Tube Picture of Polymers

T. Neuhaus

t.neuhaus@nic.fz-juelich.de

NIC

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- tube model

  - 3d tube with volume exclusion and thickness D

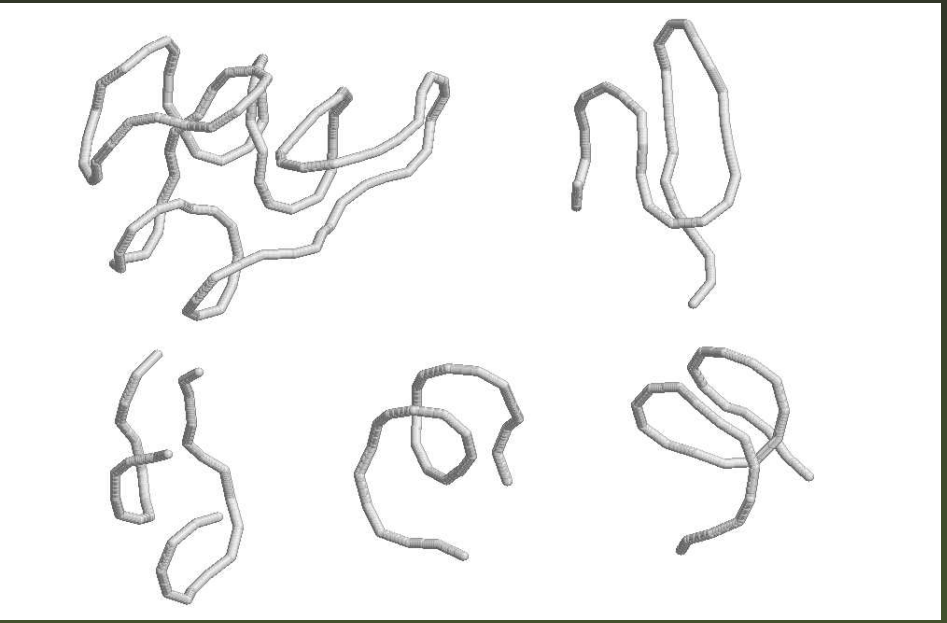
  - attractive homopolymer interaction, distance scale R_{int}

  $\rightarrow$ volume exclusion and attraction compete in a compact configuration

  , whose degree of compactness is tunable by : D/R_{int}

  J.R.Banavar, A.Flammini, D.Marenduzzo, A.Maritan and A.Trovato, J.Phys.:Cond.Matt.**15**:1787(2003)

Introduction..



from Neuhaus, Zimmermann, Hansmann, ”Ring Polymer Simulations with Global Radius of Curvature”, 2006, submitted to PRE.

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- global radius of curvature (grc)

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- conclusion

Global Radius.

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- any 3 nondegenerate points $\vec{x}, \vec{y}, \vec{z}$ define a unique circle through these points with a radius of curvature: R_{rc}
- which can be calculated easily

$$R_{rc}(\vec{x}, \vec{y}, \vec{z}) = \frac{|\vec{x} - \vec{y}| \quad |\vec{x} - \vec{z}| \quad |\vec{y} - \vec{z}|}{4A_{Triangle}(\vec{x}, \vec{y}, \vec{z})}$$

$$A_{Triangle}(\vec{x}, \vec{y}, \vec{z}) = \sqrt{s(s-a)(s-b)(s-c)}$$

$$s = \frac{a+b+c}{2}$$

$$a = |\vec{x} - \vec{y}| \; ; \; b = |\vec{x} - \vec{z}| \; ; \; c = |\vec{y} - \vec{z}|$$

Global Radius..

- we will consider $3d$ chains with length L

$$L = Na$$

$$a = 1$$

$$conf = [\vec{x}_0, ..., \vec{x}_N]$$

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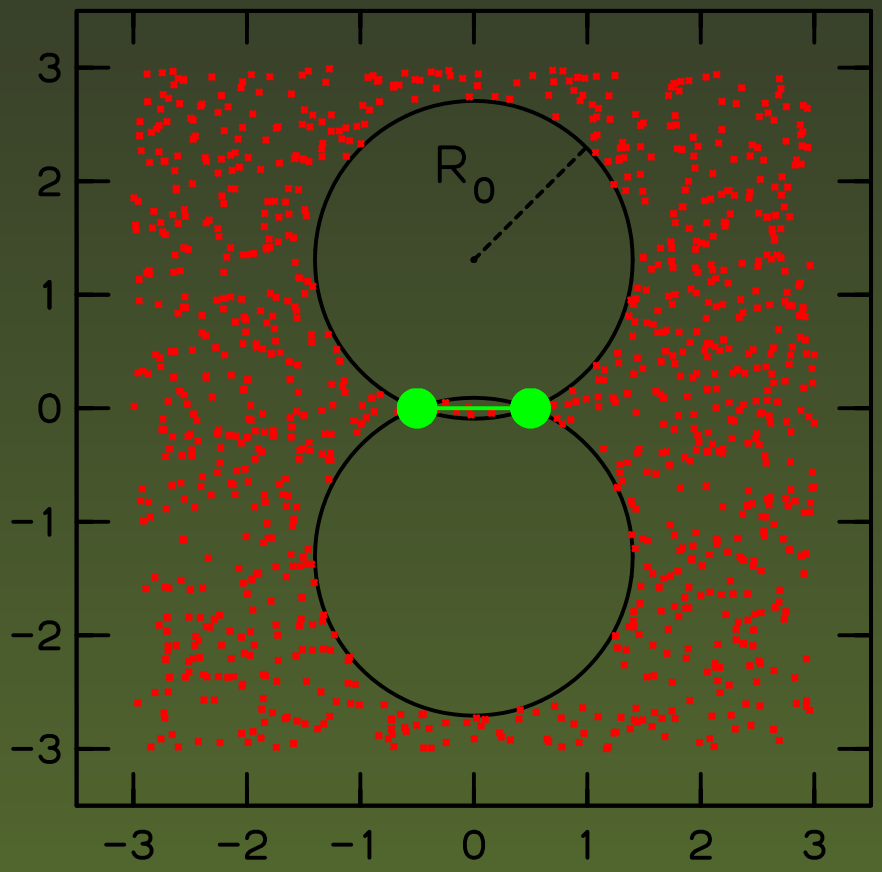
- providing a regularization of thick polymers with thickness $D \approx 2R_{grc}$

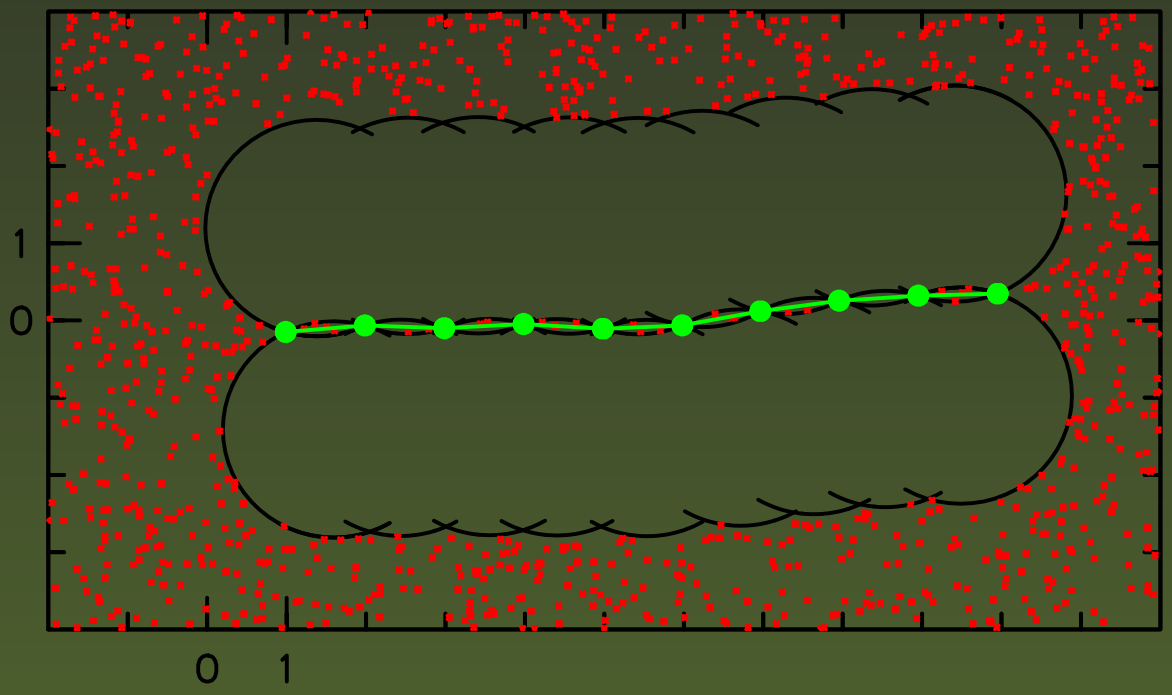
Global radius...

- solution to $R_{grc} > 1.4$ for a 3 body problem



Global radius....

- solutions to $R_{grc} > 1.4$ for a L+2 body problem



Global Radius.....

- partition function of thick polymers

$$\sum_{conf} \rightarrow \sum_{conf} \delta(2R_{grc} - D)$$

$$\sum_{conf} \rightarrow \sum_{conf} \Theta(2R_{grc} - D)$$

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- a discretized tube on a discrete chain ($a = 1$) $\rightarrow$ the tube picture breaks down at $R_{grc} = 0.5$ or $D = 1$

  however continuous tubes on discrete chains are feasable

Global Radius.....

- grc in mathematics:

  given ring of length L, thickness D with knot K

  find

$$\max D(\text{ring})\,|_{L,K\ fixed} \quad \text{for all rings}$$

  e.g. circle

$$D = \frac{1}{\pi} L(K = \text{trivial})$$

  defines the shape of ideal knots with

$$R_{lrc} \geq R_{grc} \quad \text{for non} - \text{trivial knots}$$

  O.Gonzalez and H.Maddocks, PNAS **96**:4769 (1999)

  that is : ”dense packing” of tubes with a constraint

  constraint could also be : confinement

  and : dense packing of tubes differs from dense packing of spheres

off lattice SAW.

- long chain limit : field theory

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- $N = 2, 1, 0$; correlation length divergence $\nu = .67, .63, \nu_{SAW} = 0.5877(6)$ [Li,Madras,Sokal,1995], $0.5874(2)$ [Prellberg,2001], $0.58765(20)$ [Grassberger,2004] and $0.58758(7)$ [Nickels,1997].

