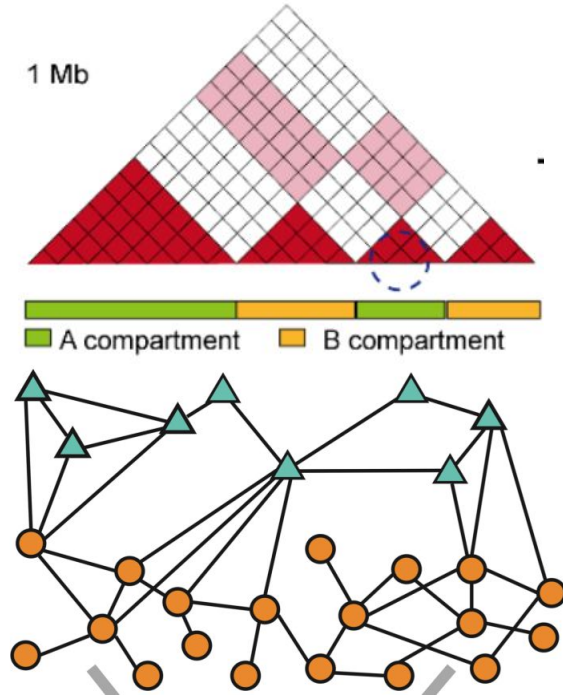# Problem
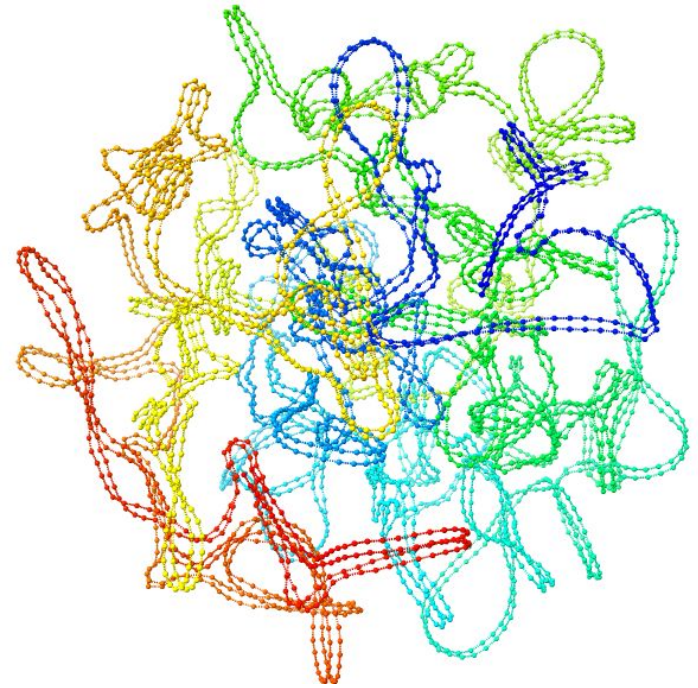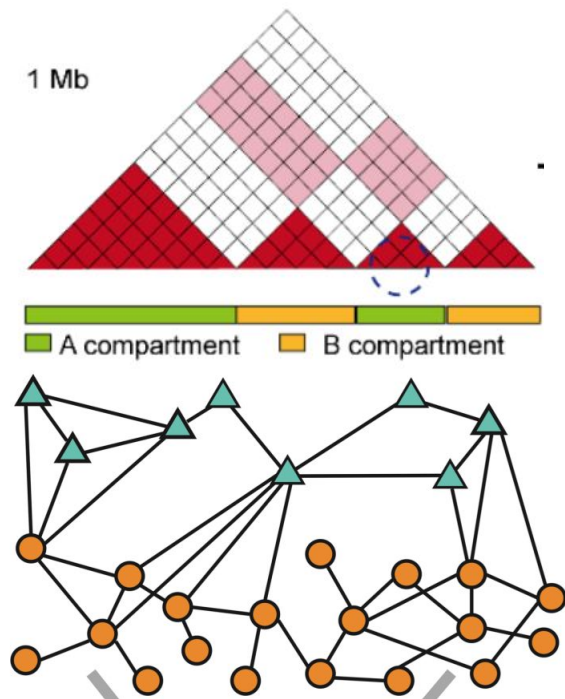

Chromatin graph model
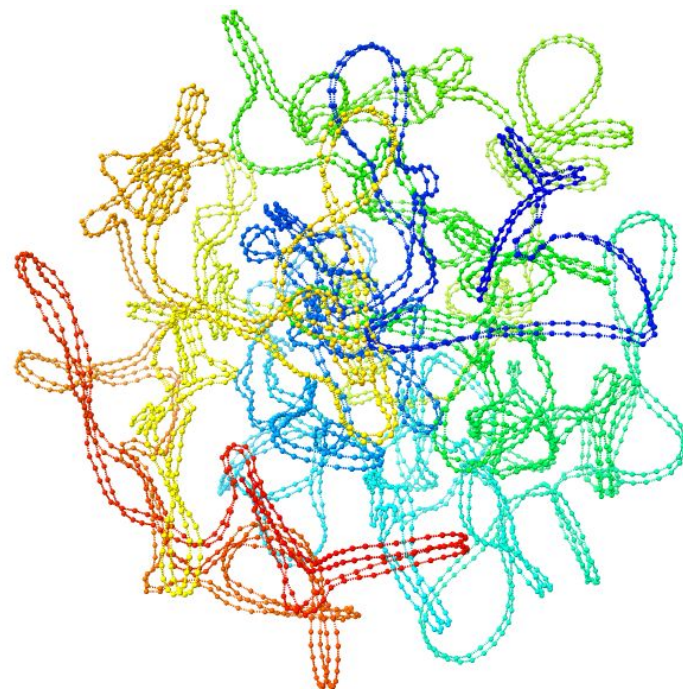
Chromatin 3D model

Currently using
Molecular Dynamics
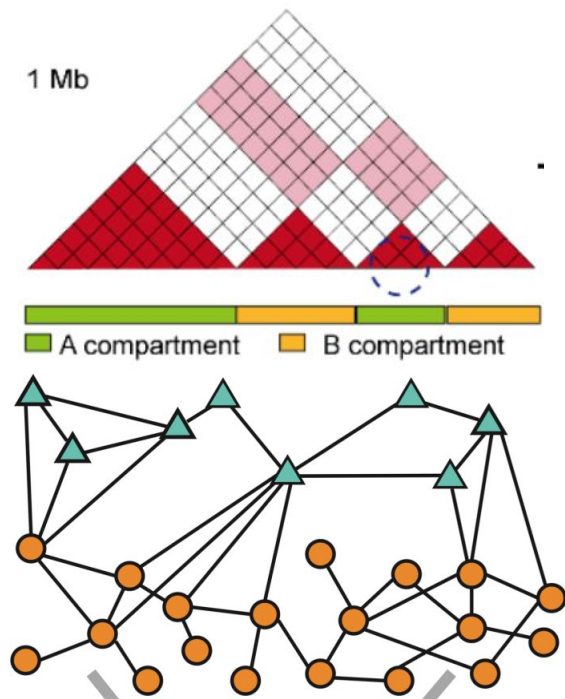
1 Mb

A compartment   B compartment

Chromatin graph model

Chromatin 3D model

Currently using
Molecular Dynamics
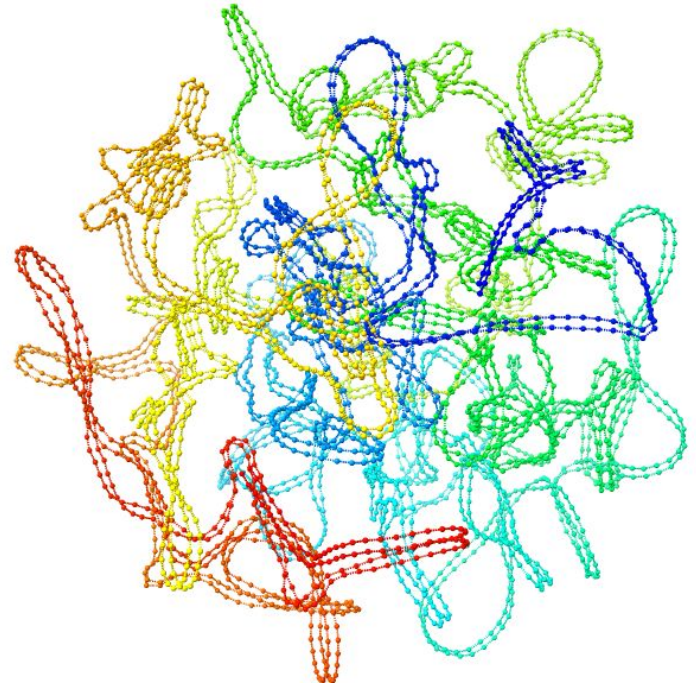
But it's slow and
computationally
expensive

