Etude théorique de la translocation de biomolécules à travers un nanopore

Timothée Menais

March 4, 2015

Translocation d'ADN à travers un nanopore

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Intérêts technologiques et fondamentaux

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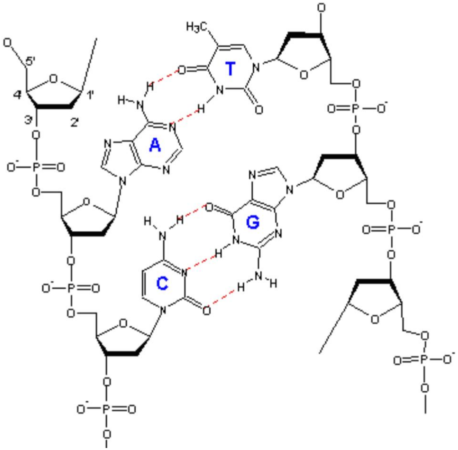
Intérêts technologiques et fondamentaux

Arrivée du graphène

Nature de l'ADN



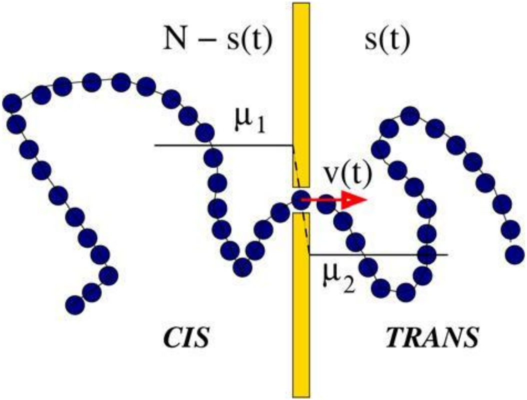
Structure

Liaisons covalentes

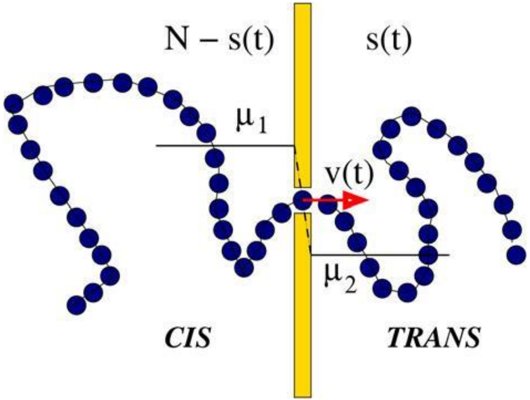
Liaisons hydrogènes

Interactions orbitalaires

Translocation

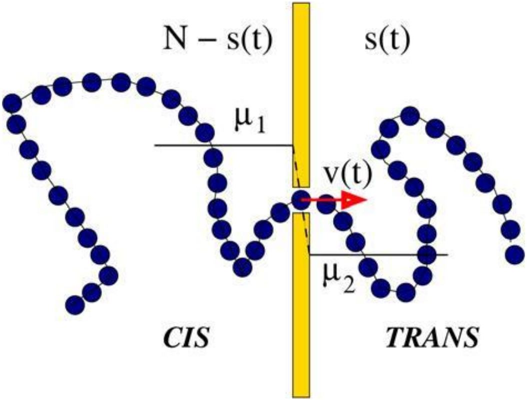


Translocation



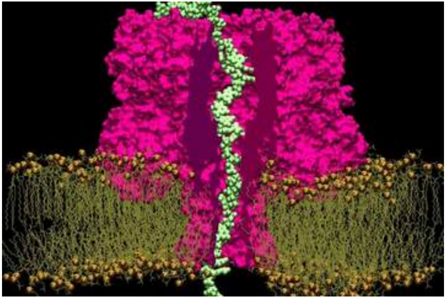
- $\tau = N^{\alpha} f^{-\delta}$

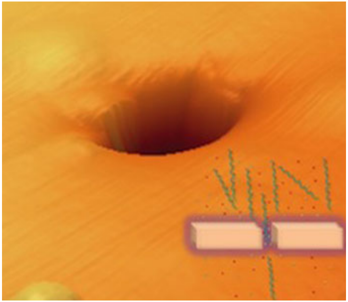
Translocation



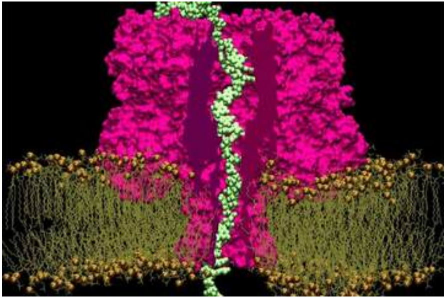
- $\tau = N^{\alpha} f^{-\delta}$
- exposants critiques