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$$Z_{Ring}(D) = \sum_{closed\ loops} 1 \quad \Theta(2R_{grc} - D)$$

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$$\sqrt{< R^2_{rms2} >} \propto L^{\nu_{SAW}}$$

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- generalized pivot update a la Sokal on the ring

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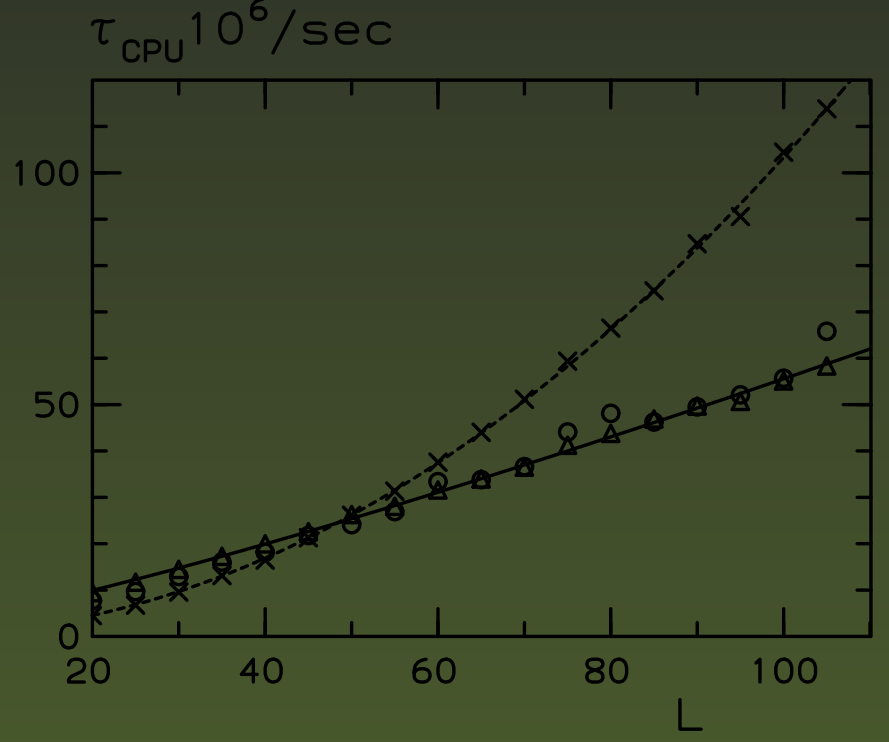


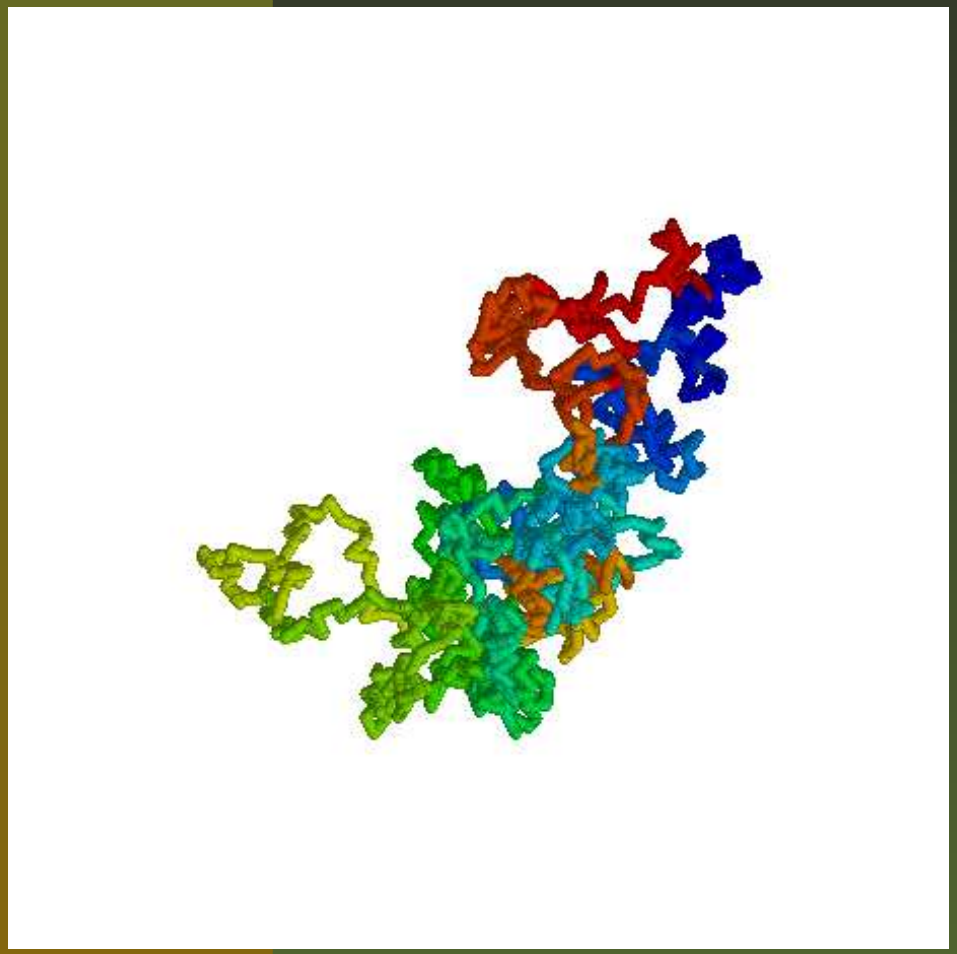
crosses : calculation of LJ potential

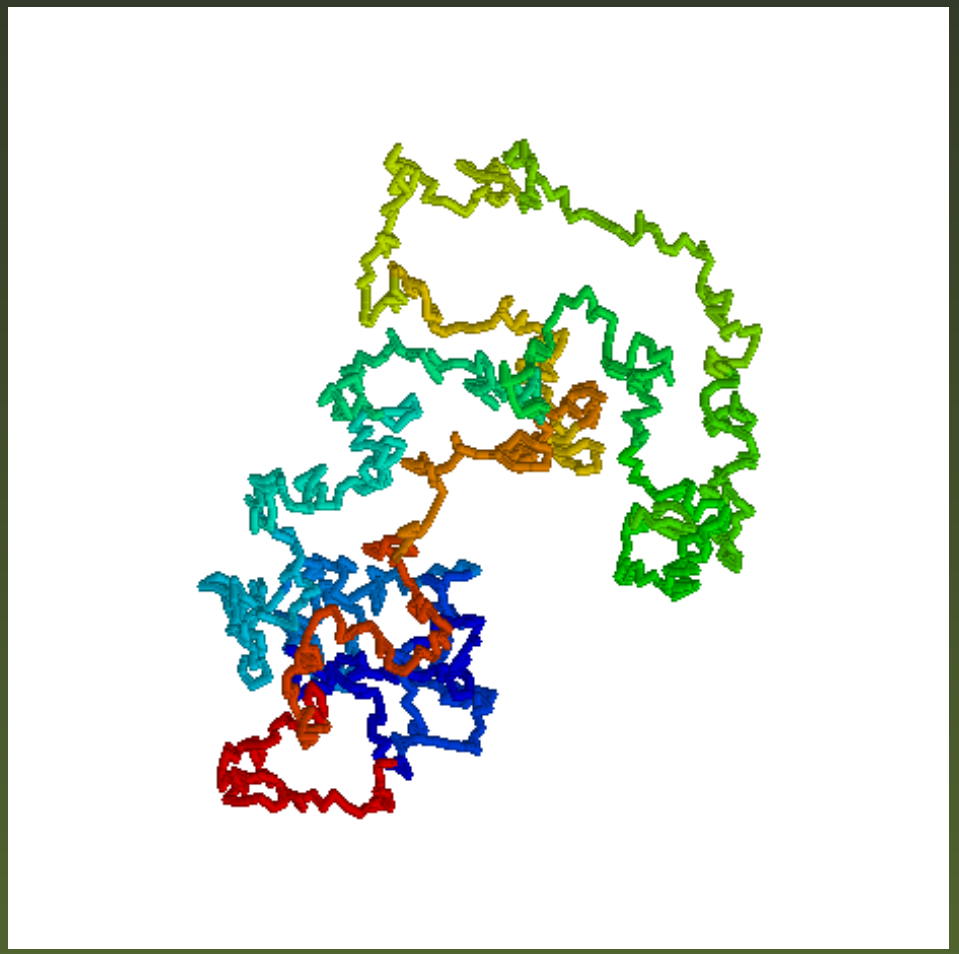
circles : grc calculation via PROJ

triangles : grc calculation via CELL LIST METHOD

off lattice SAW...