1 Mb

A compartment   B compartment

Chromatin graph model
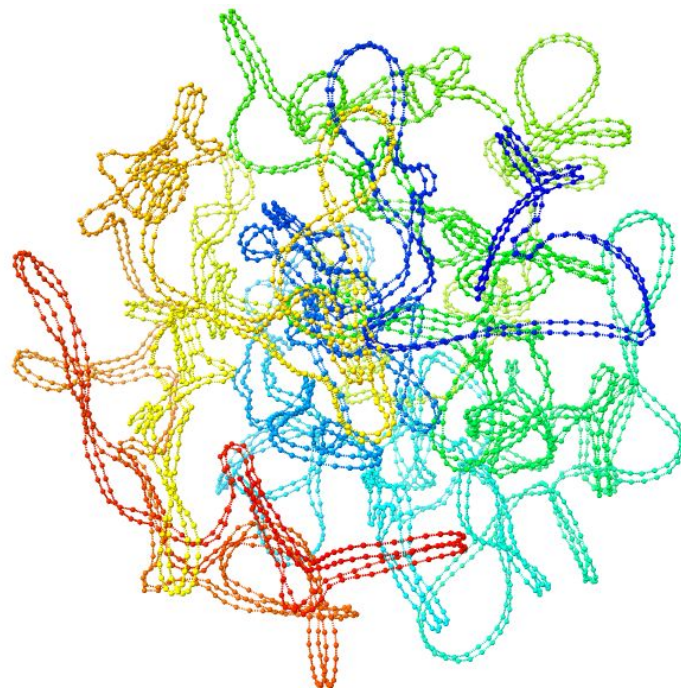
Chromatin 3D model

Can MultiDimensional Scaling (MDS) help?

Distance Matrix

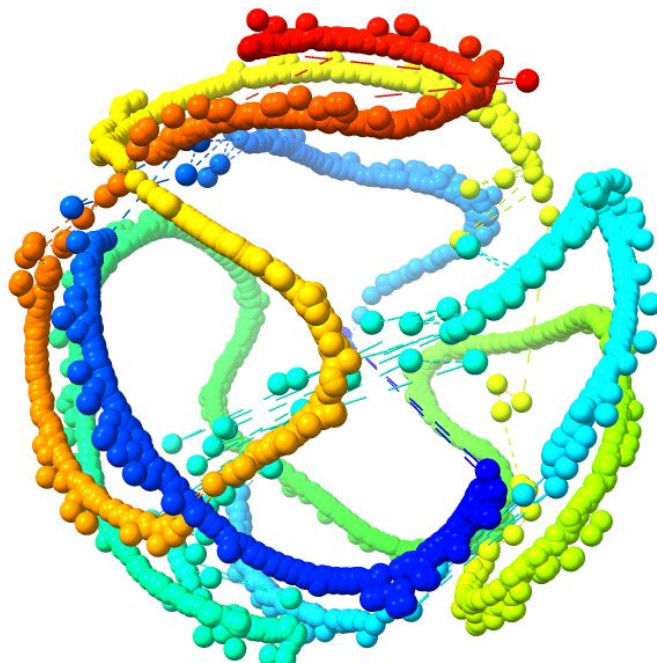|	A	B	C	D	E	F
A	0	16	47	72	77	79
B	16	0	37	57	65	66
C	47	37	0	40	30	35
D	72	57	40	0	31	23
E	77	65	30	31	0	10
F	79	66	35	23	10	0