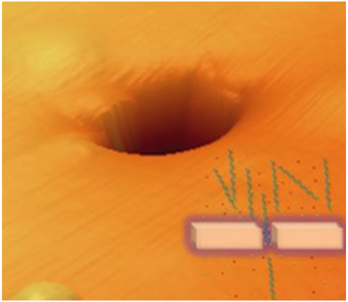
Pores classiques





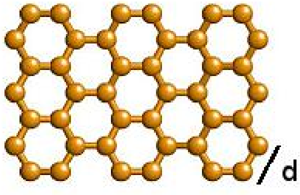
Pores classiques

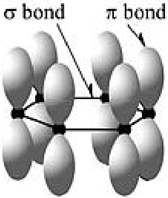




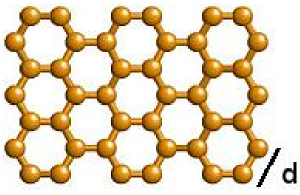
Problèmes d'épaisseur

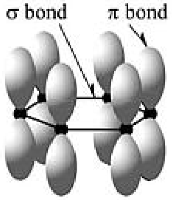
Nanopores dans le graphène



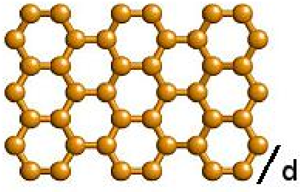


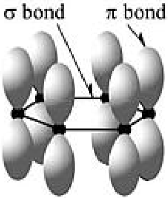
Nanopores dans le graphène





cristal bidimensionnel de carbones aromatiques





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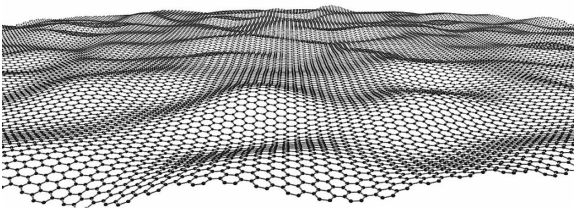
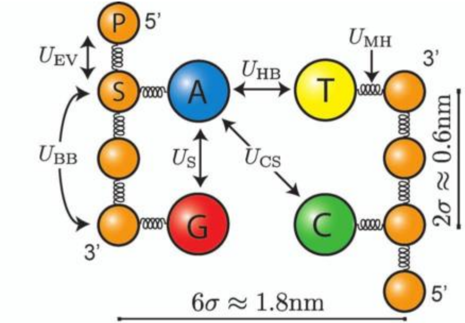


Exemple de modèle gros grain



[référence] M. C. Linak, R. Tourdot, and K. D. Dorfman. Moving beyond watson–crick models of coarse grained dna dynamics . The Journal of Chemical Physics, vol. 135, no. 20, p. 205102, 2011.

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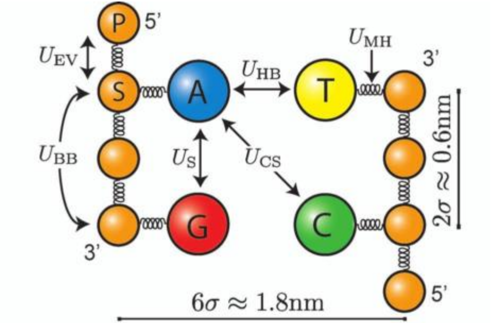

