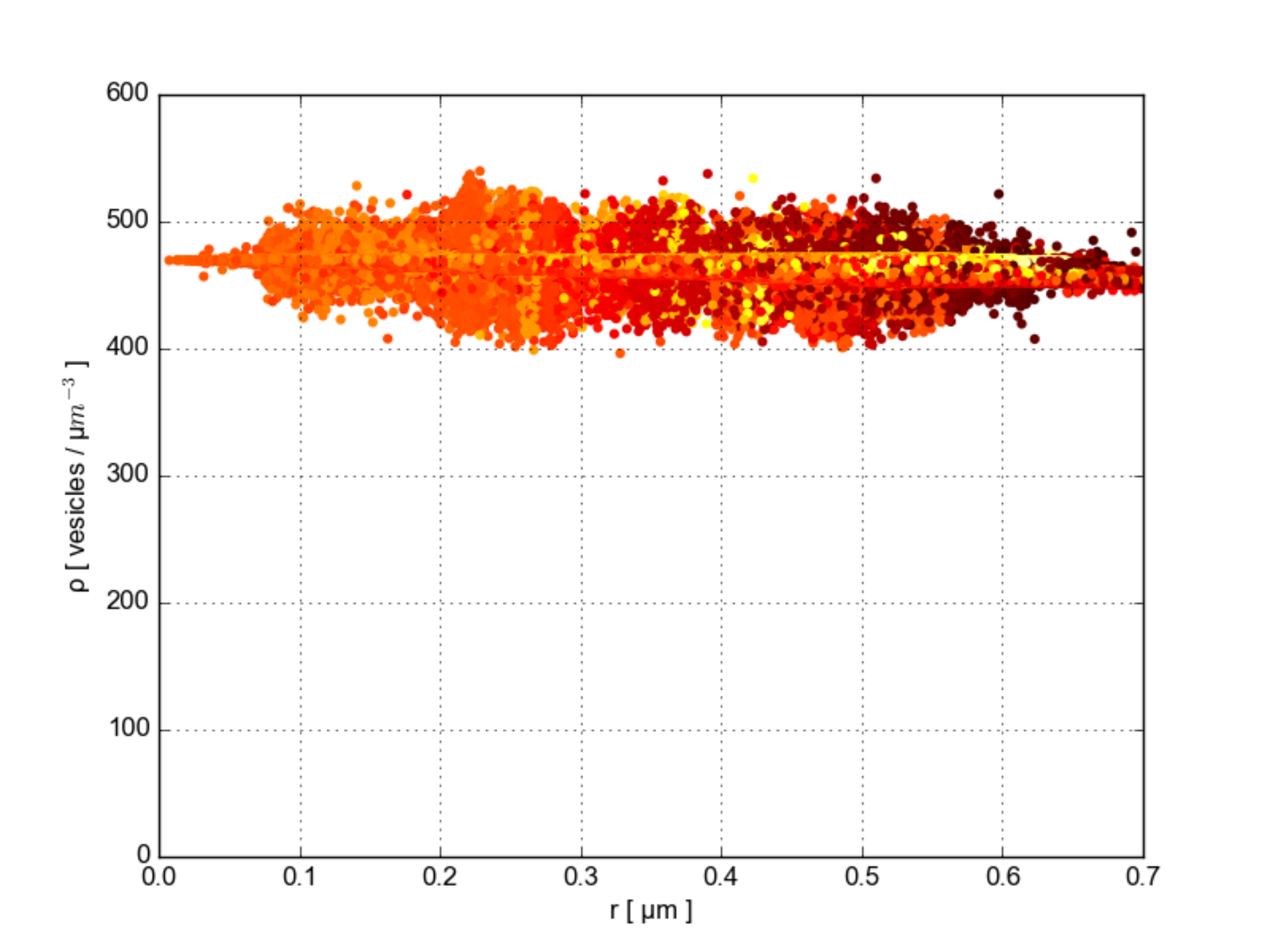
ρ [vesicles / μm^{-3}]
r [μm]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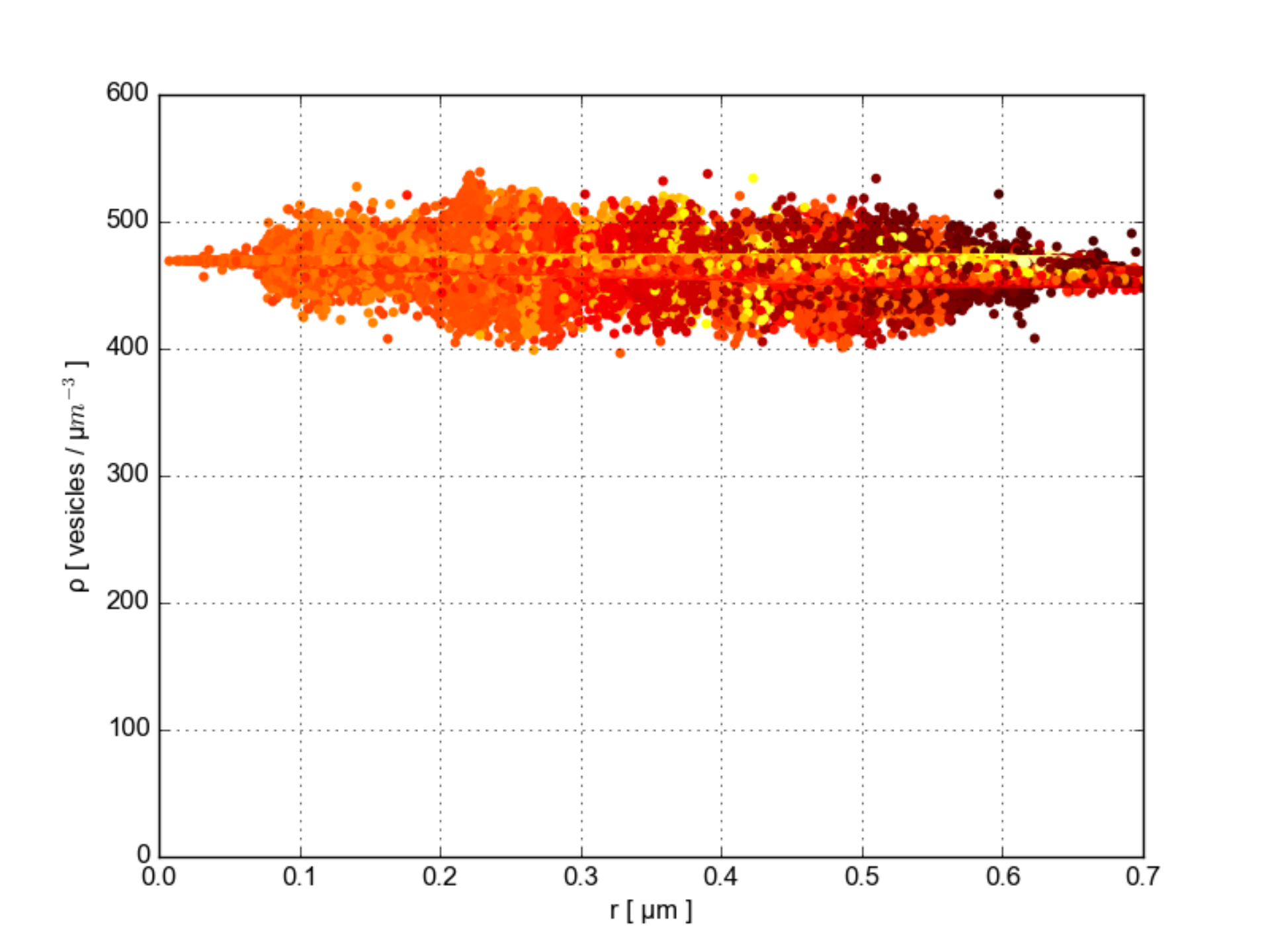
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ρ [vesicles / μm^{-3}]
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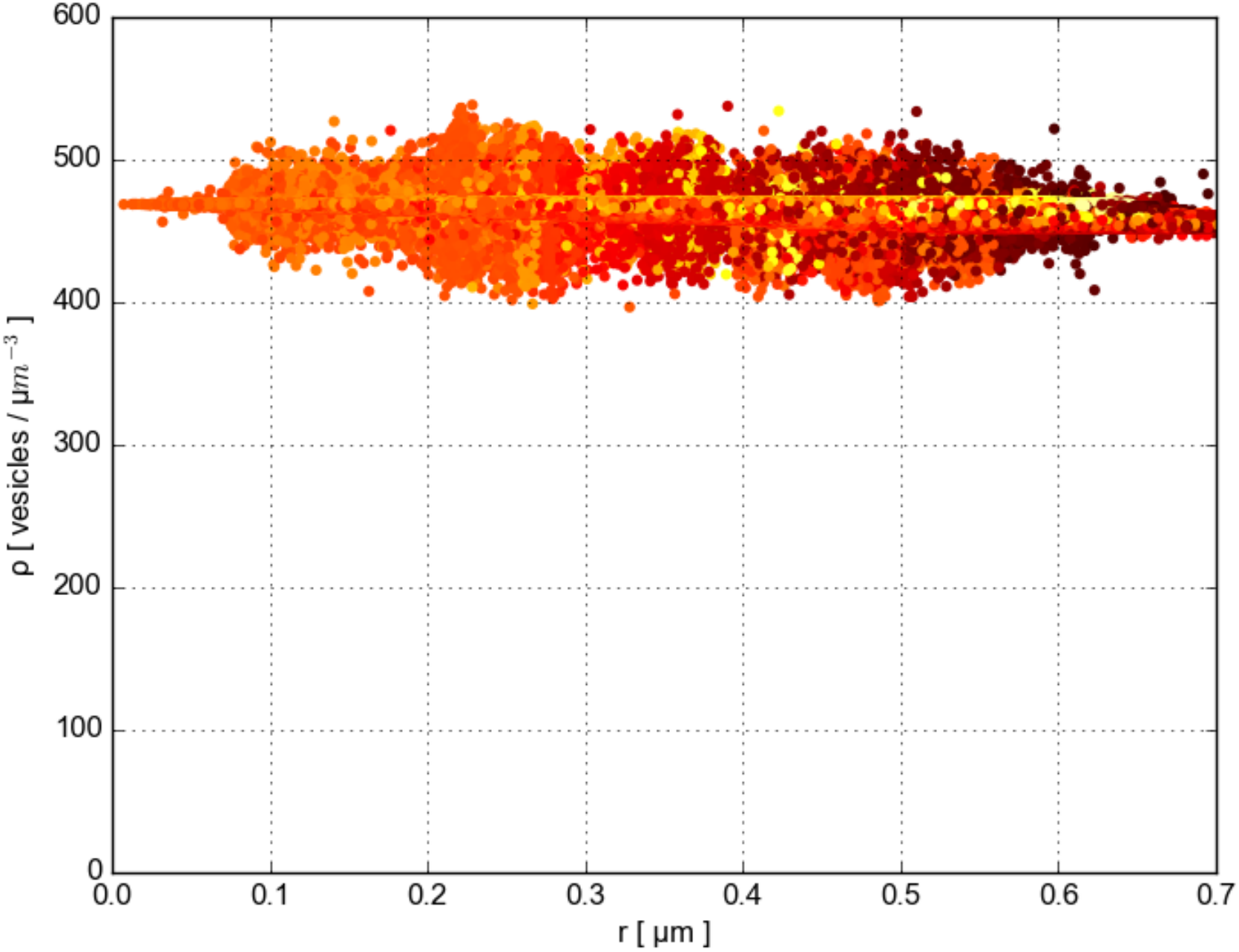
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ρ [vesicles / μm^{-3}]
