Optimization documentation for MEDYAN **v4.0**

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1 Performance updates in Medyan4.0

Medyan4.0 is optimized to carry out cache-friendly calculations in **conjugate gradient energy minimization** and **pair-wise distance search**. Pair-wise distance calculations can be accelerated further using SIMD based vectorized search. Please refer to Installation guide for more information.

The SIMD based distance search algorithm along with other optimizations described above accelerates code execution as shown below.

[Actin]=20μM, $\alpha : A$ =0.01, M:A 0.05				
Volume μm^3	**# actin monomers**	**# actin segments**	**MEDYAN4.0** d-days or h-hours	**MEDYAN3.2** d-days or h-hours
1	12000	300	2.5h	12.5h
8	9600	2400	1.5d	8d
27	3.2×10^5	8000	5.5d	40d
125	1.5×10^6	38000	26.75d	360d

Table 1: Estimated time taken by single core on a single CPU for 1000s of simulation time

[Actin]=50μM, $\alpha : A$ =0.01, M:A 0.05				
Volume μm^3	**# actin monomers**	**# actin segments**	**MEDYAN4.0** d-days or h-hours	**MEDYAN3.2** d-days or h-hours
1	30000	750	22h	3.5d
8	2.4×10^5	6000	12.25d	58d
27	8.1×10^5	20000	35d	229.5
125	3.8×10^6	94000	220d	2395d

Table 2: Estimated time taken by single core on a single CPU for 1000s of simulation time