- Interactions de contact

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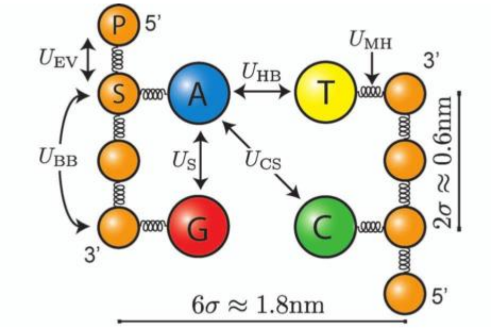

- Interactions de contact
- Liaisons covalentes

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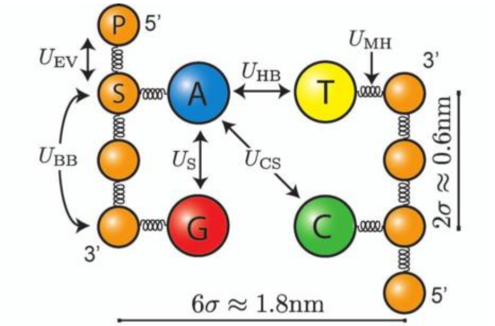

- Interactions de contact
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- Potentiel de tortion

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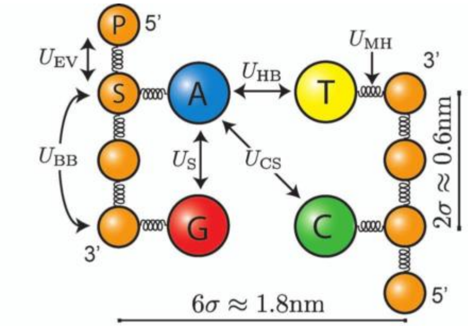

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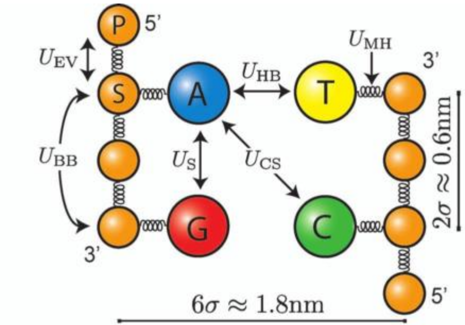

- Interactions de contact
- Liaisons covalentes
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- Interactions orbitalaires

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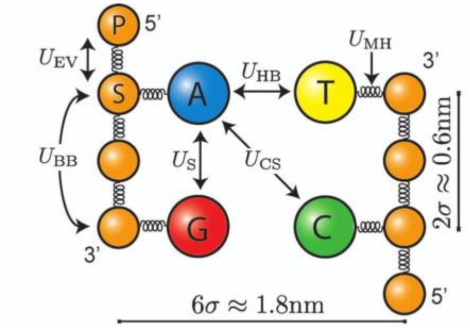

- Interactions de contact
- Liaisons covalentes
- Potentiel de tortion
- Interactions hydrogènes
- Interactions orbitalaires

Dynamique moléculaire: $\frac{d\mathbf{r}_n}{dt} = -\frac{1}{\epsilon}\frac{\partial F_{tot}}{\partial \mathbf{r}_n} + \mathbf{g}_n$

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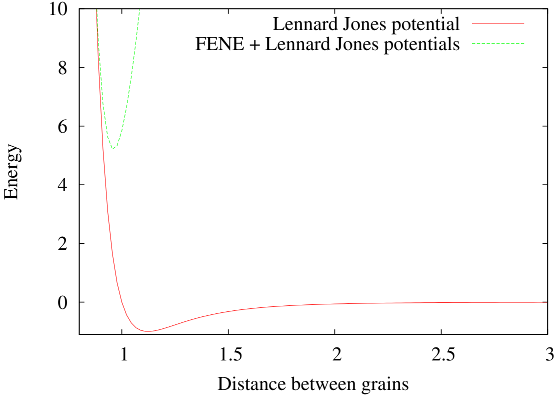
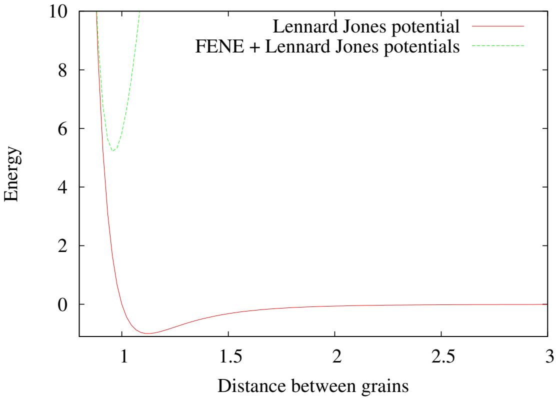
Notre modèle