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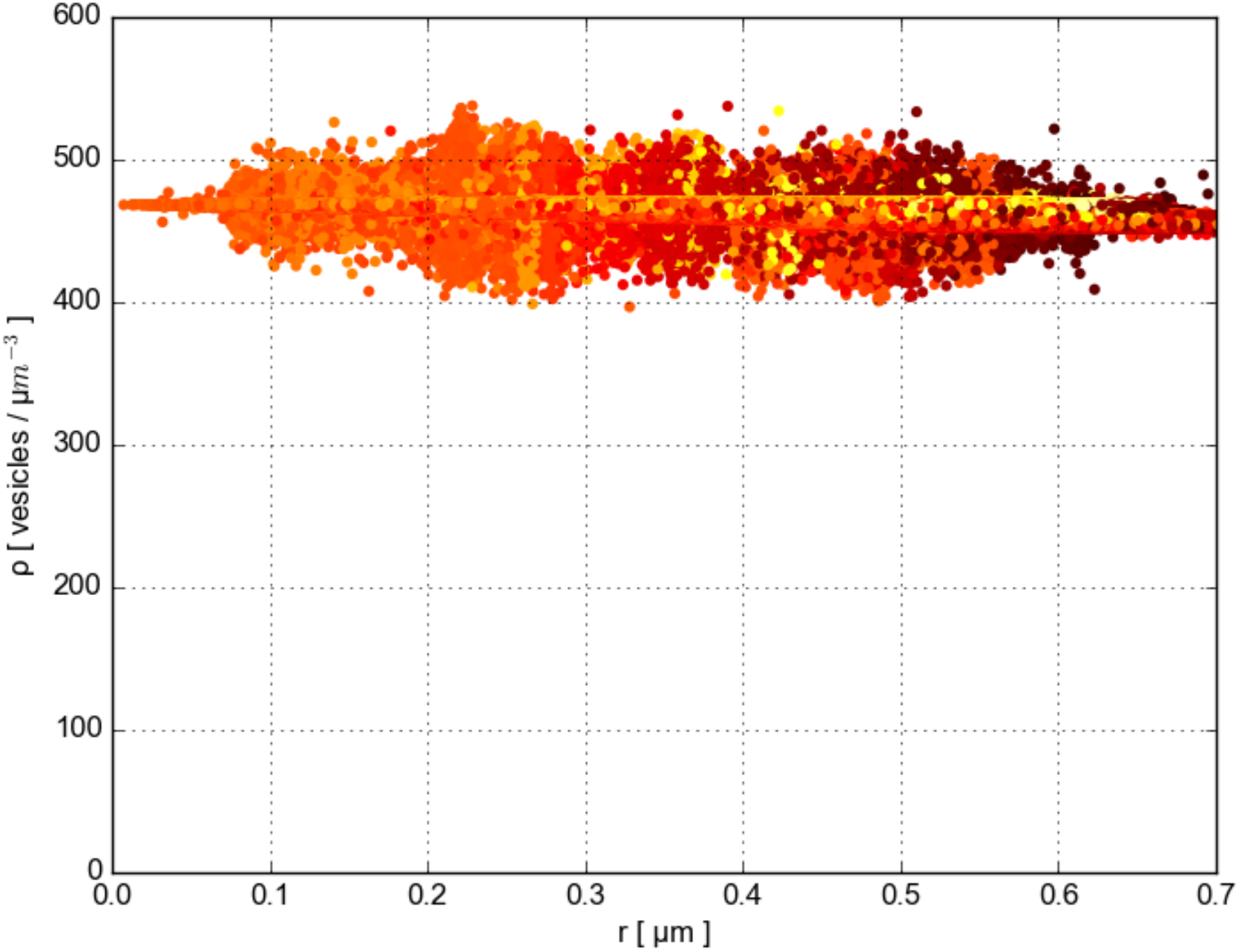
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ρ [vesicles / μm^{-3}]
