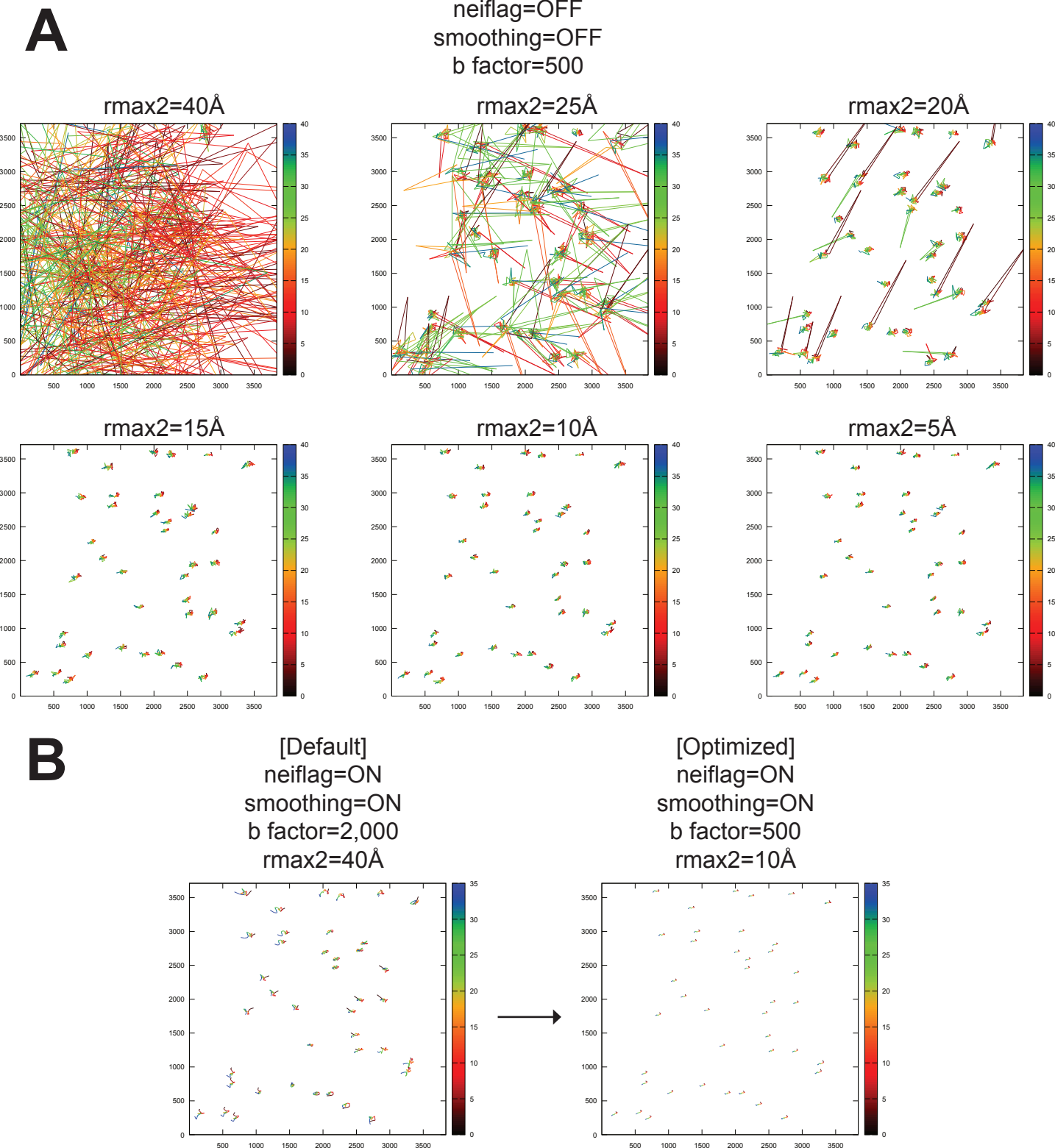
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smoothing=OFF
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rmax2=40Å
rmax2=25Å
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rmax2=15Å
rmax2=10Å
rmax2=5Å
B
[Default]
neiflag=ON
smoothing=ON
b factor=2,000
rmax2=40Å
[Optimized]
neiflag=ON
smoothing=ON
b factor=500
rmax2=10Å