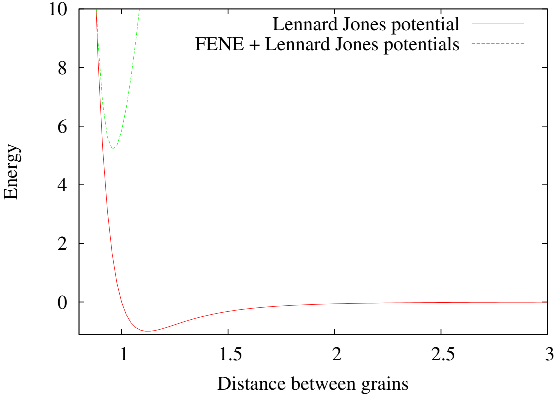


Notre modèle



Interactions de contact, coeur dur et VdW

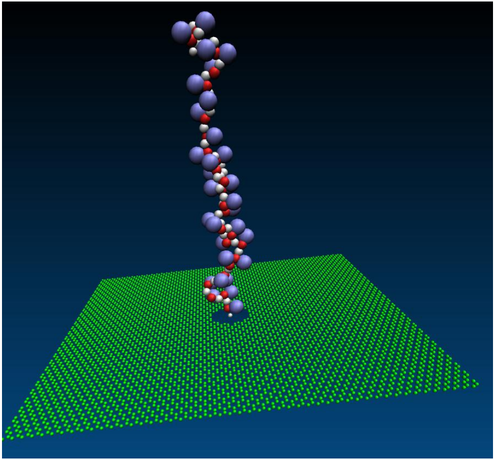
Notre modèle



Interactions de contact, coeur dur et VdW

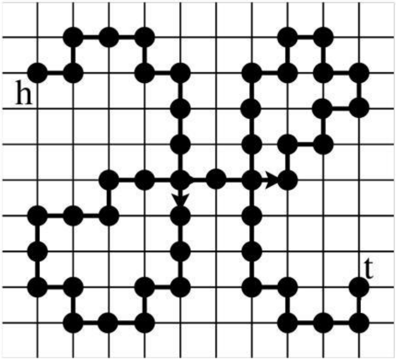
Liaisons covalentes, ajout de $\ln\left[1-(r/r_o)^2\right]$

Notre modèle



4ème grain, carbones, interactions π/σ

Statique



$$\langle \mathbf{r} \rangle = 0 \text{ et } \left\langle \mathbf{r}^2 \right\rangle = b^2 N$$

Statique

- Cas idéal
- Marche auto-évitante

Statique

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- $R_0 \propto bN^{\frac{1}{2}}$

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- $R_0 \propto bN^{\nu}$($\nu \approx 3/5$, exp. de Flory)

Statique

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- $R_0 \propto bN^{\frac{1}{2}}$
- $P(\mathbf{r}, N) = \left(\frac{3}{2\pi N b^2}\right)^{\frac{3}{2}} \exp\left(-\frac{3\mathbf{r}^2}{2Nb^2}\right)$

- Marche auto-évitante
- $R_0 \propto bN^{\nu}$($\nu \approx 3/5$, exp. de Flory)
- $P_{SAW}(R, N) \propto \exp\left[-\frac{3\mathbf{r}^2}{2Nb^2} - \frac{v_c N^2}{2\mathbf{r}^3}\right]$