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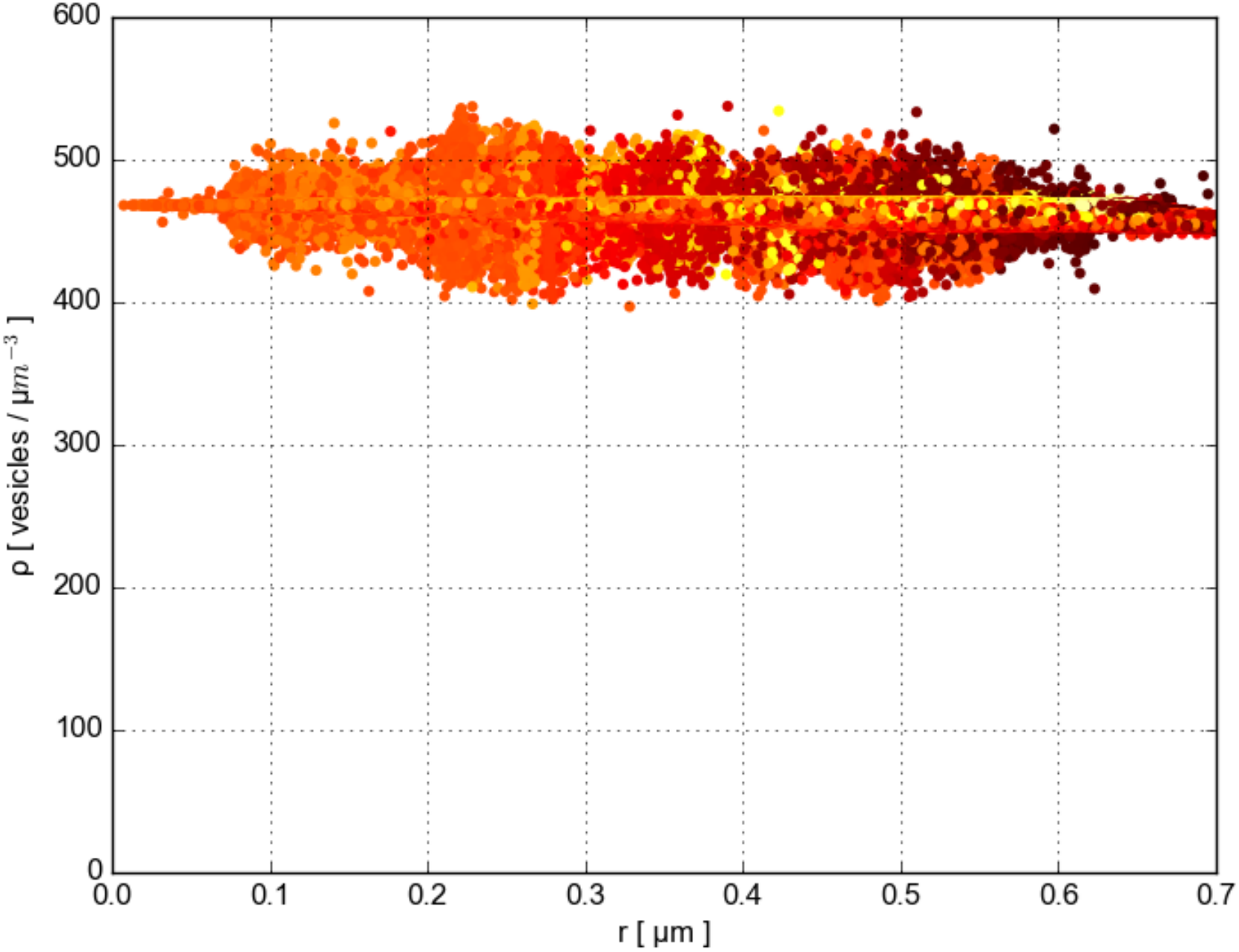
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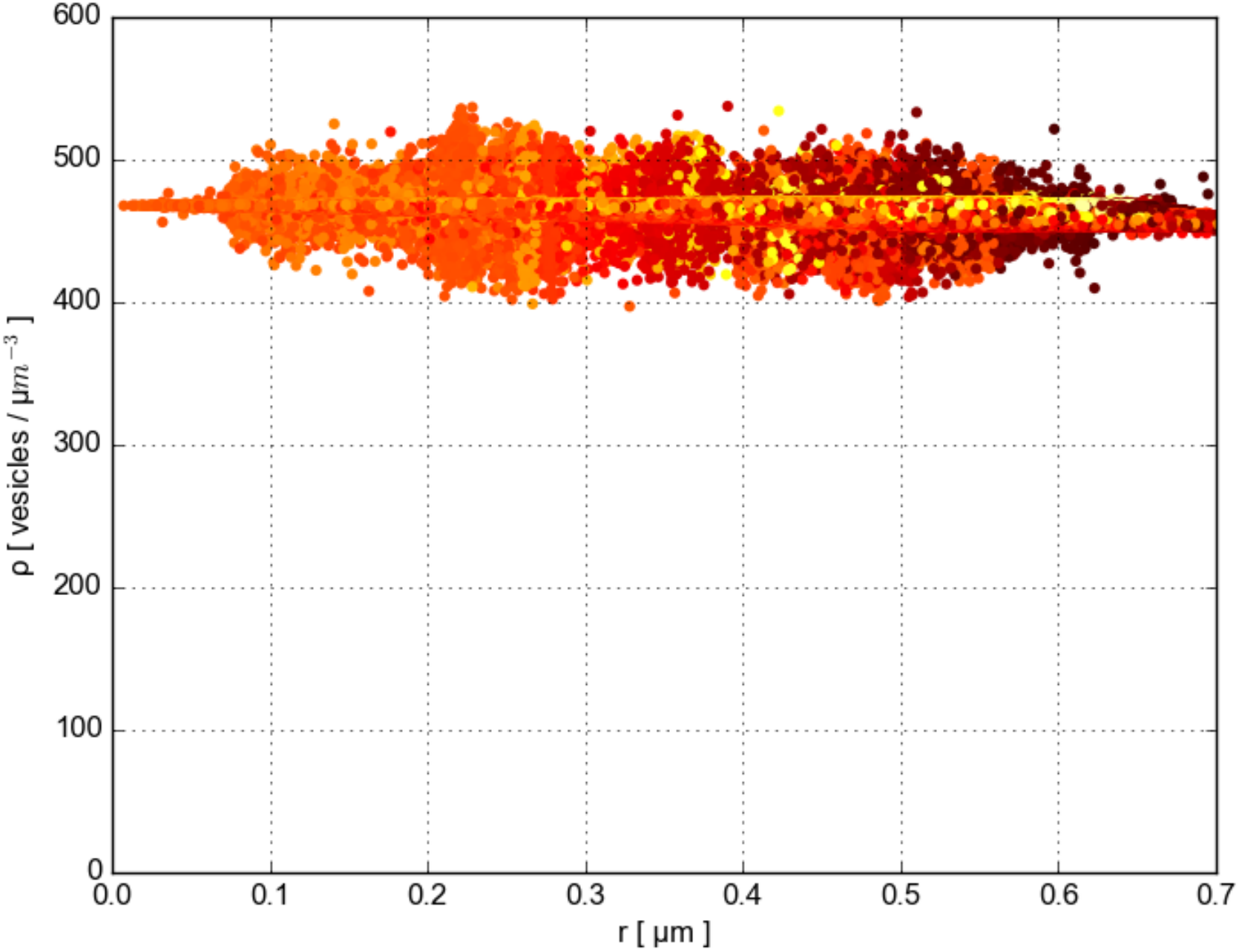