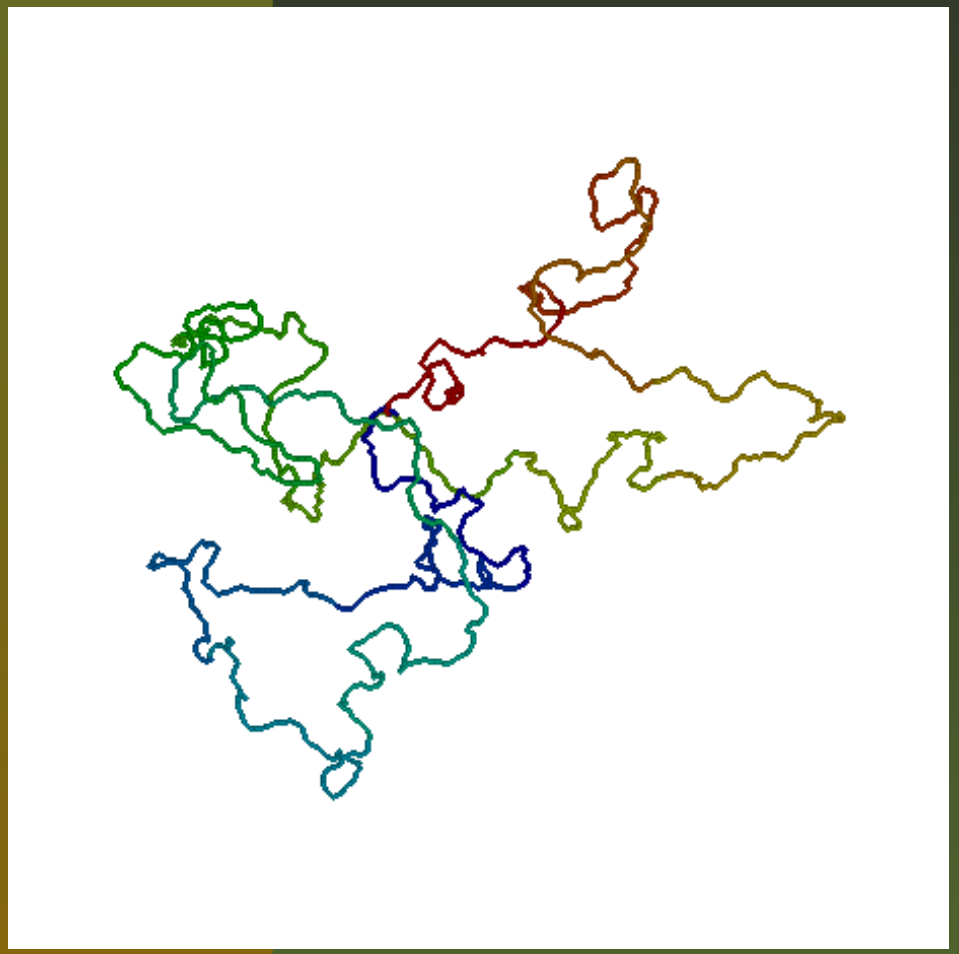
$D = 0.5$ and $D = 1$ at $L = 1000$

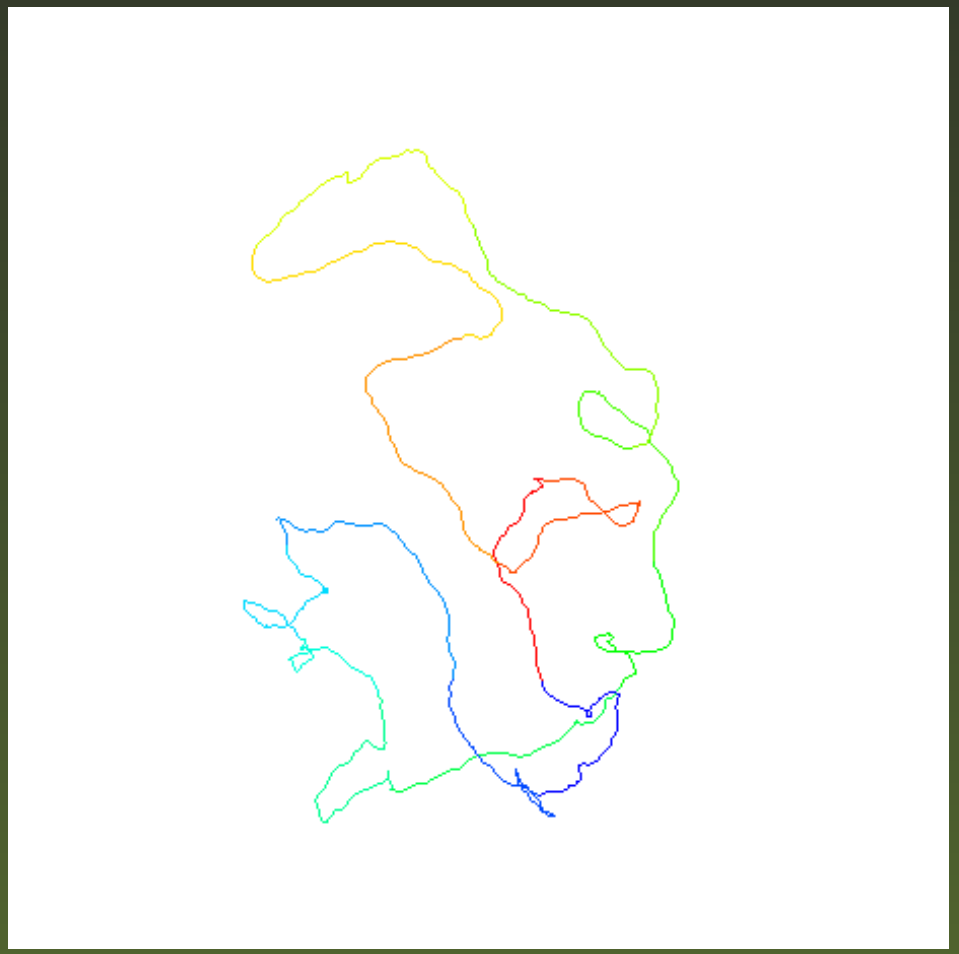




off lattice SAW....

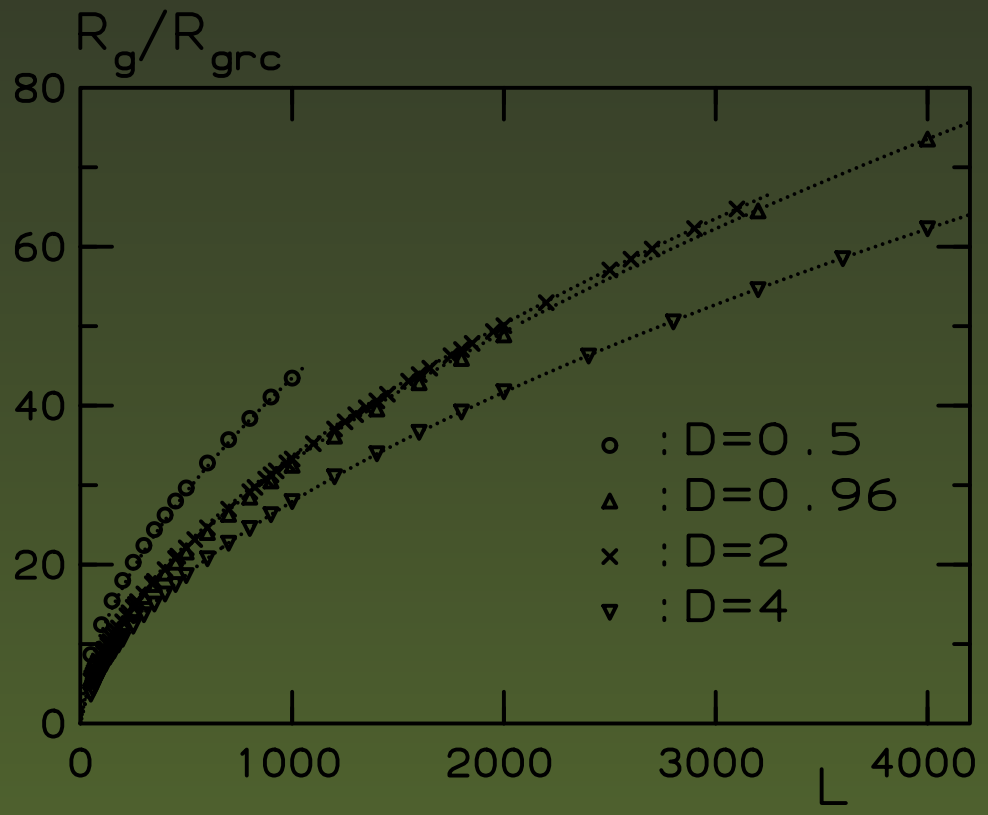
$D = 2$ and $D = 4$ at $L = 1000$





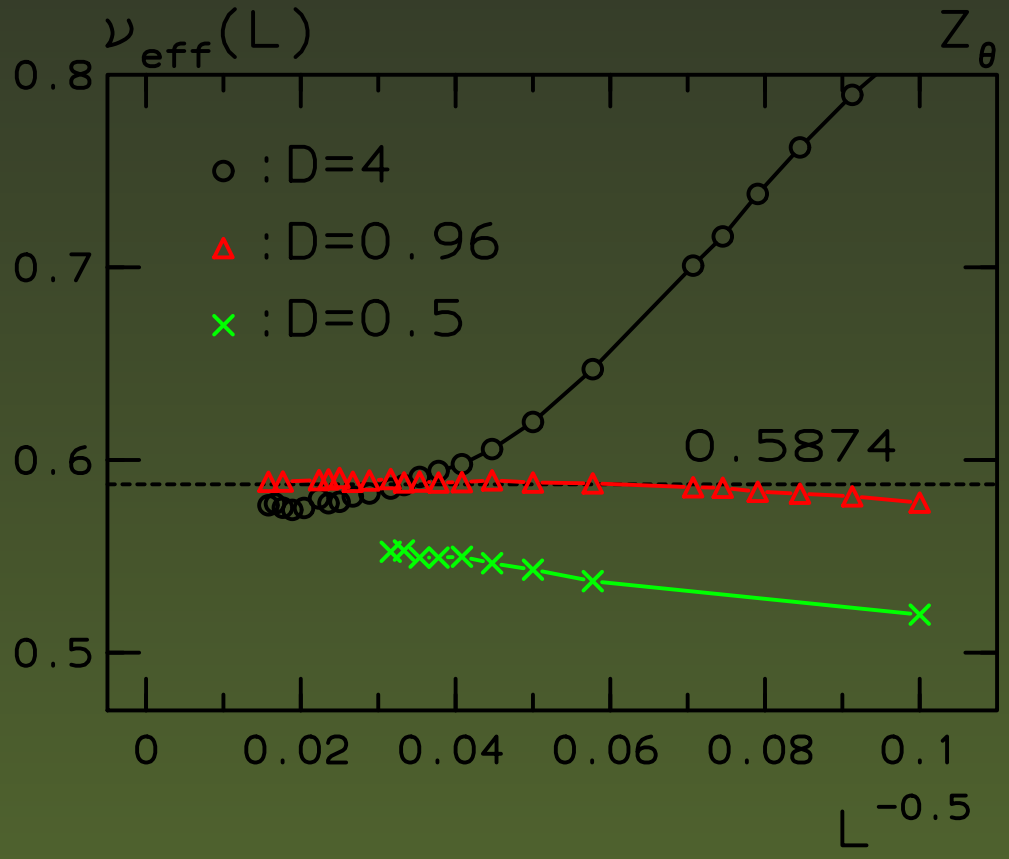
off lattice SAW.....