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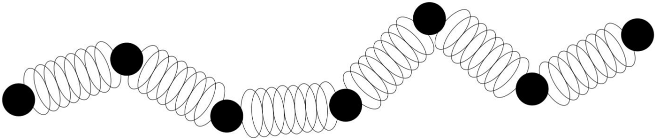
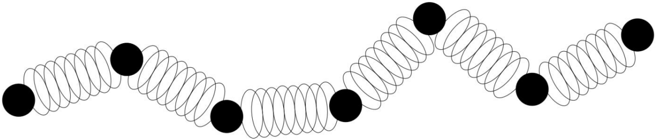
- $F(\mathbf{r}) = F(0) + \frac{3k_B T\mathbf{r}^2}{2Nb^2} + \frac{k_B T v_c N^2}{2\mathbf{r}^3}$

Dynamique de Rouse

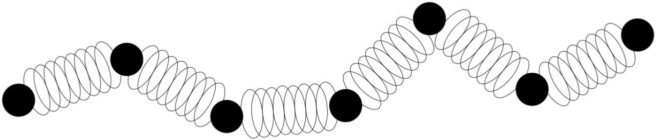


Dynamique de Rouse



- $\left\langle (\mathbf{r}_{CM}(t) - \mathbf{r}_{CM}(0))^2 \right\rangle = \frac{6 k_B T}{N \epsilon} t = 6 D t$

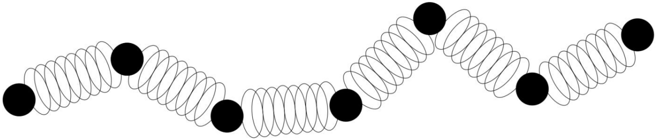
Dynamique de Rouse



- $\left\langle (\mathbf{r}_{CM}(t) - \mathbf{r}_{CM}(0))^2 \right\rangle = \frac{6k_BT}{N\epsilon}t = 6Dt$

  traction: $v \propto \eta F \propto N\epsilon F$

Dynamique de Rouse



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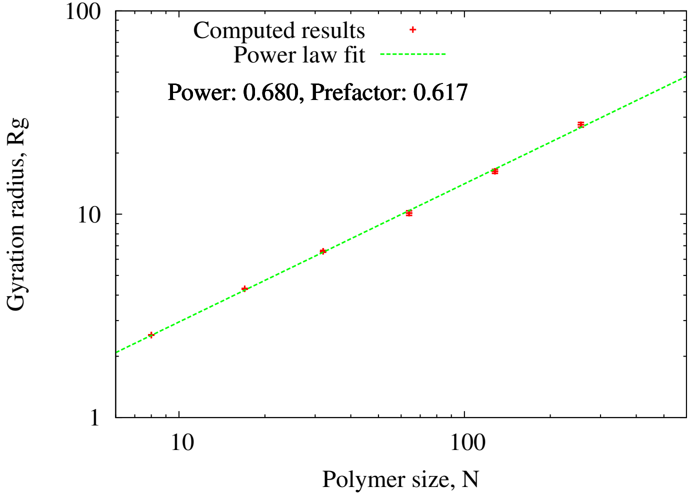
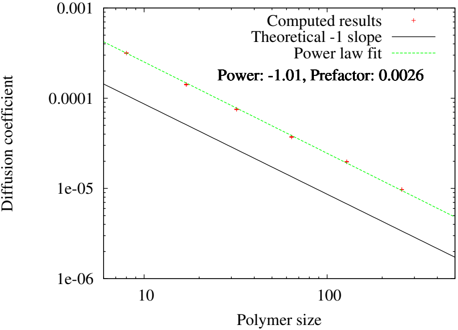
  vérifications indépendantes

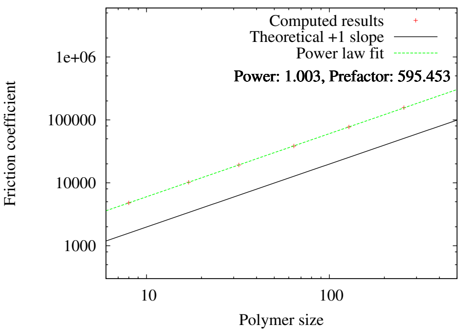
Statique



100
10
1
10
100
Gyration radius, Rg
Polymer size, N
Computed results
Power law fit
Power: 0.680, Prefactor: 0.617