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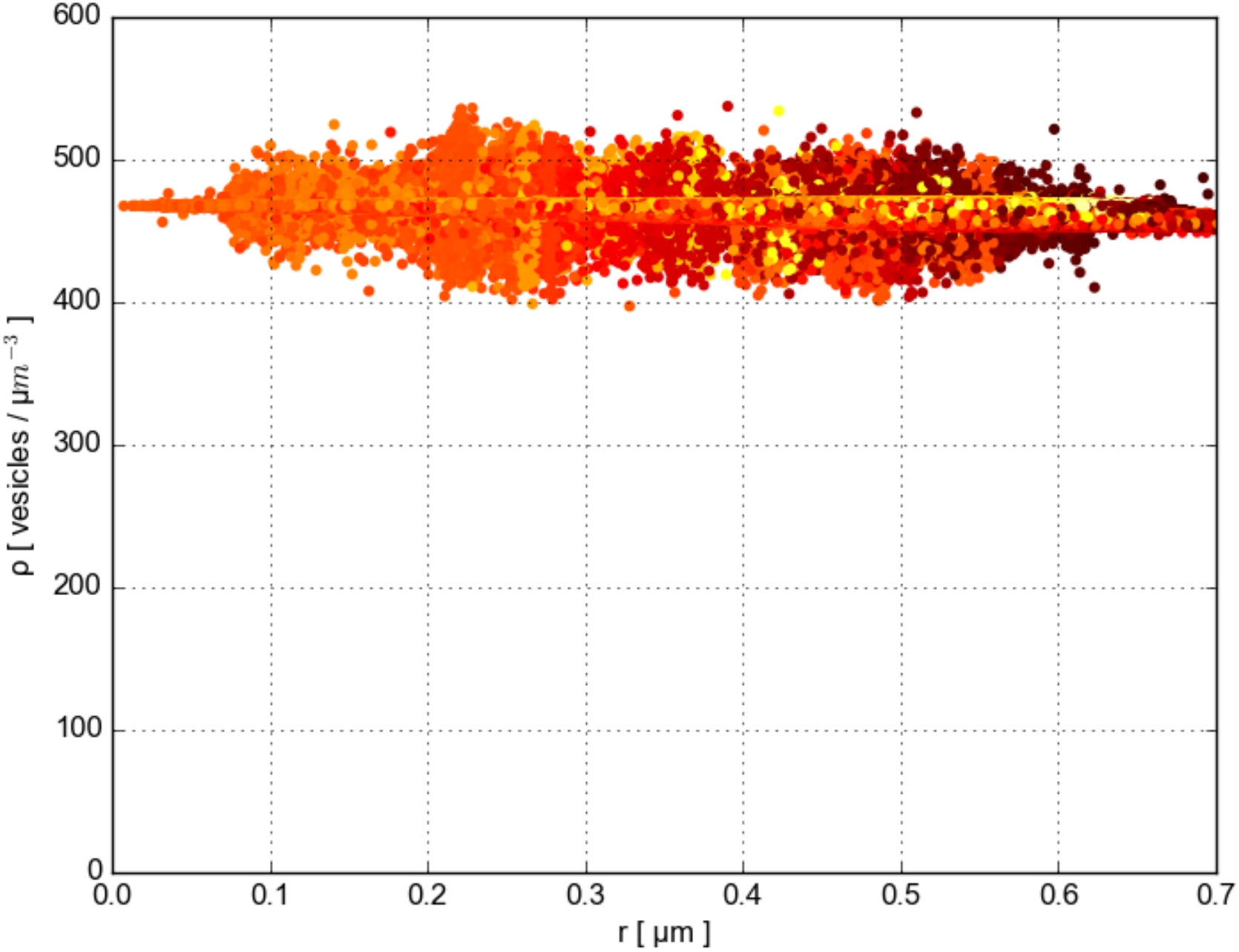
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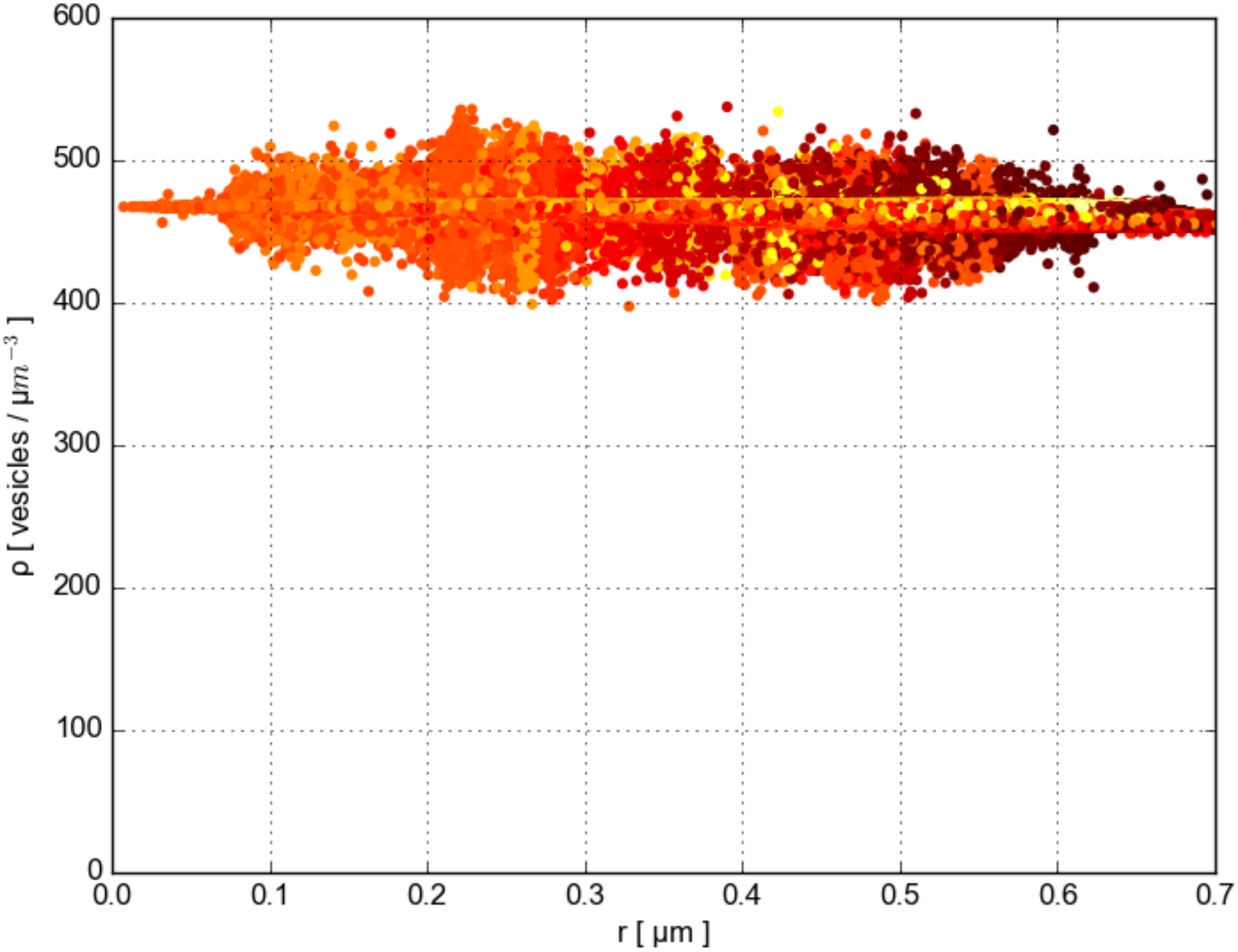