Radius of Gyration data



off lattice SAW.....

effective exponent ν_{SAW} data



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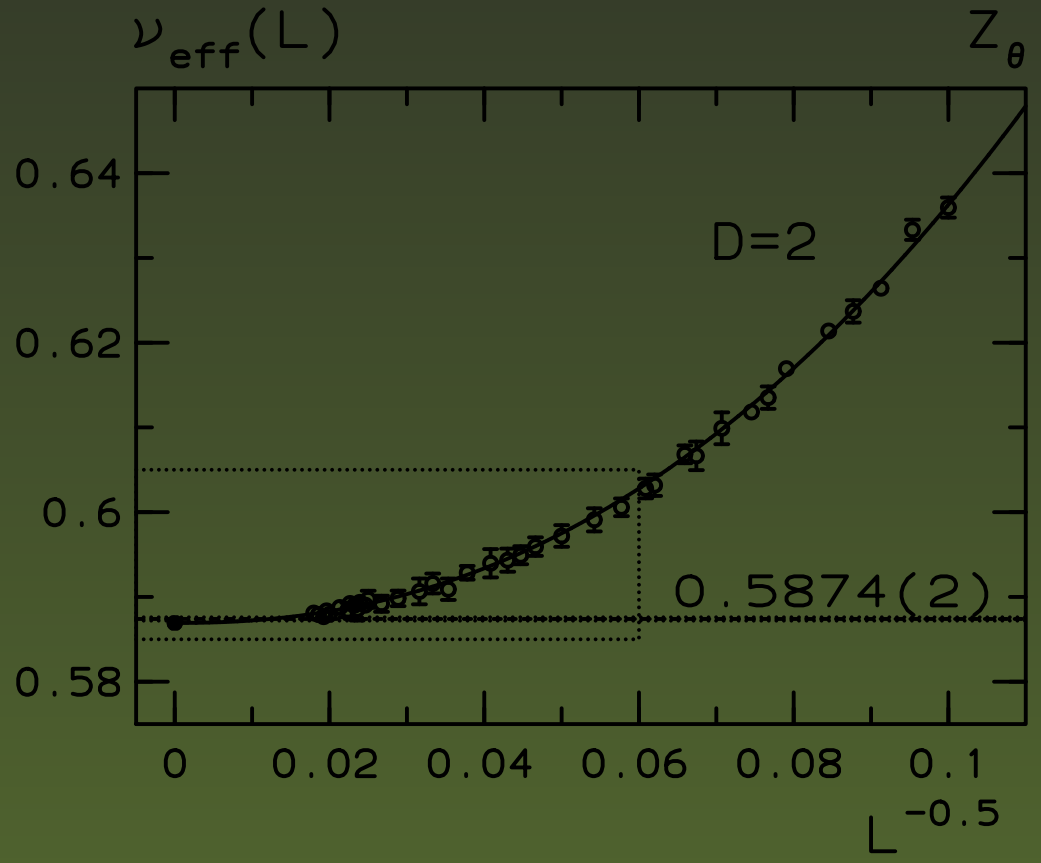

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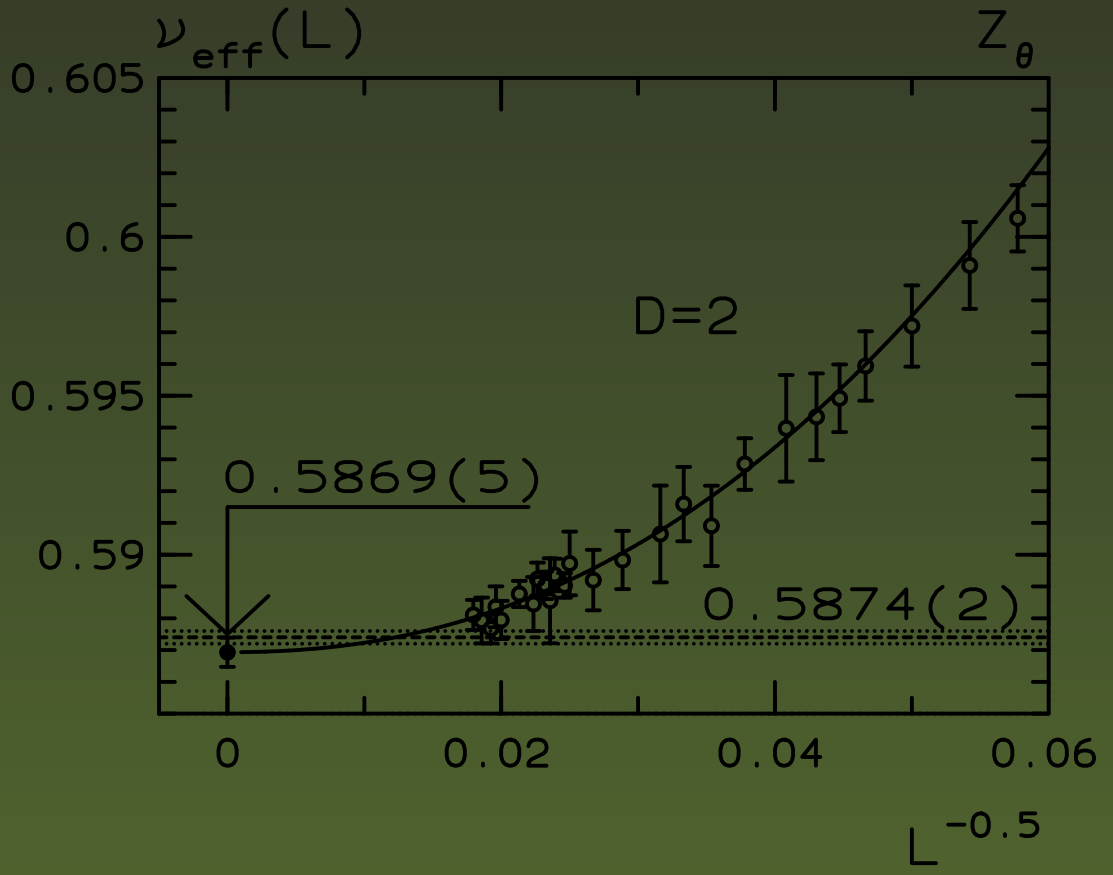

off lattice SAW.....

the fit at $D = 2$

$$\nu_{SAW,eff}(L) = 0.5869(05) + [\frac{8.2(9)}{L^{1.11(3)}}]$$

at $\chi^2_{d.o.f} = 0.72$ yields

$$\nu_{SAW} = 0.5869(5)$$

the scaling correction : $\mathrm{const}/L^{\Delta}$

has an exponent $\Delta \approx 1$

which is off from the FT value $\Delta_{FT} \approx 0.5$ [magic point ?]

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$$H_{pot} = \sum_{i=0,\ldots,N;j=0,\ldots,N;i<j} V_{int}(r_{ij})$$

$$V_{int}(r_{ij}) = 4((\frac{1.6}{2^{1/6} r_{ij}})^{12} - (\frac{1.6}{2^{1/6} r_{ij}})^{6})$$

$$90 < \theta_{bond,bond} = 102.3 \approx 104.5 < 120$$

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$$D \geq 1.6$$

$$R_{grc} \geq 0.8$$

hopefully the discretized tube does not matter too much

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- calculate ground state configurations numerically, which always are nearby the true ground state

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- parallel tempering in the end-to-end distance at temperature $T = 0.05$

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- the finding

  there are no phases for finite length chains

  the “phase dagram” is made from the following pure, as opposed to mixed, conformations

  1): $0.8 < R_{grc} < 1.2 - 1.3$: 1-dim, helix

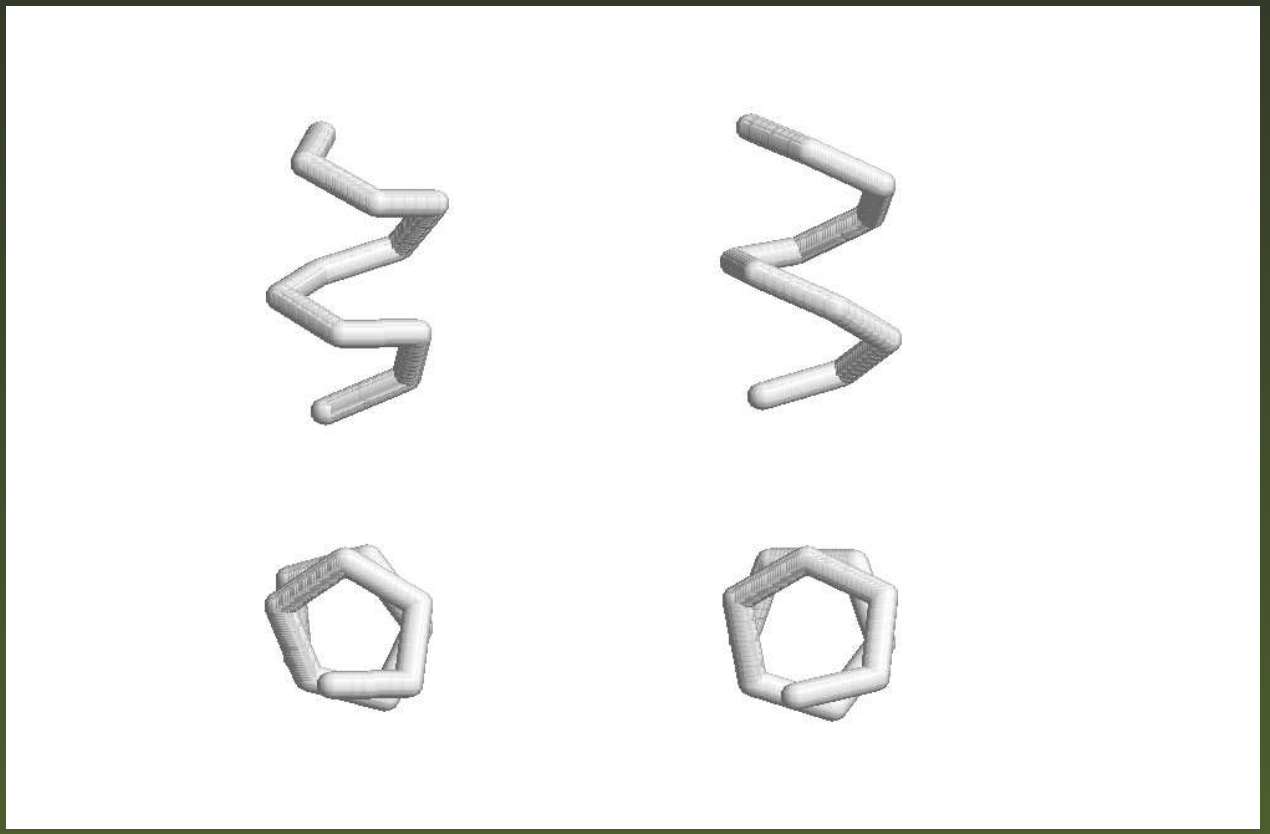
  2): $1.2 - 1.3 < R_{grc} < L/2\pi$: 3-dim, ring-polymer, twisted circle