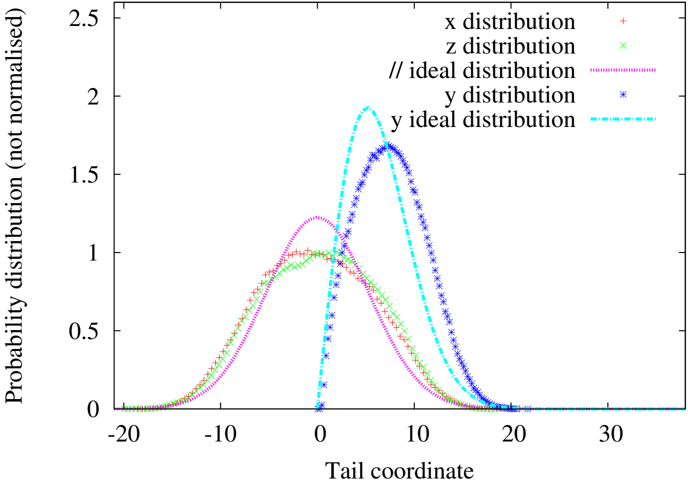
Théorème de fluctuation-dissipation





Resultats conformes à la théorie, théorème de fluctuation-dissipation vérifié.

Polymère greffé



Translocation

cas non biaisé: τ est proportionnel à $\frac{R_0^2}{D}$ ~ $N^{1+2\nu}$

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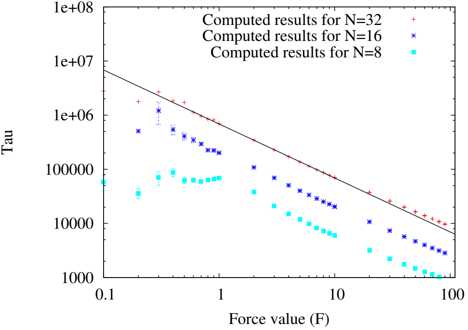
Translocation

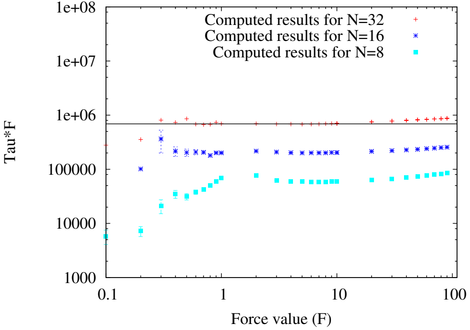
cas non biaisé: τ est proportionnel à $\frac{R_0^2}{D}$ ~ $N^{1+2\nu}$

biaisé:$\tau \propto N^{2\nu}$ à $\tau \propto N^{1+\nu}$

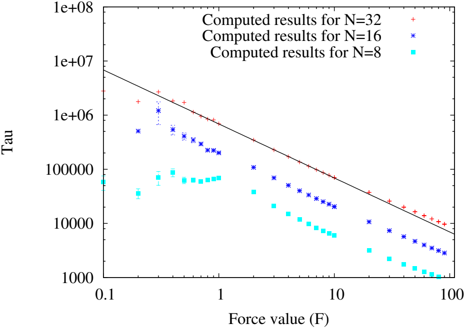
$\tau \propto F^{-1}$ à $\tau \propto F^{(1/\nu)-2}$

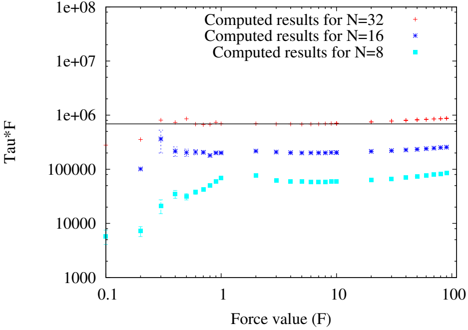
Pore large


Computed results for N=32
Computed results for N=16
Computed results for N=8
Tau
Force value (F)
1e+08
1e+07
1e+06
100000
10000
1000
0.1
1
10
100