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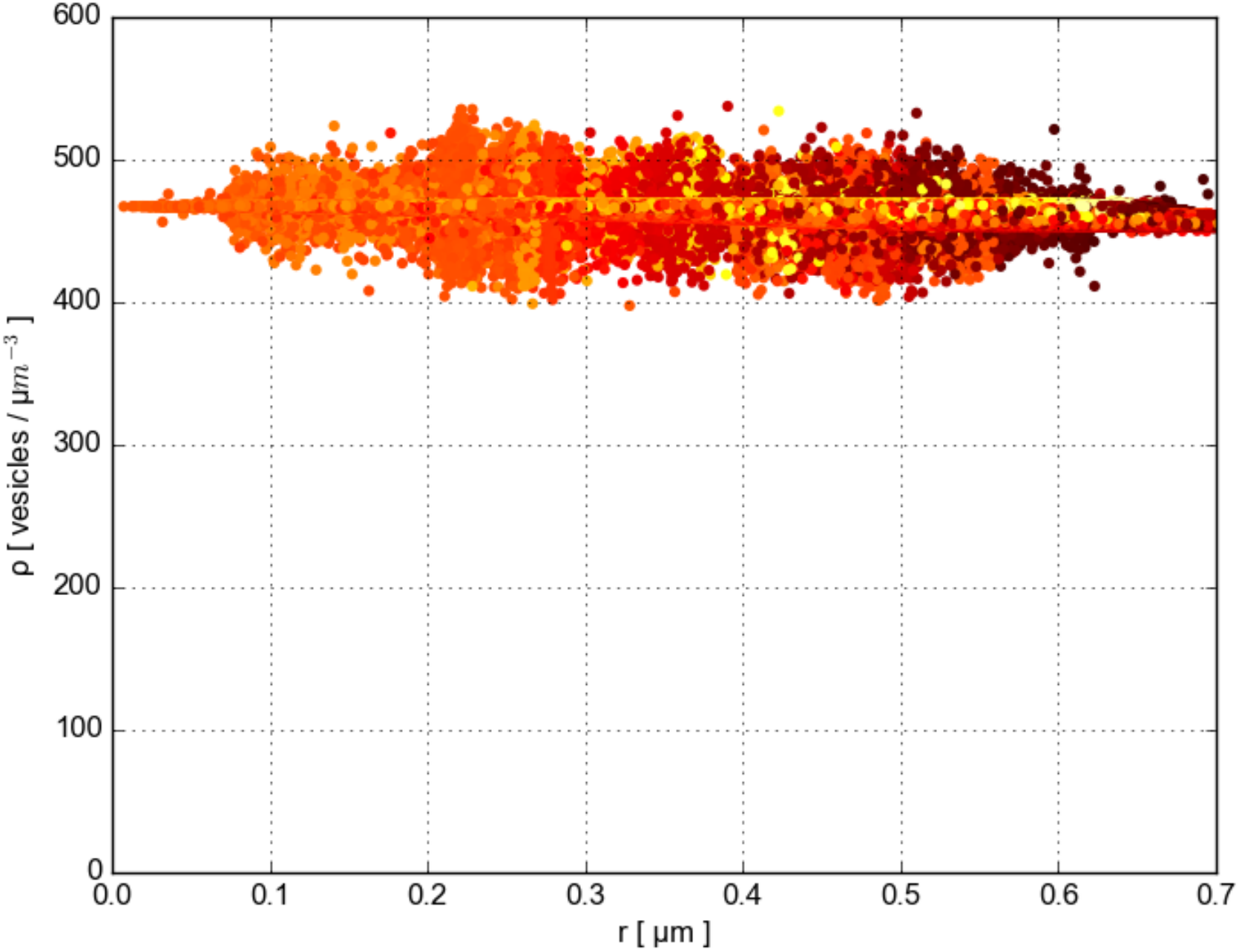
ρ [vesicles / μm^{-3}]
r [μm]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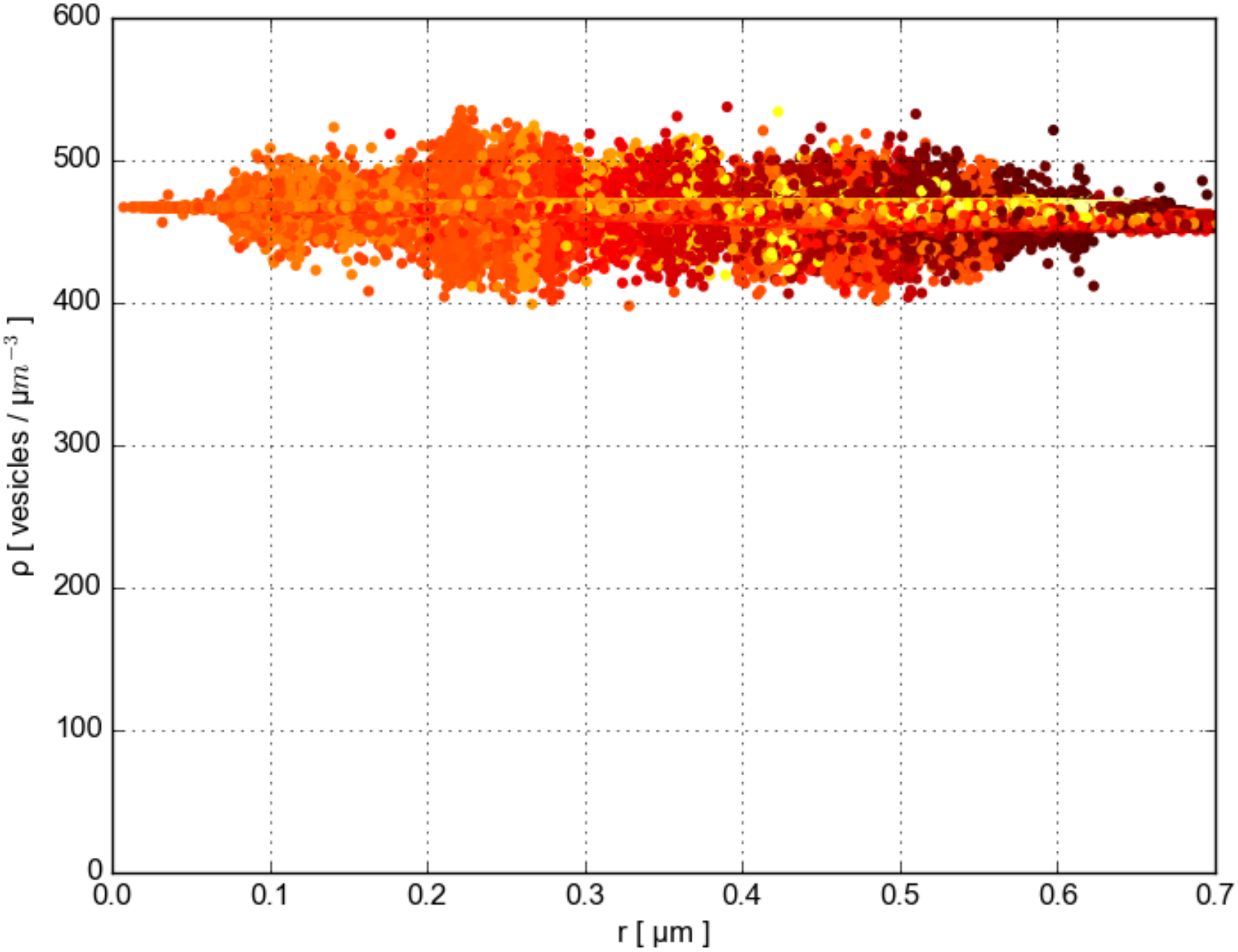