Pairwise distances NxN

3D coordinates Nx3

Progress so far
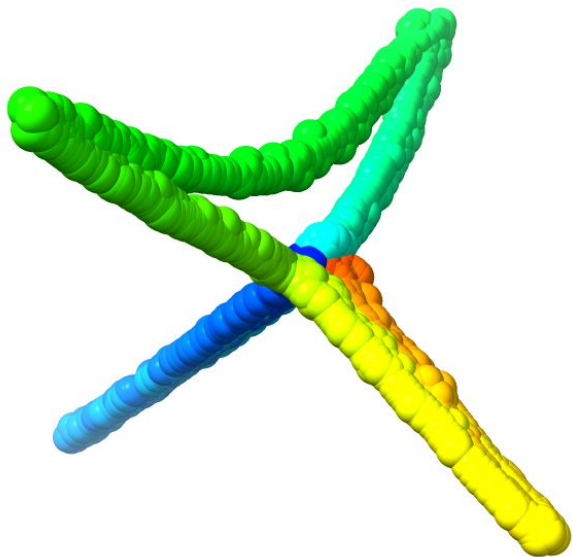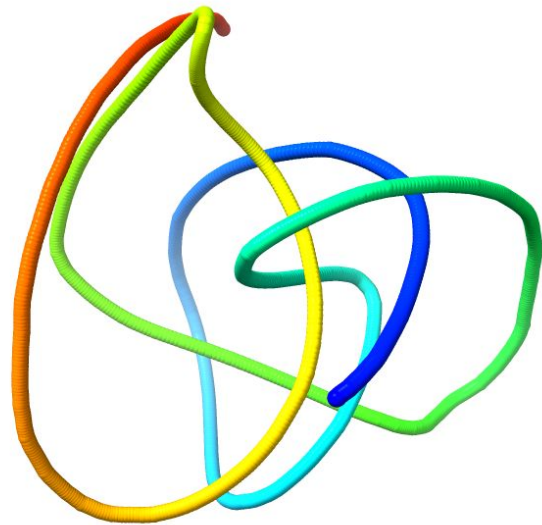

Classical MDS (PCA-like)
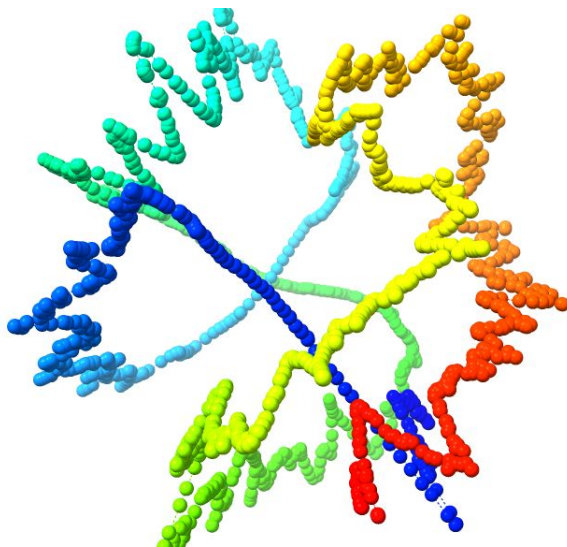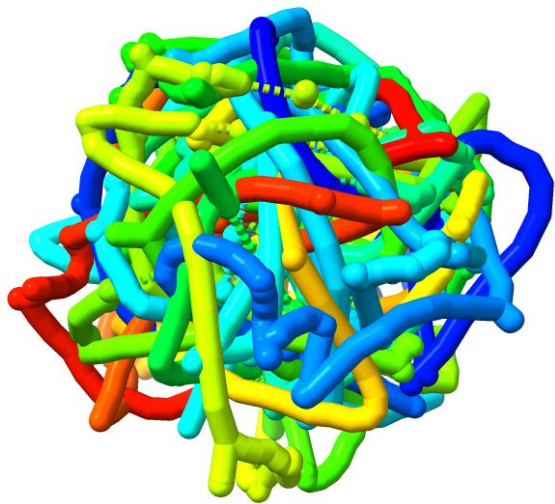- too sensitive to noise

SMACOF version
- better, but still bad

Progress so far

Weighted SMACOF
- could work, trying to configure the parameters