Computed results for N=32
Computed results for N=16
Computed results for N=8
Tau*F
Force value (F)
1e+08
1e+07
1e+06
100000
10000
1000
0.1
1
10
100

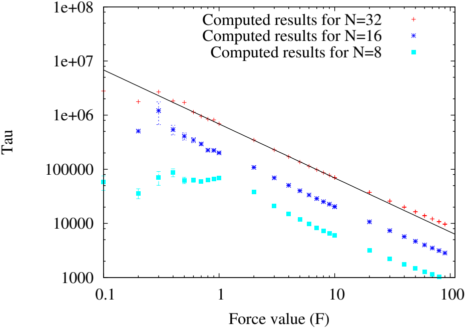
Pore large

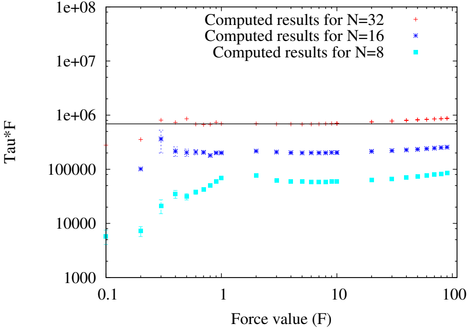




Deux régimes, $\tau \propto 1/F$ et exposant critique plus élevé

Pore large

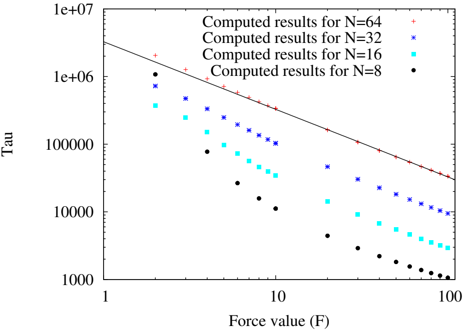




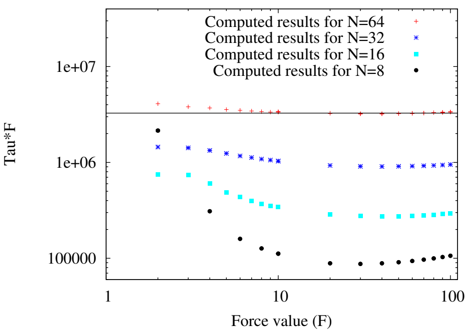
Deux régimes, $\tau \propto 1/F$ et exposant critique plus élevé

$$\tau \propto N^{1.69} \approx N^{1+\nu}$$

Pore étroit

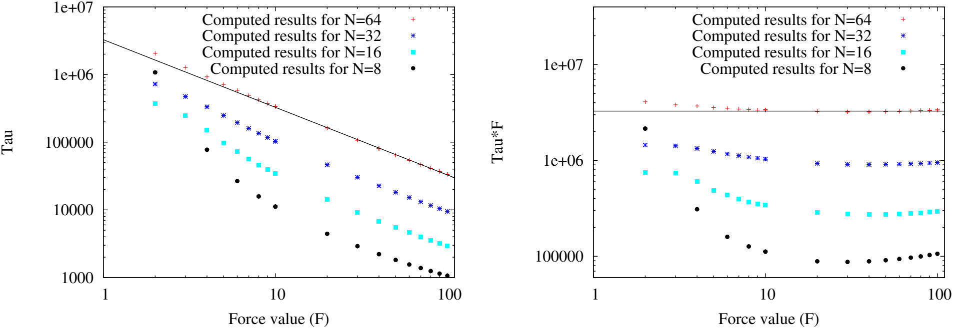


Computed results for N=64
Computed results for N=32
Computed results for N=16
Computed results for N=8
Tau
1e+07
1e+06
100000
10000
1000
1
10
100
Force value (F)