ρ [vesicles / μm^{-3}]
r [μm]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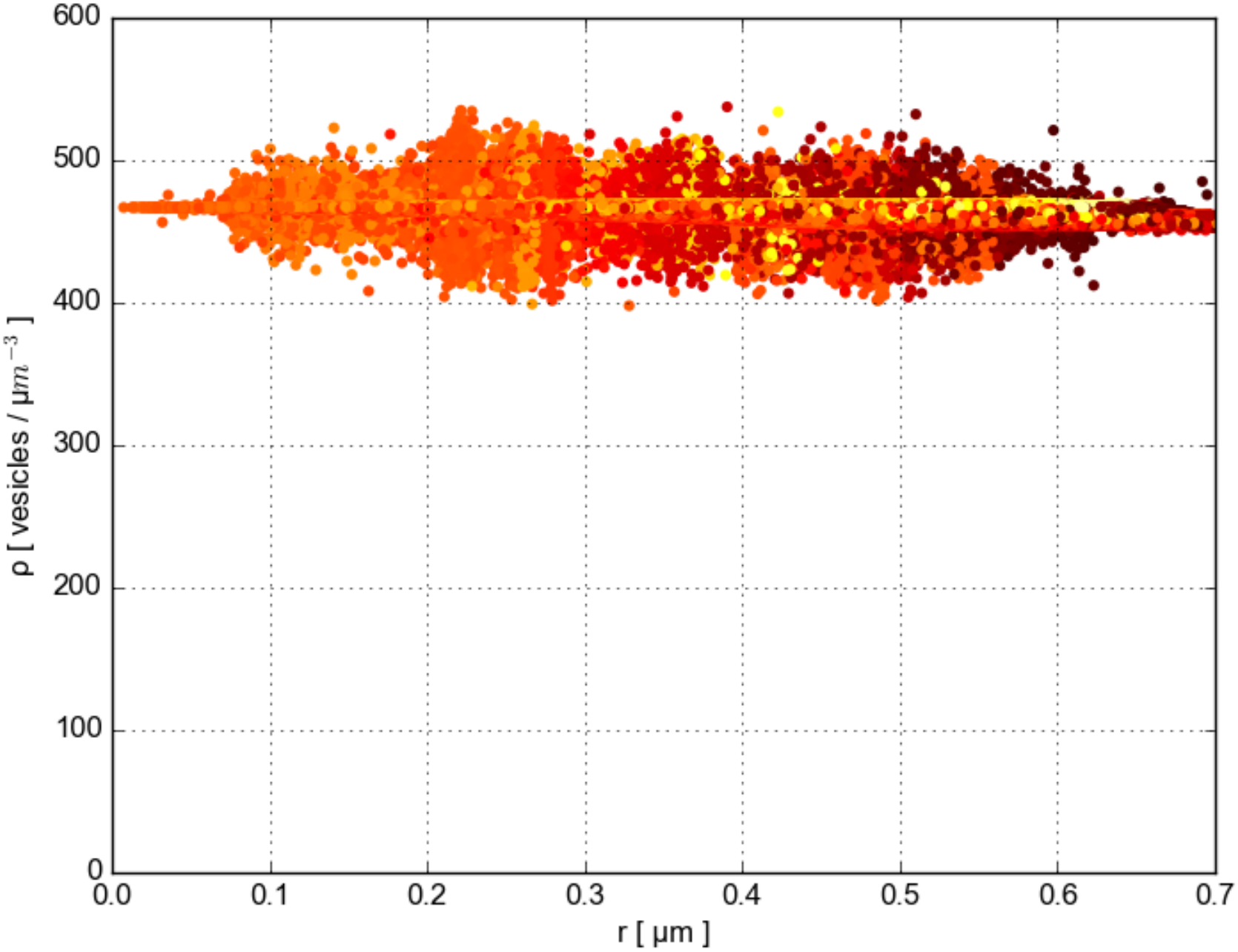
ρ [vesicles / μm^{-3}]
r [μm]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ρ [vesicles / μm^{-3}]
r [μm]

References – Quarteroni shape measure

Quarteroni A., Valli A.: Numerical Approximation of Partial Differential Equations . Springer-Verlag, 2008.

Dziękuję za uwagę.