  3): $R_{grc} = L/2\pi$: 2-dim, ring polymer, circle

  4): $R_{grc} > L/2\pi$: open ended polymer

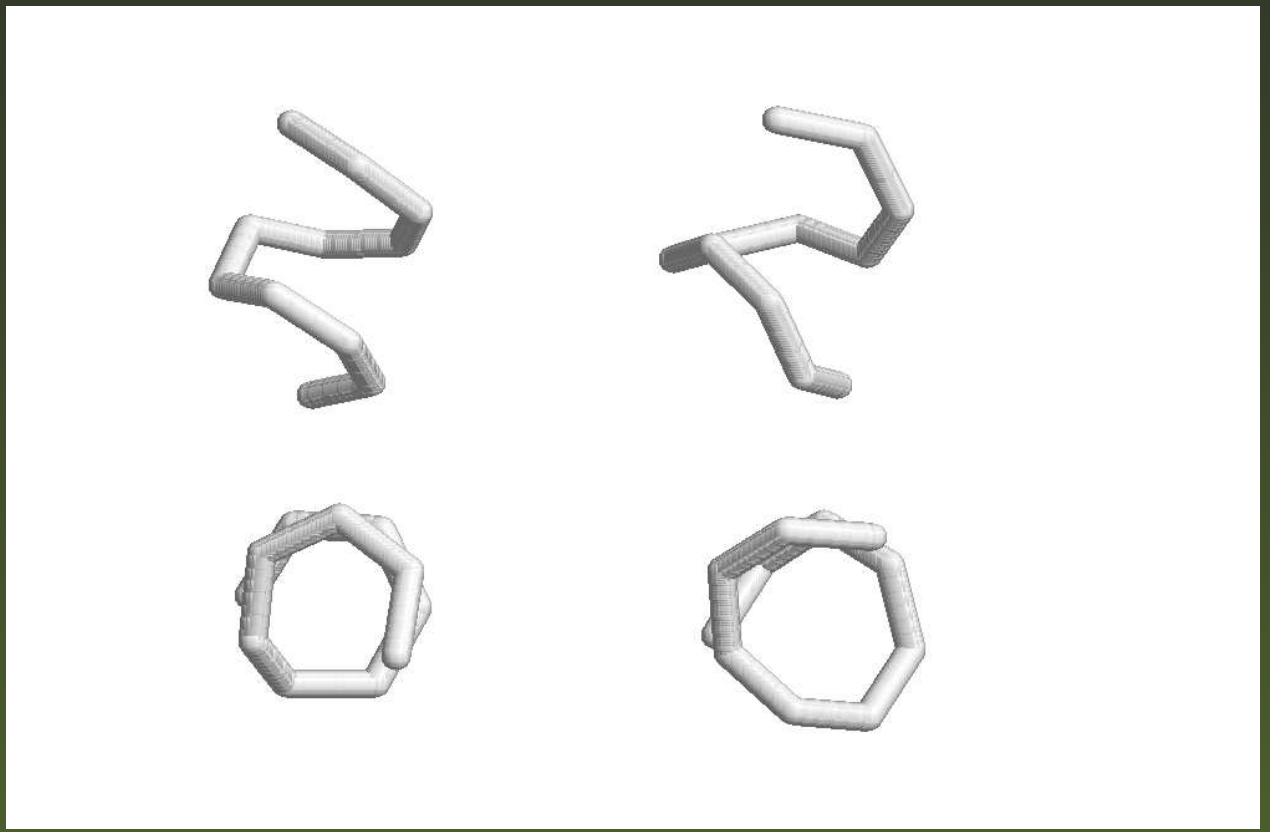
$L = 10$ chain conformations.

- $R_{grc} = 0.82$ and $R_{grc} = 0.9$: helix , helix



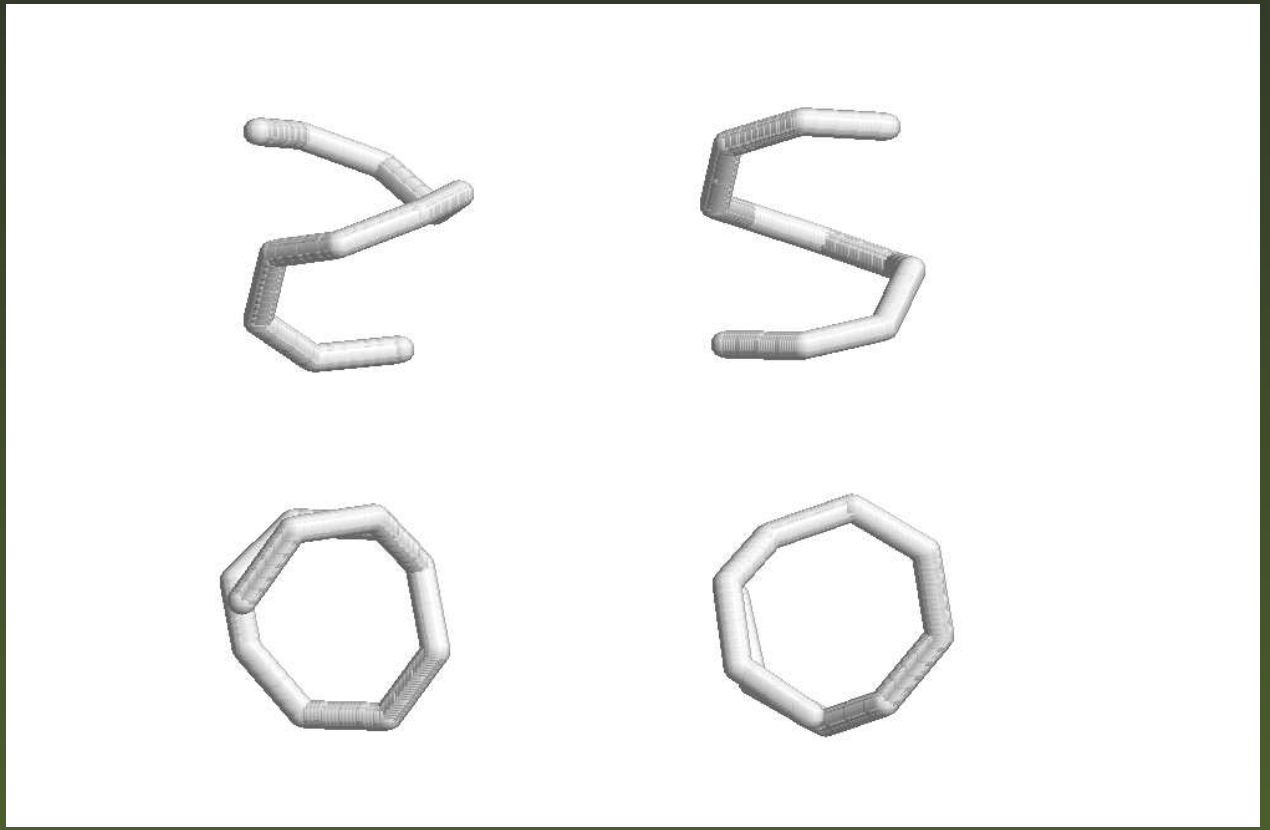
$L = 10$ chain conformations..

- $R_{grc} = 1.0$ and $R_{grc} = 1.1$: helix , helix



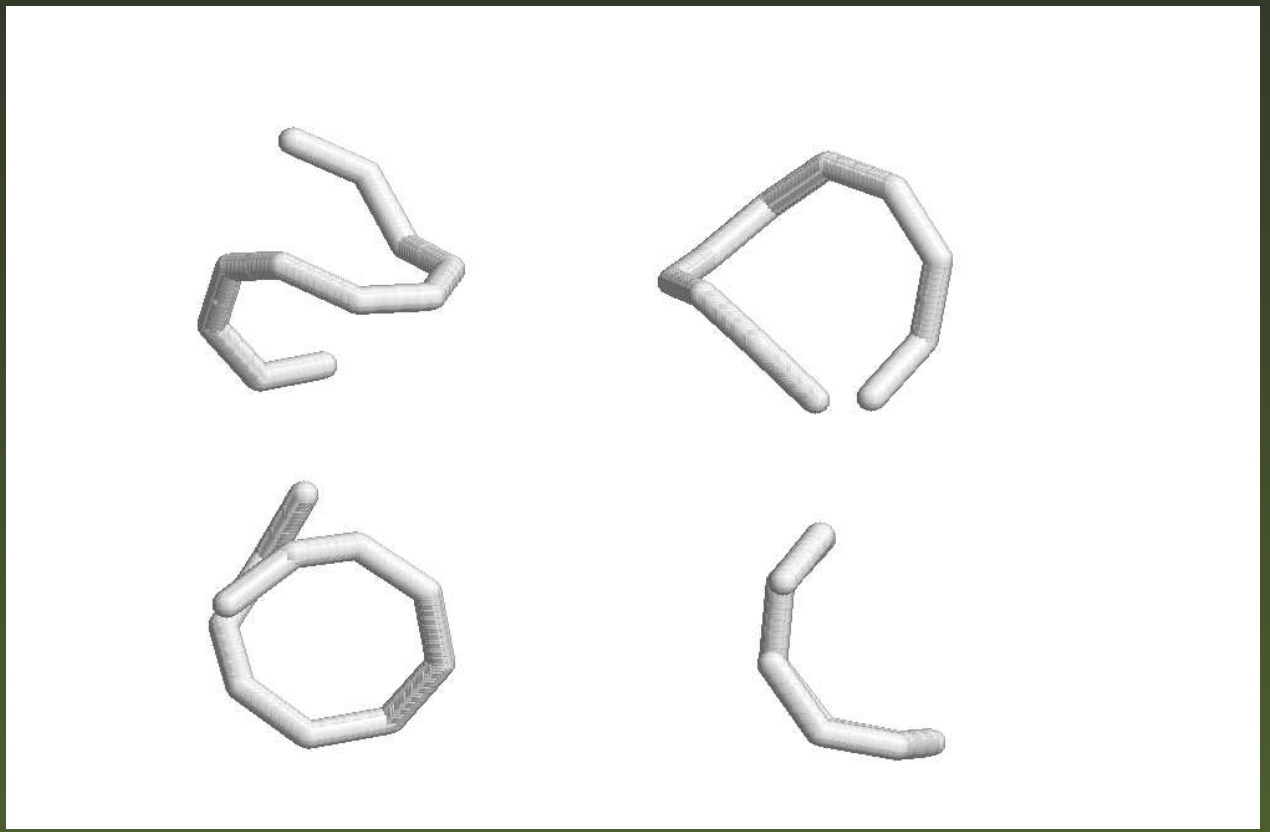
$L = 10$ chain conformations...

- $R_{grc} = 1.15$ and $R_{grc} = 1.2$: helix , helix



$L = 10$ chain conformations....