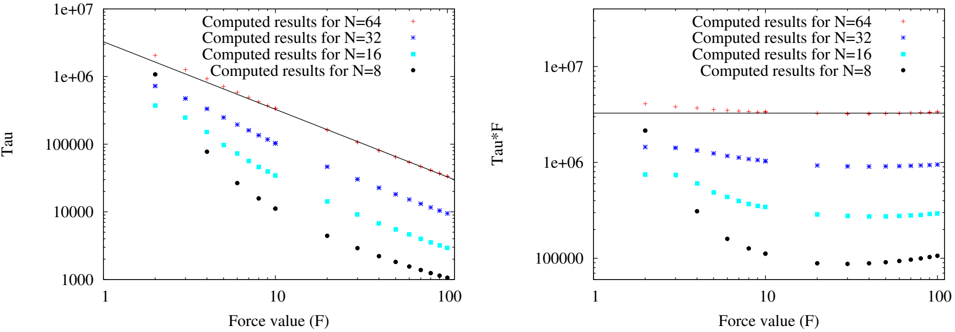
Computed results for N=64
Computed results for N=32
Computed results for N=16
Computed results for N=8
Tau*F
1e+07
1e+06
100000
1
10
100
Force value (F)

Pore étroit



Toujours deux régimes pour les forces

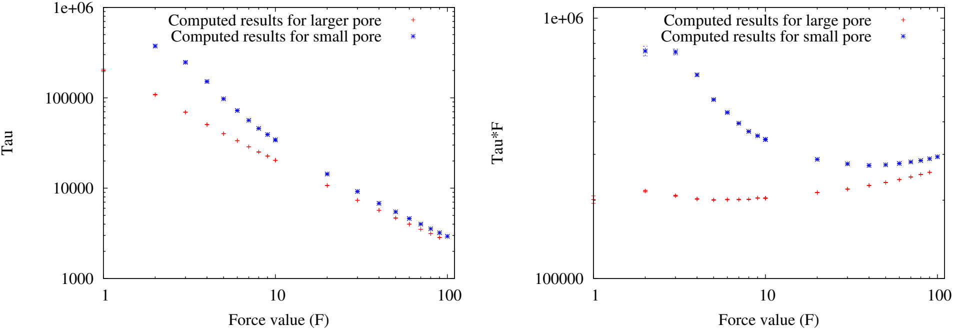
Pore étroit



Toujours deux régimes pour les forces

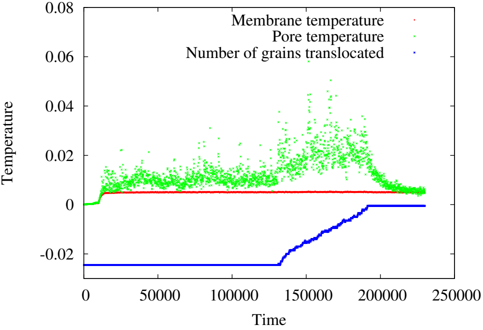
$$\tau \propto N^{1+\nu}$$

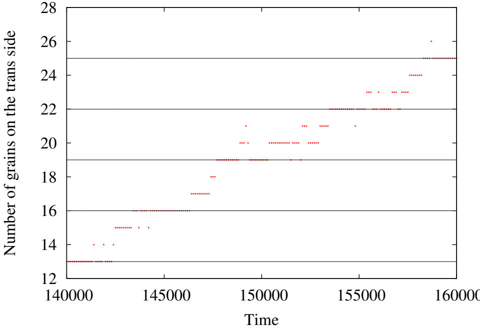
Comparaison



Ralentissement de la translocation avec un pore étroit

Pore vibrant





Echauffement du pore et translocation fractionnée

Conclusion

Utilisation d'un modèle original

Conclusion

Utilisation d'un modèle original

Détermination de lois d'échelle

Conclusion

Utilisation d'un modèle original

Détermination de lois d'échelle

Effets du frottements du pore

Conclusion

Utilisation d'un modèle original

Détermination de lois d'échelle

Effets du frottements du pore

Cas du pore vibrant?

Conclusion

Utilisation d'un modèle original

Détermination de lois d'échelle

Effets du frottements du pore

Cas du pore vibrant?

Flexibilité de l'ensemble du plan?

Conclusion

Merci de votre attention.

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Des questions ?