- $R_{grc} = 1.25$ and $R_{grc} = 1.3$: helix , twisted circle



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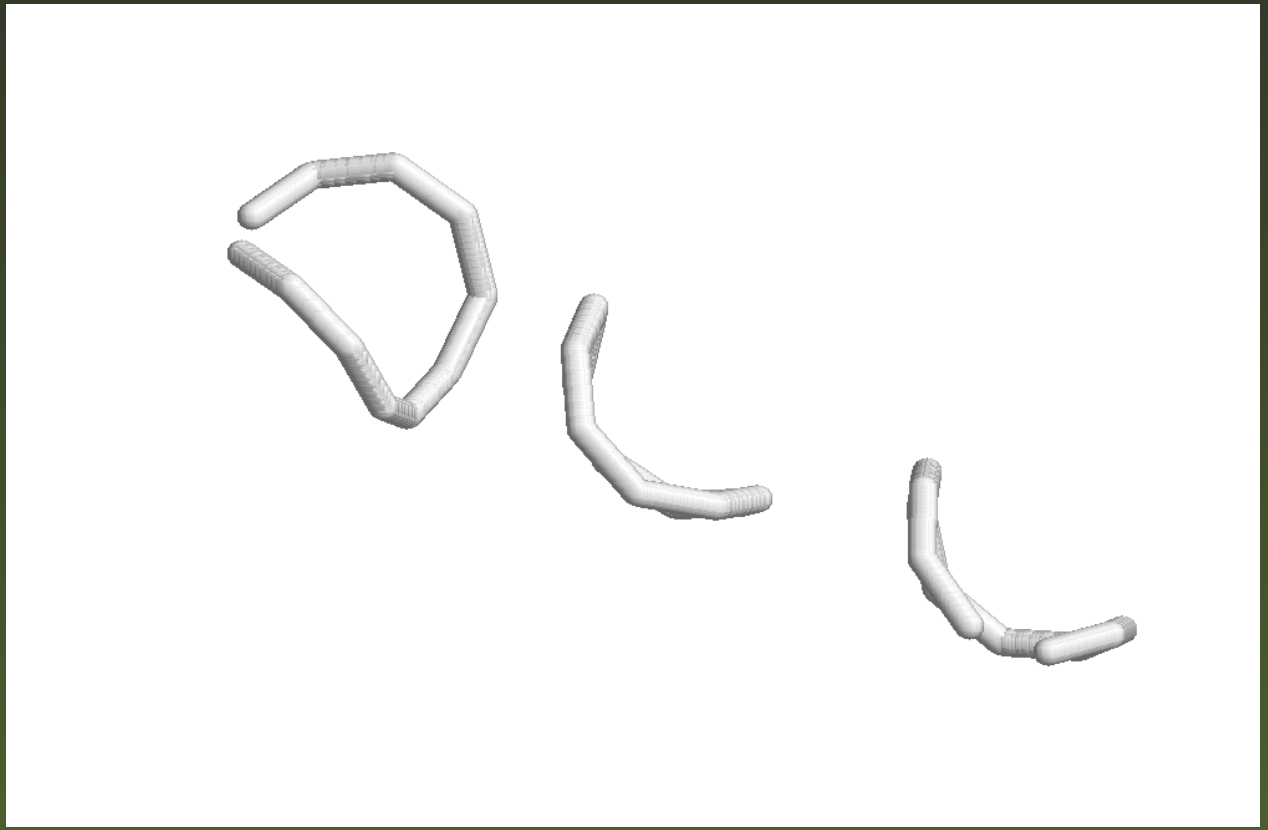
- $R_{grc} = 1.4$: twisted circle



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- the helix

$$x = R_{cyl}\,\sin(\phi) \quad y = R_{cyl}\,\cos(\phi) \quad z = p\,\frac{\phi}{2\pi}$$

p : pitch

free parameters p/R_{cyl}, D/R_{cyl}

the pitch of a helix is bounded from below by the thickness

and is saturated for the ideal helix, A.Maritan et. al., Letters to Nature, Vol 406,(2000) 288.

$$p/R_{cyl} \approx 2.516 \qquad D/2R_{cyl} \approx 1.160$$

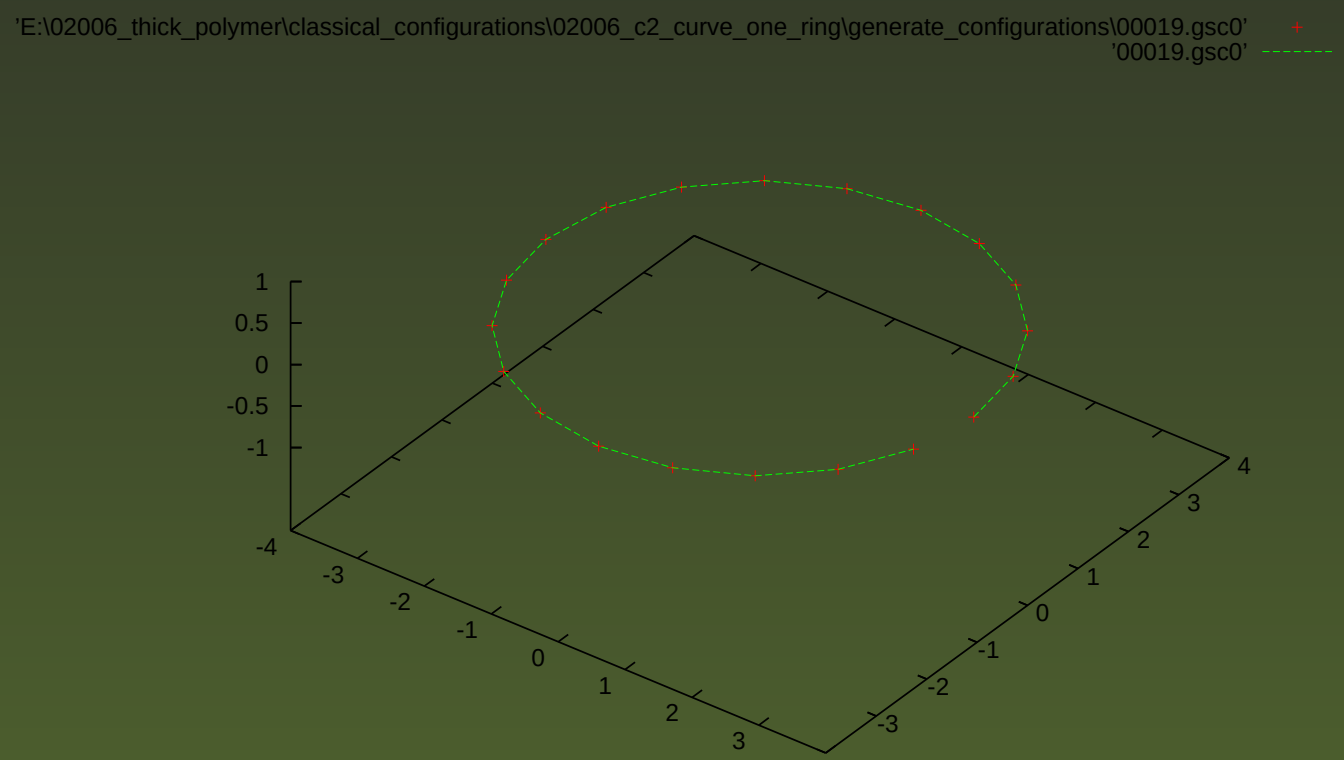
LJ homopolymer....

- twisted circles in: Koch and Engelhardt,“Closed Space Curves of Constant Curvature Consisting of Arcs of Circular Helices”, Journal for Geometry and Graphics, Vol 2, (1998), No 1, 17-31.

  “windschiefe Kreise”

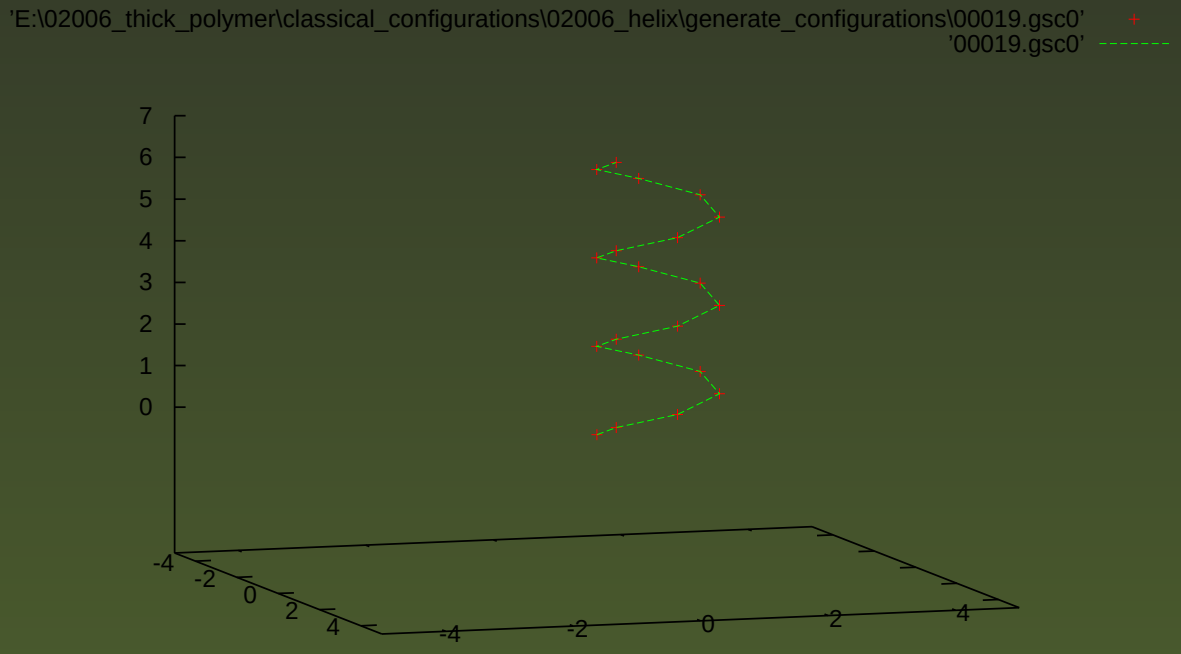
classical solution I: the circle

- planar circle



classical solution II: the ideal helix

- ideal helix



III: ring of four helix segments

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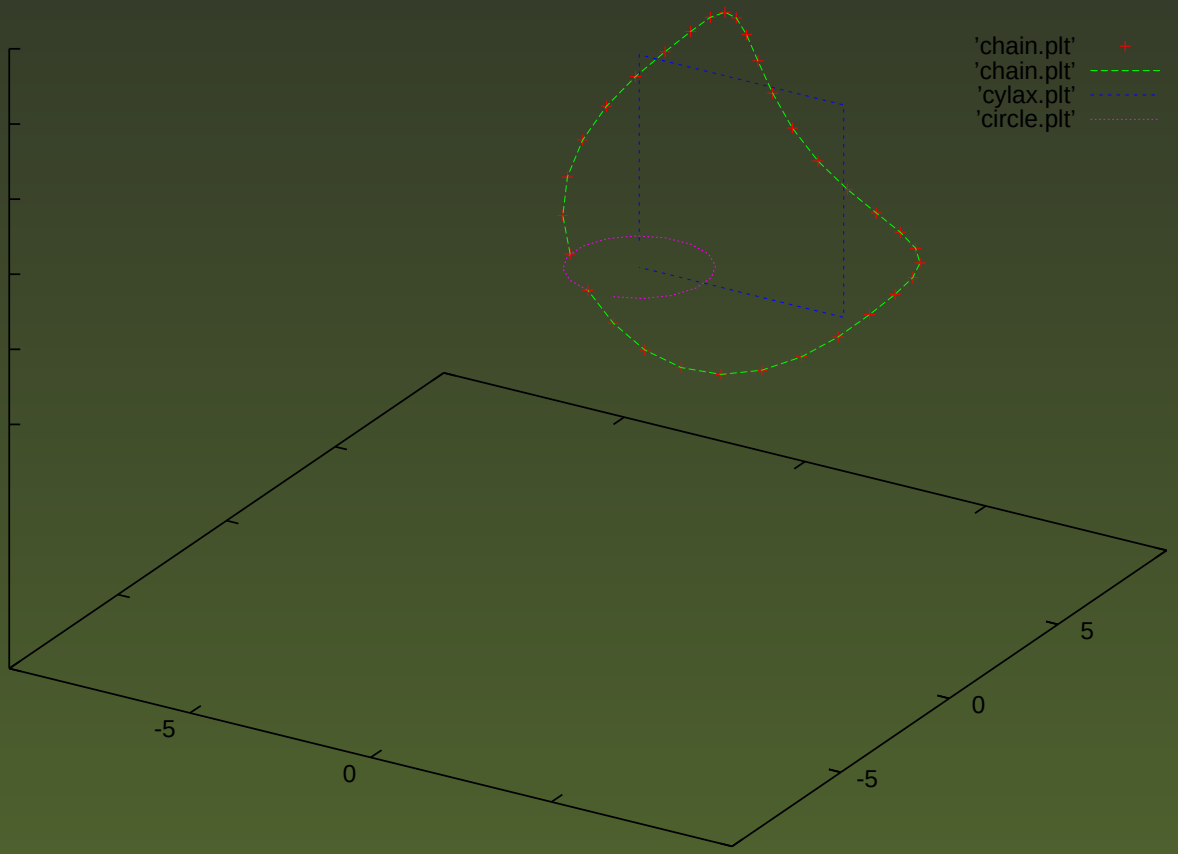

IV: ring of four circle segments

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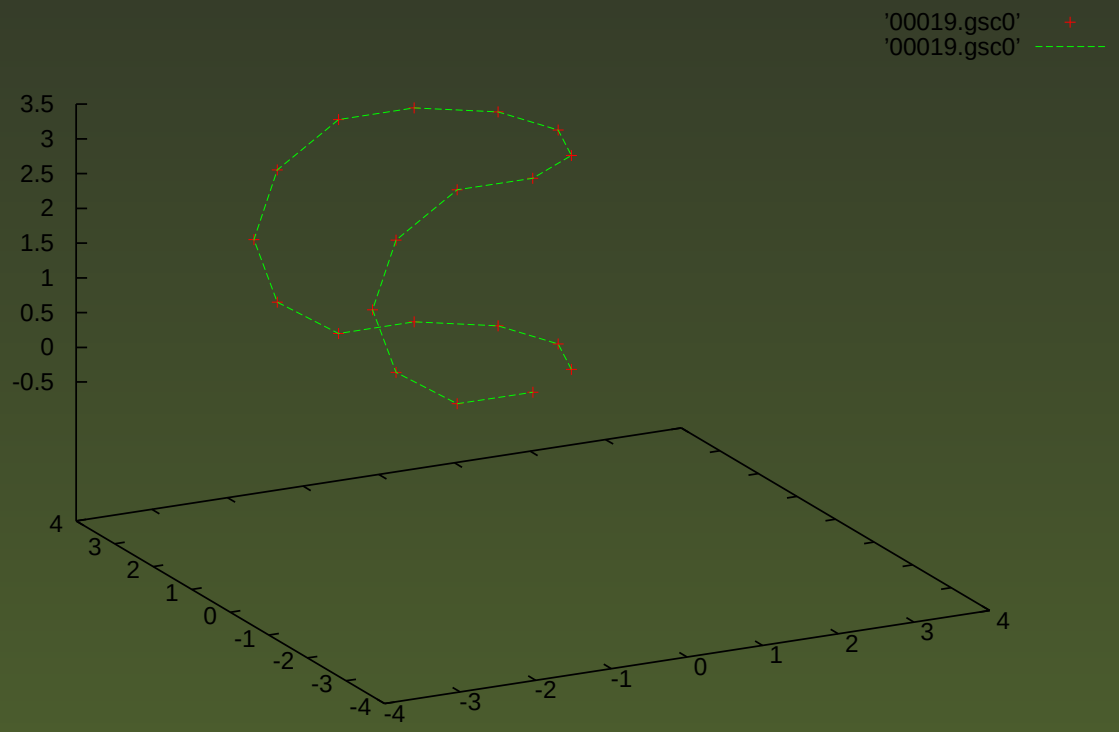
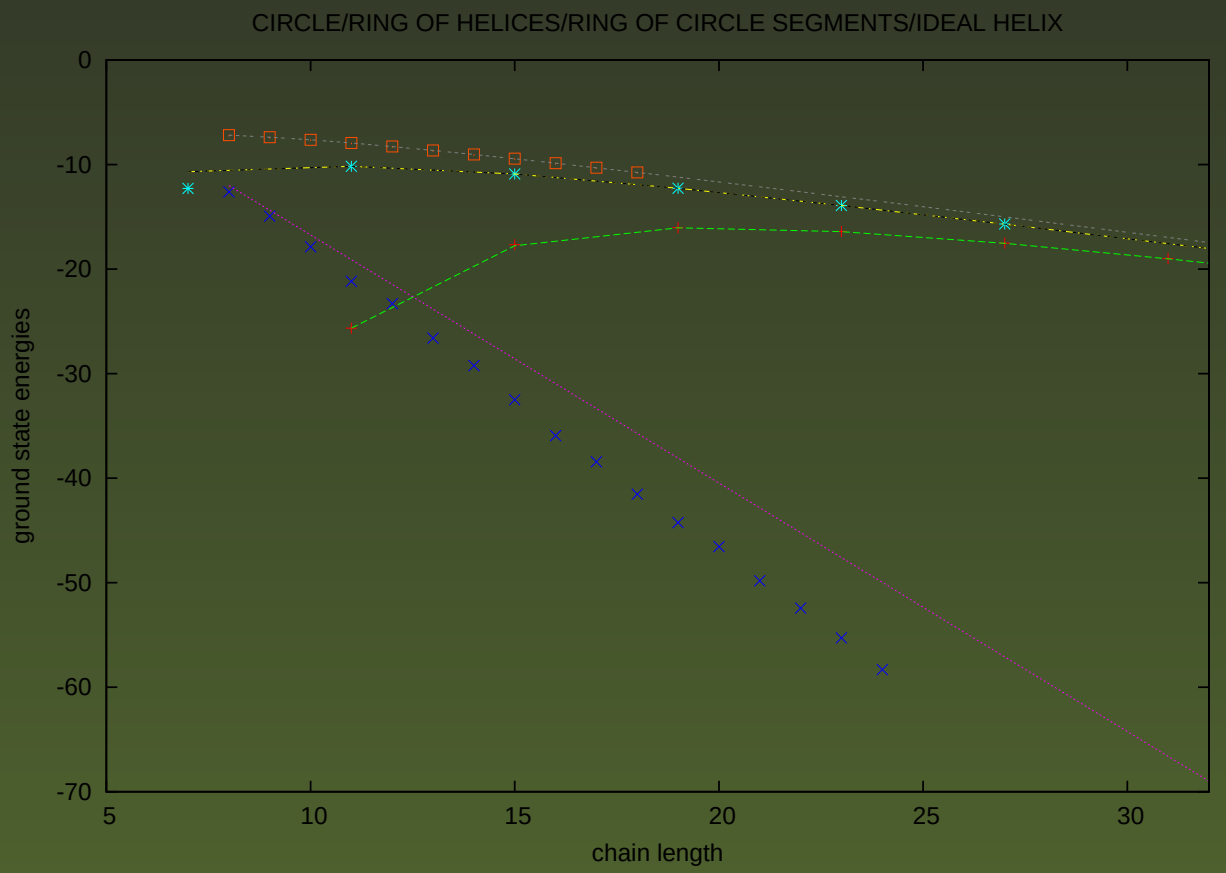


gs energies classical vs. data

- perfect match for the rings ; ideal helix at L=8,9



RMSD2 classical vs. data

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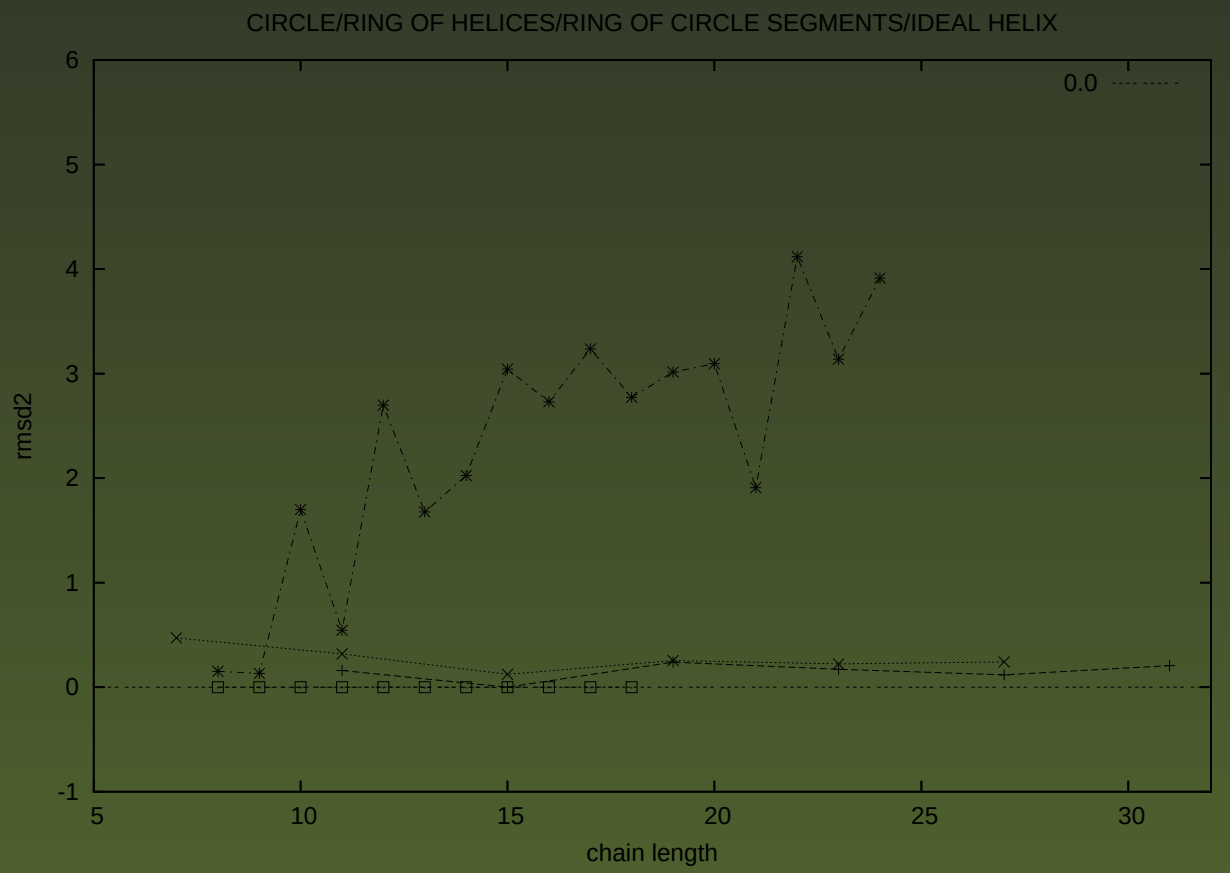
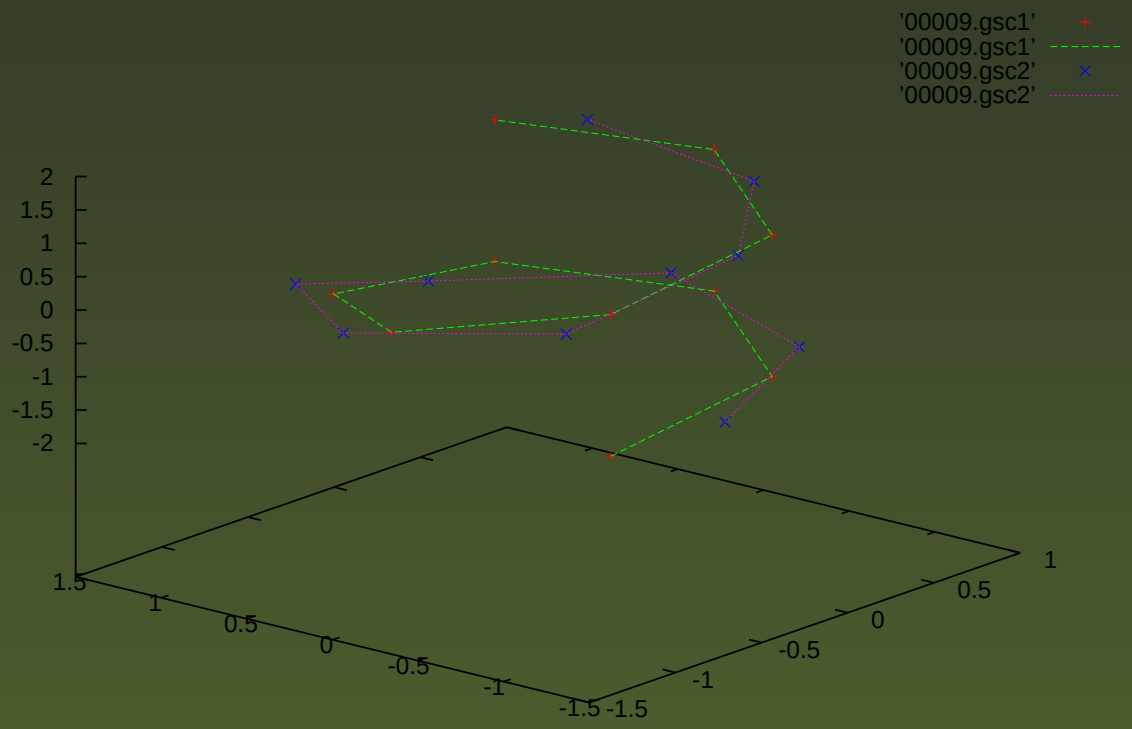


numerical : the ideal helix

- ideal helix



numerical : ring of four helix segments

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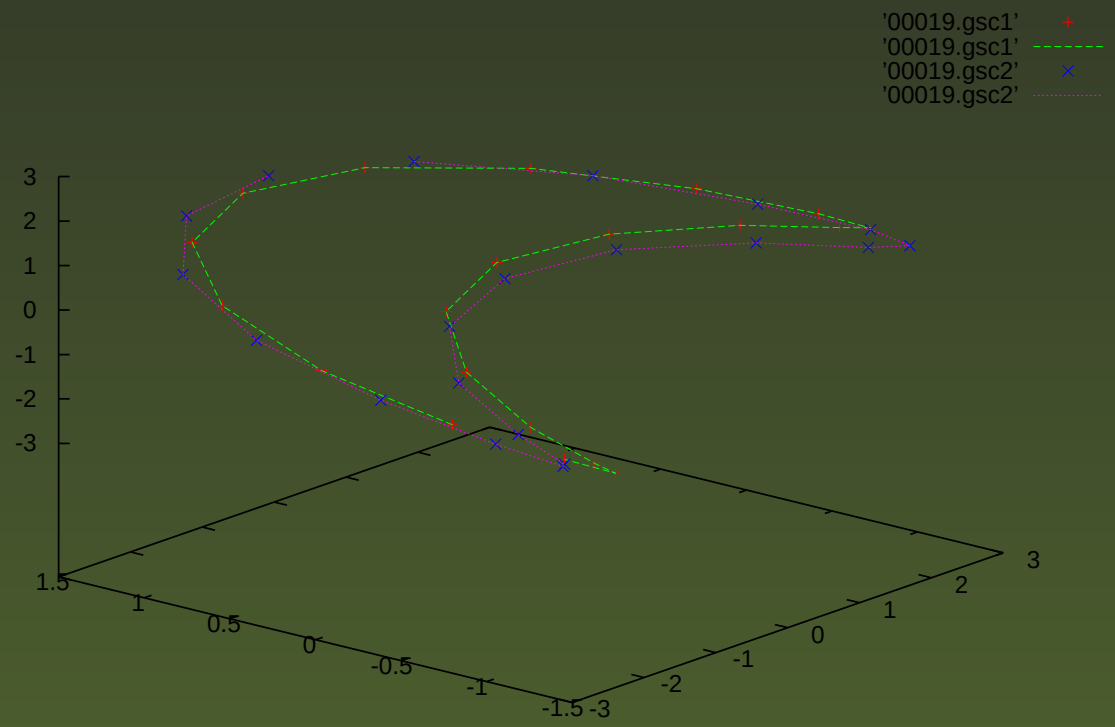

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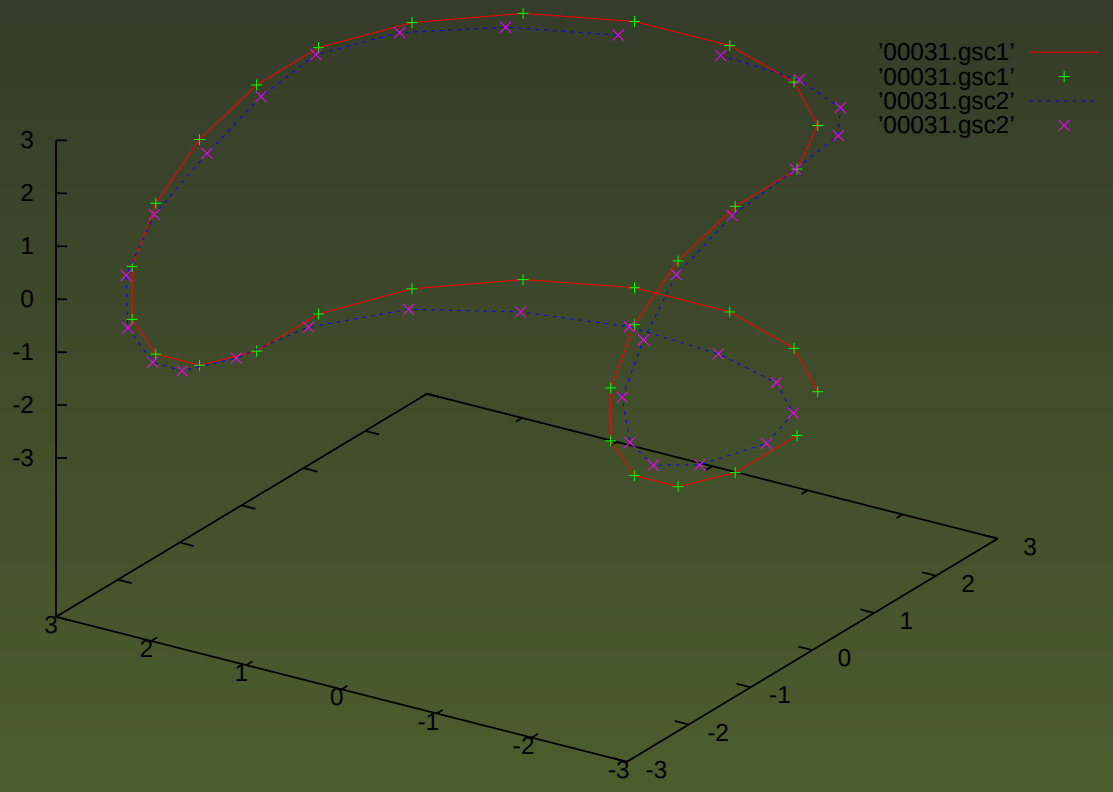

Conclusion.

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- are proteins effectively : modulated homopolymer mixed phases of tubes ?

  modulation : specific interactions in a background of constant homopolymer attraction